Reflection coupling and Wasserstein contractivity without convexity

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Abstract

We note that even if convexity of the potential U fails locally, overdamped Langevin diffusions in $\mathbb{R}^d$ are contractions w.r.t. the Kantorovich-Rubinstein-Wasserstein distance based on an appropriately chosen concave distance function equivalent to the Euclidean distance. The choice of the distance function is then optimized to obtain a large exponential decay rate. The results yield dimension-independent bounds of optimal order in $R, L \in [0, \infty)$ and $K \in (0, \infty)$ if $(x - y) \cdot (\nabla U(x) - \nabla U(y))$ is bounded from below by $-L|x - y|^2$ for $|x - y| < R$ and by $K|x - y|^2$ for $|x - y| \geq R$.

Résumé

Couplage de réflection et contractivité de Wasserstein sans convexité. On considére diffusions de Langevin sur $\mathbb{R}^d$ dans un potentiel U non convex dans un ensemble borné. A l'aide du couplage de réflection, on observe que ces diffusions sont des contractions pour la distance de Kantorovich-Rubinstein-Wasserstein basée sur une distance concave appropriée, équivalente à la distance Euclidienne. Le choix de la distance est optimisé pour obtenir un grand taux de décroissance exponentielle. Les résultats impliquent bornes optimales pour $R, L \in [0, \infty)$ et $K \in (0, \infty)$, indépendamment de la dimension, sous la condition que $(x - y) \cdot (\nabla U(x) - \nabla U(y))$ est borné inférieurement par $-L|x - y|^2$ pour $|x - y| < R$ et par $K|x - y|^2$ pour $|x - y| \geq R$.

1. Introduction

Consider a diffusion process $(X_t)_{t\geq 0}$ in $\mathbb{R}^d$ defined by a stochastic differential equation

$$dX_t \;=\; b(X_t)\,dt + \sigma\,dB_t. \tag{1}$$

Here $(B_t)_{t\geq 0}$ is a d-dimensional Brownian motion, $\sigma \in \mathbb{R}^{d\times d}$ is a constant $d \times d$ matrix with $\det \sigma > 0$, and $b : \mathbb{R}^d \to \mathbb{R}^d$ is a locally Lipschitz continuous function. We assume that the unique strong solution of (1) is non-explosive, which is essentially a consequence of the assumptions imposed further below.

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The transition kernels of the diffusion process on $\mathbb{R}^d$ defined by (1) will be denoted by $p_t(x, dy)$. We are interested in upper bounds for Kantorovich-Rubinstein-Wasserstein distances of the distributions μp_t and νp_t at a given time $t \geq 0$ w.r.t. two different initial distributions μ and ν.

*Example 1 (**Overdamped Langevin dynamics**) Suppose $\sigma = I_d$ and $b(x) = -\frac{1}{2}\nabla U(x)$ for a function $U \in C^2(\mathbb{R}^d)$ that is strictly convex (i.e. $\nabla^2 U \geq K \cdot I_d$ for some $K > 0$) outside a given ball $B \subset \mathbb{R}^d$. Then $Z := \int \exp(-U(x))dx < \infty$, and $d\mu := Z^{-1} \exp(-U)\, dx$ is a stationary distribution for the diffusion process (X_t). The results below imply upper bounds for the L^1 Wasserstein distances between the law νp_t of X_t and μ for an arbitrary initial distribution ν and $t \geq 0$.*

A *coupling by reflection* of two solutions of (1) with initial distributions μ and ν is a diffusion process (X_t, Y_t) with values in $\mathbb{R}^{2d}$ defined by $(X_0, Y_0) \sim \eta$ where η is a coupling of μ and ν,

$$\begin{aligned} dX_t &= b(X_t)\, dt + \sigma\, dB_t && \text{for } t \geq 0, \\ dY_t &= b(Y_t)\, dt + \sigma(I - 2e_t e_t^\top)\, dB_t && \text{for } t < T, \qquad Y_t \;=\; X_t \quad \text{for } t \geq T. \end{aligned} \tag{2}$$

