

Global contractivity for Langevin dynamics with distribution-dependent forces and uniform in time propagation of chaos

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Second-order Langevin dynamics: $(X_t, V_t)_{t \geq 0}$

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

where $\gamma > 0$ is the friction parameter.

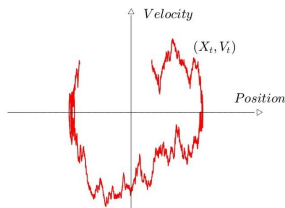
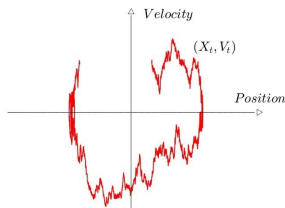


Figure: Trajectory in \mathbb{R}^2 , $U(x) = |x|^2/2$, $\gamma = 1$.

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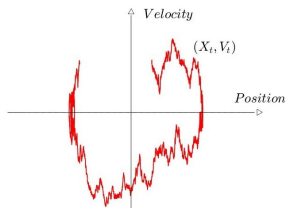
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- Analyse long-time behaviour;
- Understand the long-time behaviour of interacting particle systems and its limit behaviour if the number of particles goes to infinity;

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Applications:

- Statistical physics, deep learning, biology, ...

- 1 Second-order nonlinear Langevin dynamics - Model
- 2 Couplings
- 3 Contraction results
- 4 Propagation of chaos

Section 1

Second-order nonlinear Langevin dynamics - Model

Second-order nonlinear Langevin dynamics of McKean-Vlasov type

$$\begin{cases} dX_t = V_t dt \\ dV_t = u(b(X_t) + \int_{\mathbb{R}^d} \tilde{b}(X_t, x) \mu_t^X(dx)) dt - \gamma V_t dt + \sqrt{2\gamma u} dB_t, \end{cases}$$

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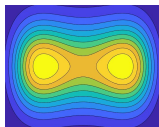
Probabilistic counterpart of the Vlasov-Fokker-Planck equation

$$\begin{aligned} \partial_t f_t(x, v) = & \nabla_v \cdot \left[\gamma \nabla_v f_t(x, v) + \gamma v f_t(x, v) + u \left(b(x) + \int_{\mathbb{R}^d} \tilde{b}(x, z) \mu_t^x(dz) \right) f_t(x, v) \right] \\ & - u \nabla_x \cdot [y f_t(x, v)], \end{aligned}$$

where f_t time dependent density function on \mathbb{R}^{2d} .

For 'classical' second-order Langevin dynamics, i.e., $b = -\nabla U$ and $\tilde{b} \equiv 0$, the unique invariant probability measure on $\mathbb{R}^d \times \mathbb{R}^d$ is given by the Boltzmann-Gibbs measure

$$\mu_*(dx dv) \propto \exp(-U(x) - |v|^2/(2u)) dx dv.$$



Questions: Under which conditions does the above process have a unique invariant measure? How does the long-time behaviour of the process behave?

Goal:

- Conditions for existence of a unique invariant probability measure
- Exponential contractivity, i.e.,

$$\mathcal{W}_{1,\rho}(\mu_t, \nu_t) \leq e^{-ct} \mathcal{W}_{1,\rho}(\mu_0, \nu_0)$$

$$\mathcal{W}_1(\mu_t, \nu_t) \leq M e^{-ct} \mathcal{W}_1(\mu_0, \nu_0),$$

for some distance $\rho : \mathbb{R}^{2d} \times \mathbb{R}^{2d} \rightarrow [0, \infty)$,

where $\mu_t = \text{Law}(X_t, V_t)$ with $(X_0, V_0) \sim \mu_0$ and $\nu_t = \text{Law}(\bar{X}_t, \bar{V}_t)$ with $(\bar{X}_0, \bar{V}_0) \sim \nu_0$.

$$(\mathcal{W}_1(\mu, \nu) = \inf_{(X,V) \sim \mu, (\bar{X}, \bar{V}) \sim \nu} \mathbb{E}[|(X, V) - (\bar{X}, \bar{V})|];$$

$$\mathcal{W}_{1,\rho}(\mu, \nu) = \inf_{(X,V) \sim \mu, (\bar{X}, \bar{V}) \sim \nu} \mathbb{E}[\rho((X, V), (\bar{X}, \bar{V}))])$$

Section 2

Couplings

Short recap:

Definition: Coupling of two measures

A coupling of measures $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ is a probability measure $\gamma \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$ with marginals μ and ν .

Definition: Coupling of two stochastic processes

A coupling of two stochastic processes $((X_t), P)$ and $((Y_t), P')$ with state spaces \mathbb{R}^d , respectively, is realized by a process $((\tilde{X}_t, \tilde{Y}_t), \tilde{P})$ with state space $\mathbb{R}^d \times \mathbb{R}^d$ such that the laws of $\tilde{X} = (\tilde{X}_t)_{t \geq 0}$ and $\tilde{Y} = (\tilde{Y}_t)_{t \geq 0}$ under \tilde{P} coincide with the laws of $X = (X_t)_{t \geq 0}$ under P and $Y = (Y_t)_{t \geq 0}$ under P' , respectively.

Consider

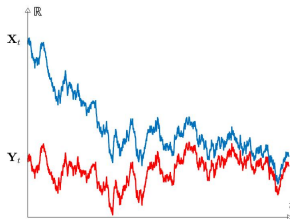
$$dX_t = -\nabla U(X_t)dt + \sqrt{2}dB_t$$

Example 1: Synchronous coupling

Assume U is κ -strongly convex ($\langle \nabla U(x) - \nabla U(y), x - y \rangle \geq \kappa|x - y|^2$ for all $x, y \in \mathbb{R}^d$).

$$\begin{cases} dX_t = -\nabla U(X_t)dt + \sqrt{2}dB_t \\ dY_t = -\nabla U(Y_t)dt + \sqrt{2}dB_t \end{cases}$$

with $(X_0, Y_0) = (x, y)$.



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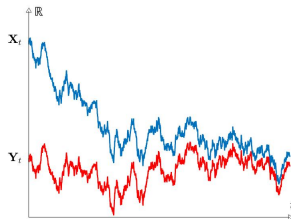
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Then,

$$\begin{aligned} d|X_t - Y_t|^2 &= 2\langle X_t - Y_t, \nabla U(X_t) - \nabla U(Y_t) \rangle dt \leq -2\kappa|X_t - Y_t|^2 dt \\ \Rightarrow |X_t - Y_t|^2 &\leq e^{-2\kappa t}|X_0 - Y_0|^2. \end{aligned}$$

Hence for $p \geq 1$

$$\mathcal{W}_p(\mu_t, \nu_t) \leq e^{-\kappa t} \mathcal{W}_p(\mu_0, \nu_0).$$

Example 2: Reflection coupling

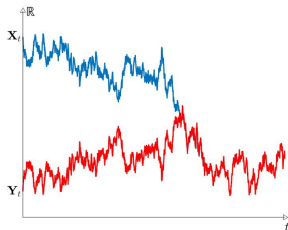
Assume U is κ -strongly convex outside a Euclidean ball of radius $R > 0$, i.e.,

$$-\langle \nabla U(x) - \nabla U(y), x - y \rangle \leq (-\kappa \mathbb{1}_{|x-y| > R} + L \mathbb{1}_{|x-y| \leq R}) |x - y|^2.$$

$$dX_t = -\nabla U(X_t)dt + \sqrt{2}dB_t$$

$$dY_t = \begin{cases} -\nabla U(Y_t)dt + \sqrt{2}dB_t & \text{if } t \geq \tau \\ -\nabla U(Y_t)dt + \sqrt{2}(I_d - 2e_t e_t^T)dB_t & \text{if } t < \tau \end{cases}$$

where $(X_0, Y_0) = (x, y)$, $\tau = \inf\{t \geq 0 : X_t = Y_t\}$ first coupling time and $e_t = (X_t - Y_t)/|X_t - Y_t|$.