Here $e_t e_t^\top$ is the orthogonal projection onto the unit vector $e_t := \sigma^{-1}(X_t - Y_t)/|\sigma^{-1}(X_t - Y_t)|$, and $T = \inf\{t \geq 0 \,:\, X_t = Y_t\}$ is the coupling time, i.e., the first hitting time of the diagonal $\Delta = \{(x, y) \in \mathbb{R}^{2d} \,:\, x = y\}$, cf. [5,1]. The reflection coupling can be realized as a diffusion process in $\mathbb{R}^{2d}$, and the marginal processes $(X_t)_{t\geq 0}$ and $(Y_t)_{t\geq 0}$ are solutions of (1) w.r.t. the Brownian motions B_t and $\tilde{B}_t = \int_0^t (I_d - 2I_{\{s<T\}} e_s e_s^\top)\, dB_s$. The difference vector $Z_t := X_t - Y_t$ solves the s.d.e.

$$dZ_t \;=\; (b(X_t) - b(Y_t))\, dt + 2|\sigma^{-1} Z_t|^{-1} Z_t\, dW_t \quad \text{for } t < T, \qquad Z_t = 0 \quad \text{for } t \geq T, \tag{3}$$

w.r.t. the *one-dimensional* Brownian motion $W_t \;=\; \int_0^t e_s^\top\, dB_s$.

Lindvall and Rogers [5] introduced coupling by reflection in order to derive upper bounds for the total variation distance of the distributions of X_t and Y_t at a given time $t \geq 0$. Here we are instead considering the Kantorovich-Rubinstein (L^1-Wasserstein) distances

$$W_f(\mu, \nu) \;=\; \inf_\eta \int d_f(x, y)\, \eta(dx\, dy), \qquad d_f(x, y) \;=\; f(\|x - y\|) \quad (x, y \in \mathbb{R}^d), \tag{4}$$

of probability measures μ, ν on $\mathbb{R}^d$, where the infimum is over all couplings η of μ and ν, $f : [0, \infty) \to [0, \infty)$ is an appropriately chosen concave increasing function with $f(0) = 0$, and $\|z\| = \sqrt{z \cdot Gz}$ with $G \in \mathbb{R}^{d\times d}$ symmetric and strictly positive definite. Typical choices for the norm are the Euclidean norm $\|z\| = |z|$ and the intrinsic metric $\|z\| = |\sigma^{-1} z|$ corresponding to $G = I_d$ and $G = (\sigma\sigma^\top)^{-1}$ respectively.

2. Results

Similarly to Lindvall and Rogers [5], we define for $r \in (0, \infty)$:

$$\kappa(r) \;=\; \inf\left\{-2\, \frac{|\sigma^{-1}(x - y)|^2}{\|x - y\|^2}\, \frac{(x - y) \cdot G(b(x) - b(y))}{\|x - y\|^2} \;:\; x, y \in \mathbb{R}^d \text{ with } \|x - y\| = r\right\}.$$

Note that the factor $|\sigma^{-1}(x - y)|^2/\|x - y\|^2$ equals 1 if $\|\cdot\|$ is the intrinsic metric. In Example 1 with $G = I_d$, we have $\kappa(r) = \inf\left\{\int_0^1 \partial^2_{(x-y)/|x-y|} U((1 - t)x + ty)\, dt : x, y \in \mathbb{R}^d \text{ s.t. } |x - y| = r\right\}$. We assume from now on that $\liminf_{r\to\infty} \kappa(r) > 0$, and we define constants $R_0, R_1 \in [0, \infty)$ with $R_0 \leq R_1$ by

$$R_0 \;=\; \inf\{R \geq 0 \,:\, \kappa(r) \geq 0\ \forall\, r \geq R\}, \qquad R_1 \;=\; \inf\{R \geq R_0 \,:\, \kappa(r)R(R - R_0) \geq 8\ \forall\, r \geq R\}.$$

We consider the particular distance function $d_f(x,y)=f(\|x-y\|)$ given by

$$f(r)=\int_0^r \varphi(s)g(s)\,ds,\quad \varphi(r)=\exp\left(-\frac{1}{4}\int_0^r s\kappa(s)^-\,ds\right),\quad g(r)=1-\frac{1}{2}\int_0^{r\wedge R_1}\frac{\Phi(s)}{\varphi(s)}\,ds\Big/\int_0^{R_1}\frac{\Phi(s)}{\varphi(s)}\,ds, \quad (5)$$

where $\Phi(r)=\int_0^r\varphi(s)\,ds$. Note that Φ and f are concave, because φ and g are decreasing. Moreover, $\Phi(r)/2\le f(r)\le\Phi(r)$ for any $r\ge 0$. Hence d_f and d_Φ as well as W_f and W_Φ differ at most by a factor 2. The choice of f is obtained by trying to maximize the decay rate of W_f, cf. the proof below.

Theorem 1 *Let $\alpha:=\sup\{|\sigma^{-1}z|^2\ :\ z\in\mathbb{R}^d \text{ with } \|z\|=1\}$, and define $c\in(0,\infty)$ by*

$$\frac{1}{c}\;=\;\alpha\int_0^{R_1}\Phi(s)\varphi(s)^{-1}\,ds\;=\;\alpha\int_0^{R_1}\int_0^{s}\exp\left(\frac{1}{4}\int_t^s u\kappa(u)^-\,du\right)dt\,ds\,. \quad (6)$$

Then for d_f given by (4) and (5), the function $t\mapsto e^{ct}\mathbb{E}[d_f(X_t,Y_t)]$ is decreasing on $[0,\infty)$.

The theorem yields exponential contractivity at rate $c>0$ for the transition kernels p_t of (1) w.r.t. the Kantorovich-Rubinstein-Wasserstein distance W_f. Moreover, it implies upper bounds for the standard KRW distance $W=W_{\mathrm{id}}$ w.r.t. the distance function $d(x,y)=\|x-y\|$:

Corollary 2.1 *For any $t\ge 0$ and any probability measures μ,ν on $\mathbb{R}^d$,*

$$W_f(\mu p_t,\nu p_t)\;\le\;e^{-ct}W_f(\mu,\nu),\quad \textit{and}\quad W(\mu p_t,\nu p_t)\;\le\;2\varphi(R_0)^{-1}e^{-ct}W(\mu,\nu). \quad (7)$$

The second estimate follows from the first, because $\varphi(R_0)\|x-y\|/2\le d_f(x,y)\le\|x-y\|$ for any $x,y\in\mathbb{R}^d$. For the Wasserstein mixing times, the corollary yields the upper bound

$$\tau_W(\varepsilon)\;:=\;\inf\{t\ge 0\ :\ W(\mu p_t,\nu p_t)\le\varepsilon W(\mu,\nu)\ \forall\,\mu,\nu\}\;\le\;c^{-1}\log(2/(\varepsilon\varphi(R_0)))\quad \text{for any } \varepsilon>0.$$

Proof of Theorem 1. Let $r_t=\|Z_t\|=\|X_t-Y_t\|$. By (3) and Itô's formula,

$$df(r_t)=2|\sigma^{-1}Z_t|^{-1}r_tf'(r_t)\,dW_t+r_t^{-1}Z_t\cdot G(b(X_t)-b(Y_t))f'(r_t)\,dt+2|\sigma^{-1}Z_t|^{-2}r_t^2f''(r_t)\,dt \quad (8)$$

a.s. for $t<T$. The drift is bounded from above by $B_t:=2|\sigma^{-1}Z_t|^{-2}r_t^2\,(f''(r_t)-r_t\kappa(r_t)f'(r_t)/4)$. We show that by our choice of f, this expression is smaller than $-cf(r_t)$. Indeed, for $r<R_1$,

$$f''(r)\;=\;-\frac{1}{4}r\kappa(r)^-\varphi(r)g(r)-\frac{1}{2}\Phi(r)\Big/\int_0^{R_1}\frac{\Phi(s)}{\varphi(s)}\,ds\;\le\;\frac{1}{4}r\kappa(r)f'(r)-\frac{1}{2}f(r)\Big/\int_0^{R_1}\frac{\Phi(s)}{\varphi(s)}\,ds\,. \quad (9)$$