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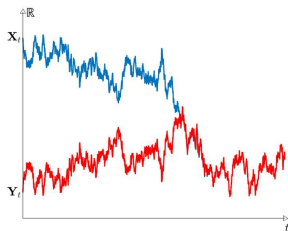
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For $r_t = |X_t - Y_t|$ and 'appropriate' f [Eberle '16]

$$df(r_t) \leq \underbrace{(f'(r_t)(-\kappa \mathbb{1}_{r_t \geq R} + L \mathbb{1}_{r_t < R}) r_t + 4f''(r_t))}_{\text{drift}} dt + 2f'(r_t) 2e_t^T dB_t$$



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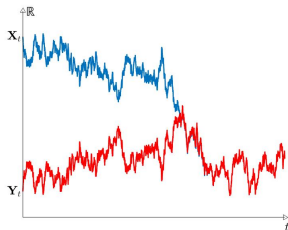
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Take expectation and apply Grönwall's inequality

$$\mathcal{W}_f(\mu_t, \nu_t) \leq \mathbb{E}[f(r_t)] \leq e^{-ct} \mathbb{E}[f(r_0)].$$



Section 3

Contraction results

Results: using analytic approaches/ hypercoercivity

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

Results: using probabilistic approaches/ coupling approaches

- Riou-Durand/Dalalyan '20 ('classical' LD, strongly convex case, synchronous coupling)
- Bolley/Guillin/Malrieu '10 (nonlinear LD, synchronous coupling)
- Eberle/Guillin/Zimmer '19 ('classical' LD, via Lyapunov function, semimetric)

$$\rho((x, v), (\bar{x}, \bar{v})) = f(\alpha|x - \bar{x}| + |v - \bar{v}|)(1 + \epsilon G(x) + \epsilon G(\bar{x})) \quad (1)$$

- Le Bris/Monmarché/Guillin '22, Kazeykina/Ren/Tan/Yang (nonlinear LD, via Lyapunov function)

Contraction result for second-order Langevin dynamics

Consider

$$\begin{cases} dX_t = V_t dt \\ dV_t = u(b(X_t) + \int_{\mathbb{R}^d} \tilde{b}(X_t, x) \mu_t^X(dx)) dt - \gamma V_t dt + \sqrt{2\gamma u} dB_t, \end{cases}$$

- (A) • b is Lipschitz continuous and there exist $R \in [0, \infty)$, a positive definite matrix $K \in \mathbb{R}^{d \times d}$ (with smallest eigen value $\kappa > 0$ and largest eigenvalue $L_K > 0$) and a function $g : \mathbb{R}^d \rightarrow \mathbb{R}^d$ such that

$$\begin{aligned} b(x) &= -Kx + g(x) && \text{for all } x \in \mathbb{R}^d, \text{ and} \\ \langle x - y, g(x) - g(y) \rangle &\leq 0 && \text{for all } x, y \in \mathbb{R}^d \text{ s.t. } |x - y| \geq R. \end{aligned}$$

- \tilde{b} is Lipschitz continuous and is Lipschitz constant \tilde{L} satisfies $\tilde{L} \leq C_{(\kappa, L_g, u, \gamma)}$, where L_g is the Lipschitz constant of g .

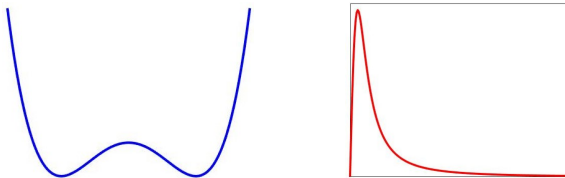


Figure: $b = -\nabla U$ with U doublewell; \tilde{b} gradient of a mollified Coulomb potential

Theorem (KS 2022)

Let $\mu_0, \nu_0 \in \mathcal{P}_2(\mathbb{R}^{2d})$. Let μ_t and ν_t be the law of (X_t, V_t) and (X'_t, V'_t) , resp. Suppose (A) holds and $L_g u \gamma^{-2} \leq \kappa / (2L_g)$. Then for all $t \geq 0$,

$$\mathcal{W}_{1,\rho}(\mu_t, \nu_t) \leq e^{-ct} \mathcal{W}_{1,\rho}(\mu_0, \nu_0), \quad \mathcal{W}_1(\mu_t, \nu_t) \leq M e^{-ct} \mathcal{W}_1(\mu_0, \nu_0),$$

where c and M are explicit constants depending on γ, u, κ, L_g and R .

Moreover, there exists a unique invariant probability measure μ_* and convergence in L^1 Wasserstein distance to μ_* holds.