For $r\ge R_1$, we have $f'(r)=\varphi(r)/2=\varphi(R_0)/2$ and $\kappa(r)R_1(R_1-R_0)\ge 8$ by definition of R_1, whence

$$\begin{aligned}f''(r)-\frac{1}{4}r\kappa(r)f'(r)&\le-\frac{1}{8}r\kappa(r)\varphi(R_0)\;\le\;-\frac{\varphi(R_0)}{R_1-R_0}\cdot\frac{r}{R_1}\;\le\;-\frac{\varphi(R_0)}{R_1-R_0}\cdot\frac{\Phi(r)}{\Phi(R_1)}\\&\le-\frac{1}{2}\Phi(r)\Big/\int_{R_0}^{R_1}\Phi(s)\varphi(s)^{-1}\,ds\;\le\;-\frac{1}{2}f(r)\Big/\int_0^{R_1}\Phi(s)\varphi(s)^{-1}\,ds\,. \quad (10)\end{aligned}$$

Here we have used that for $r\ge R_0$, we have $\varphi(r)=\varphi(R_0)$, $\Phi(r)=\Phi(R_0)+(r-R_0)\varphi(R_0)$, and hence

$$\begin{aligned}&\int_{R_0}^{R_1}\Phi(s)\varphi(s)^{-1}\,ds\;=\;\int_{R_0}^{R_1}(\Phi(R_0)+(s-R_0)\varphi(R_0))\varphi(R_0)^{-1}\,ds\;=\;\frac{\Phi(R_0)}{\varphi(R_0)}(R_1-R_0)+\frac{1}{2}(R_1-R_0)^2\\&\ge(R_1-R_0)(\Phi(R_0)+(R_1-R_0)\varphi(R_0))\varphi(R_0)^{-1}/2\;\ge\;(R_1-R_0)\Phi(R_1)\varphi(R_0)^{-1}/2.\end{aligned}$$

By (9) and (10), we conclude that $B_t \le -cf(r_t)$. Optional stopping in (8) at $T_k = \inf\{t \ge 0 : r_t \notin (k^{-1}, k)\}$ now implies $\mathbb{E}[f(r_t)\,;\, t < T_k] \le -c\int_0^t \mathbb{E}[f(r_s)\,;\, s < T_k]\,ds$ for any $k \in \mathbb{N}$ and $t \ge 0$. The assertion follows for $k \to \infty$ since $r_t = 0$ for $t \ge T$, and $T = \sup T_k$ by non-explosiveness. □

A first application. To illustrate that the bounds derived above are fairly sharp, let us suppose that $\kappa(r) \ge -L$ for $r \le R$ and $\kappa(r) \ge K$ for $r > R$ with constants $R, L \in [0,\infty)$ and $K \in (0,\infty)$. Then, since $\varphi(r) = \varphi(R_0)$ and $\Phi(r) = \Phi(R_0) + (r - R_0)\varphi(R_0)$ for $r \ge R_0$,

$$\alpha^{-1}c^{-1} \;=\; \int_0^{R_1} \Phi(s)\varphi(s)^{-1}\,ds \;=\; \int_0^{R_0} \Phi(s)\varphi(s)^{-1}\,ds + (R_1 - R_0)\Phi(R_0)\varphi(R_0)^{-1} + (R_1 - R_0)^2/2. \quad (11)$$