- c and M and the bound on \tilde{L} are dimension independent
- for $\tilde{b} \equiv 0$ and $b(x) = -\kappa x$

$$c = \min(\gamma/8, \kappa u \gamma^{-1}/2)$$

L^2 spectral gap of the generator: $c_{gap} = (1 - \sqrt{(1 - 4\kappa u \gamma^{-2})^+})\gamma/2$ [Pavliotis '14]
 \Rightarrow Rate is of the same order

Consider

$$\begin{cases} dX_t = V_t dt \\ dV_t = (-\gamma V_t + ub(X_t))dt + \sqrt{2\gamma u} dB_t, \end{cases}$$

$$\begin{cases} d\bar{X}_t = \bar{V}_t dt \\ d\bar{V}_t = (-\gamma \bar{V}_t + ub(\bar{X}_t))dt + \sqrt{2\gamma u} d\bar{B}_t, \end{cases}$$

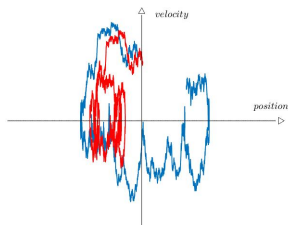
where $(B_t)_{t \geq 0}$ and $(\bar{B}_t)_{t \geq 0}$ are two Brownian motions.

Difference process: $(Z_t, W_t) := (X_t - \bar{X}_t, V_t - \bar{V}_t)$

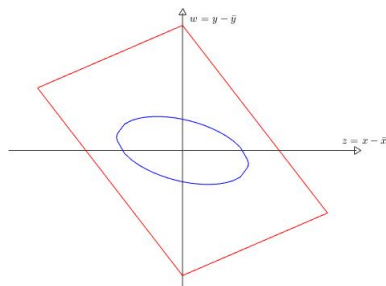
$$\begin{cases} dZ_t = W_t dt \\ dW_t = (-\gamma W_t + u(b(X_t) - b(\bar{X}_t)))dt + \sqrt{2\gamma u}(dB_t - d\bar{B}_t) \end{cases}$$

Aim: find distance ρ and coupling, such that

$$d\rho((X_t, V_t), (\bar{X}_t, \bar{V}_t)) \leq -c\rho((X_t, V_t), (\bar{X}_t, \bar{V}_t))dt + dM_t.$$



Phase space



Goal: Contractivity for

- region outside the blue ellipse
- region inside the red rectangle

Consider

$$r_l(t) = (Z_t \cdot (AZ_t) + Z_t \cdot (BW_t) + W_t \cdot (CW_t))^{1/2}$$

where $A, B, C \in \mathbb{R}^{d \times d}$ are symmetric positive definite matrices given by $A = K\gamma^2 u + (1/2)(1 - 2\tau)I_d$, $B = \gamma^{-1}(1 - 2\tau)I_d$, $C = \gamma^{-2}I_d$ with $\tau = \min(1/8, \gamma^{-2}\kappa u/2 - \gamma^{-4}L_g^2 u^2)$.

By Ito's formula and (A),

$$dr_l(t)^2 \leq -\tau\gamma r_l(t)^2 dt + dM_t$$

if $L_g u \gamma^{-2} < \kappa/(2L_g)$ and $r_l(t)^2 \geq \mathcal{R}$ for $\mathcal{R} = (1/\tau)(L_g R^2 + 8\mathbb{1}_{R>0})\gamma^{-2}$.

Coupling and metric: for small distances

Consider $(Z_t, Q_t) = (Z_t, Z_t + \gamma^{-1}W_t)$ [Eberle, Guillin, Zimmer '19]

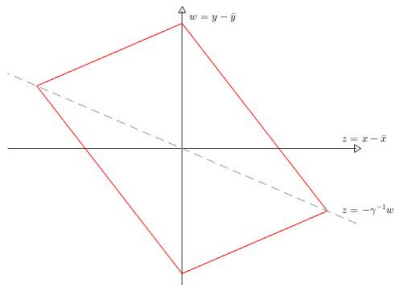
$$\begin{cases} dZ_t = -\gamma Z_t dt + \gamma Q_t dt \\ dQ_t = \gamma^{-1}u(b(X_t) - b(\bar{X}_t))dt + \sqrt{2\gamma^{-1}u}(dB_t - d\bar{B}_t) \end{cases}$$