The lower bounds on the function κ imply the upper bounds $R_0 \le R$, $R_1 - R_0 \le \min(8/(KR_0), \sqrt{8/K})$, $\Phi(r)\varphi(r)^{-1} \;\le\; \int_0^r \exp(L(r^2 - t^2)/8)\,dt \;\le\; \min(\sqrt{2\pi/L}, r)\exp(Lr^2/8)$ for $r \le R_0$, and

$$\int_0^{R_0} \Phi(r)\varphi(r)^{-1}\,dr \;\le\; \begin{cases} 4L^{-1}(\exp(LR_0^2/8) - 1) \;\le\; (e-1)R_0^2/2 & \text{if } LR_0^2/8 \le 1, \\ 8\sqrt{2\pi}L^{-3/2}R_0^{-1}\exp(LR_0^2/8) & \text{if } LR_0^2/8 \ge 1. \end{cases}$$

Combining these estimates, we obtain by (11),

$$\alpha^{-1}c^{-1} \;\le\; \begin{cases} (e-1)R^2/2 + e\sqrt{8/K}R + 4/K \;\le\; (3e/2)\max(R^2, 8/K) & \text{if } LR_0^2/8 \;\le\; 1, \\ 8\sqrt{2\pi}R^{-1}L^{-1/2}(L^{-1} + K^{-1})\exp(LR^2/8) + 32R^{-2}K^{-2} & \text{if } LR_0^2/8 \ge 1. \end{cases}$$

In the first case, c is at least of order $\min(R^{-2}, K)$. Even if $L = 0$ (convex case), this order can not be improved as one-dimensional Langevin diffusions with potential $U(x) = Kx^2/2$, or, respectively, with vanishing drift on $(-R/2, R/2)$ demonstrate. In the second case ($LR_0^2 \ge 8$), if $K \ge \text{const.} \cdot L$ then the upper bound for c^{-1} is of order $R^{-1}L^{-3/2}\exp(LR^2/8)$. This order in R and L is again optimal:

Example 2 (***Double-well with $U''(x) = -L$ for $|x| \le R/2$***) *Consider a Langevin diffusion in $\mathbb{R}^1$ with a symmetric potential $U \in C^2(\mathbb{R})$ satisfying $U(x) = -Lx^2/2$ for $x \in [-R/2, R/2]$, $U'' \ge -L$, and $\liminf_{|x|\to\infty} U''(x) > 0$. If $\|\cdot\|$ is the Euclidean norm then $\kappa(r) = -L$ for $r \in (0, R]$. On the other hand,*

$$\lim_{t\to\infty} t^{-1}\log\, P_{R/2}[T_0 > t] \;=\; -\lambda_1(0,\infty) \;\ge\; -(2e-2)^{-1}(eL)^{3/2}R\exp(-LR^2/8) \quad \text{for } LR^2 \ge 4, \qquad (12)$$

where T_0 denotes the first hitting time of 0 for the process starting at $R/2$, and $\lambda_1(0,\infty)$ is the lowest Dirichlet eigenvalue of the generator on $(0,\infty)$, cf. [3]. The bound for λ_1 follows by inserting the function $g(x) = \min(\sqrt{L}x, 1)$ into the variational characterization of the Dirichlet eigenvalue. By (12), the L^1 Wasserstein distance $W(\delta_{-R/2}p_t, \delta_{R/2}p_t)$ decays at most with a rate of order $L^{3/2}R\exp(-LR^2/8)$.

Remark. The idea to study Wasserstein contractivity w.r.t. concave distance functions goes back to Chen and Wang [2], where it is implicitly contained in the proofs. Indeed, in [2] and [6], Chen and Wang apply very similar methods to estimate spectral gaps of diffusion generators on $\mathbb{R}^d$ and on manifolds. Related arguments have also been applied in [4] to quantify exponential ergodicity in infinite dimensional situations. The techniques presented have natural extensions to non-constant diffusion coefficients and diffusions on manifolds, Euler discretizations of s.d.e., and high and infinite dimensional diffusions (dimension-independent bounds) that will be studied in detail in forthcoming work.

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