Synchronous coupling: $dB_t = d\bar{B}_t$ for $Q_t = 0$

Reflection coupling: $d\bar{B}_t = (I_d - 2e_t e_t^T)dB_t$, $e_t = Q_t/|Q_t|$
 \bar{B} Brownian motion by Lévy's characterization; for $|Q_t| \neq 0$

For $r_s(t) = \alpha|Z_t| + |Q_t| < R_1$
($\alpha, R_1 \in \mathbb{R}_+$), there exists a concave,
increasing function $f : \mathbb{R}_+ \rightarrow \mathbb{R}_+$
with $f(0) = 0$ s.t.

$$df(r_s(t)) \leq -c_1 f(r_s(t))dt + dM_t.$$



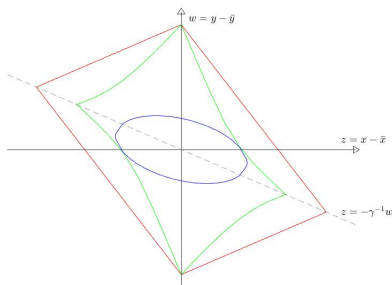
$$z = x - \bar{x}, \quad w = v - \bar{v},$$

$$r_s = \alpha|z| + |z + \gamma^{-1}w| \text{ and}$$

$$r_l = (z \cdot (Az) + z \cdot (Bw) + w \cdot (Cw))^{1/2}$$

$$\rho((x, v), (x', v')) = f(r_s \wedge (D_{\mathcal{K}} + \epsilon r_l))$$

with appropriate constants $\epsilon, D_{\mathcal{K}}, R_1$.



Combine the **couplings** for the two regions:

$$dB'_t = (\text{Id} - \mathbb{1}_{\{Q_t \neq 0, r_s \leq D_{\mathcal{K}} + \epsilon r_l\}} 2e_t e_t^T) dB_t, \quad e_t = Q_t / |Q_t|$$

Contractivity for $\rho(t) = \rho((X_t, V_t), (\bar{X}_t, \bar{V}_t))$:

$$d\rho(t) \leq -c\rho(t)dt + dM_t$$

By Grönwall,

$$\mathcal{W}_{1,\rho}(\mu_t, \nu_t) \leq \mathbb{E}[\rho(t)] \leq e^{-ct} \mathbb{E}[\rho(0)].$$

For the **nonlinear Langevin dynamics**

$$\begin{cases} dX_t = V_t dt \\ dV_t = u(b(X_t) + \int_{\mathbb{R}^d} \tilde{b}(X_t, x) \mu_t^X(dx)) dt - \gamma V_t dt + \sqrt{2\gamma} u dB_t, \end{cases}$$

we obtain by Lipschitz continuity of \tilde{b}

$$\frac{d}{dt} \mathbb{E}[\rho(t)] \leq -c \mathbb{E}[\rho(t)] + \tilde{L} \gamma^{-1} u \mathbb{E}[|Z_t|] \leq -(c/2) \mathbb{E}[\rho(t)],$$

if \tilde{L} is sufficiently small.

Section 4

Propagation of chaos

- Mean-field particle system with N particles of the second-order Langevin dynamics

$$\begin{cases} dX_t^{i,N} = V_t^{i,N} dt \\ dV_t^{i,N} = (ub(X_t^{i,N}) + N^{-1} \sum_{j=1}^N u\tilde{b}(X_t^{i,N}, X_t^{j,N}) - \gamma V_t^{i,N}) dt + \sqrt{2\gamma u} dB_t^i \end{cases}$$

for $i = 1, \dots, N$.

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for $i = 1, \dots, N$.

Theorem (KS 2022)

Fix $N \in \mathbb{N}$. Under the assumption of the previous convergence theorem, it holds for $t \geq 0$,

$$\mathcal{W}_{1, \bar{l}_N^1}(\mu_t^N, \mu_t^{\otimes N}) \leq CN^{-1/2},$$

where $\mu_t^{\otimes N}$ denotes the product law of N independent copies of (\bar{X}_t, \bar{V}_t) with $(\bar{X}_0, \bar{V}_0) \sim \mu_0$, μ_t^N denotes the law of the mean-field system $\{X_t^{i,N}, V_t^{i,N}\}_{i=1}^N$ with initial distribution $\mu_0^{\otimes N}$. The distance \bar{l}_N^1 is given by $\bar{l}_N^1(\{x^i, v^i\}_{i=1}^N, \{\bar{x}^i, \bar{v}^i\}_{i=1}^N) = N^{-1} \sum_{i=1}^N |(x^i, v^i) - (\bar{x}^i, \bar{v}^i)|$.

Sketch of the proof: similar to [Durmus/Eberle/Guillin/Zimmer '20]

- Couple

$$\begin{cases} d\bar{X}_t^i &= \bar{V}_t^i dt \\ d\bar{V}_t^i &= (ub(\bar{X}_t^i) + \int u\tilde{b}(\bar{X}_t^i, \bar{x})d\mu_t(\bar{x}) - \gamma\bar{V}_t^i)dt + \sqrt{2\gamma u}d\bar{B}_t^i \end{cases}$$

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Sketch of the proof: similar to [Durmus/Eberle/Guillin/Zimmer '20]

- Couple

$$\begin{cases} d\bar{X}_t^i &= \bar{V}_t^i dt \\ d\bar{V}_t^i &= (ub(\bar{X}_t^i) + \int \tilde{u}\tilde{b}(\bar{X}_t^i, \bar{x})d\mu_t(\bar{x}) - \gamma\bar{V}_t^i)dt + \sqrt{2\gamma u}d\bar{B}_t^i \\ &+ \sum_{j=1}^d \tilde{u}(\bar{X}_t^i, \bar{X}_t^j)dt - \sum_{j=1}^d \tilde{u}(\bar{X}_t^i, \bar{X}_t^j)dt \\ dX_t^i &= V_t^i dt \\ dV_t^i &= (ub(X_t^i) + N^{-1} \sum_{j=1}^N \tilde{u}\tilde{b}(X_t^i, X_t^j) - \gamma V_t^i)dt + \sqrt{2\gamma u}dB_t^i \end{cases}$$

- take expectation and use previous coupling construction and distance function

$$\frac{d}{dt} \mathbb{E} \left[\sum_{i=1}^d \rho((\bar{X}_t^i, \bar{V}_t^i), (X_t^i, V_t^i)) \right] \leq -c \mathbb{E} \left[\rho((\bar{X}_t^i, \bar{V}_t^i), (X_t^i, V_t^i)) \right] + \frac{u}{\gamma} (*)$$

- bound

$$(*) = \mathbb{E} \left[\left| \sum_{j=1}^N \tilde{b}(\bar{X}_t^i, \bar{X}_t^j) - \int \tilde{b}(\bar{X}_t^i, \bar{x})d\mu_t(\bar{x}) \right| \right] \leq 4\tilde{L}N^{-1/2} \mathbb{E}[|\bar{X}_t^1|^2]^{1/2}$$

Sketch of the proof: similar to [Durmus/Eberle/Guillin/Zimmer '20]

- Couple

$$\begin{cases} d\bar{X}_t^i &= \bar{V}_t^i dt \\ d\bar{V}_t^i &= (ub(\bar{X}_t^i) + \int \tilde{u}\tilde{b}(\bar{X}_t^i, \bar{x})d\mu_t(\bar{x}) - \gamma\bar{V}_t^i)dt + \sqrt{2\gamma u}d\bar{B}_t^i \\ &+ \sum_{j=1}^d \tilde{u}(\bar{X}_t^i, \bar{X}_t^j)dt - \sum_{j=1}^d \tilde{u}(\bar{X}_t^i, \bar{X}_t^j)dt \\ dX_t^i &= V_t^i dt \\ dV_t^i &= (ub(X_t^i) + N^{-1} \sum_{j=1}^N \tilde{u}(X_t^i, X_t^j) - \gamma V_t^i)dt + \sqrt{2\gamma u}dB_t^i \end{cases}$$

- take expectation and use previous coupling construction and distance function

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- compute uniform second moment bound and take Grönwall's inequality

Conclusion:

- second-order nonlinear Langevin dynamics:
 - contraction in an L^1 Wasserstein distance
 - uniform in time propagation of chaos bounds
- using coupling approaches and suitable distance functions

Open questions:

- $\gamma \rightarrow 0$?
- relax Lipschitz bound on the interaction force?

Thank you for your attention!

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