

Uniform-in-time propagation of chaos for mean-field Langevin dynamics with convex energy

Songbo Wang

CMAP, École polytechnique

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Joint work with F. Chen and Z. Ren

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Scaling transformation on (X, t) ((X, V, t) resp.) allows one to fix constants

$$\sigma = \sqrt{2}$$

$$(\alpha, \gamma, \sigma) = (1, 1, \sqrt{2}), \text{ resp.}$$

upon a redefinition of U .

Fokker–Planck equation

In the overdamped case, the probability density of $\text{Law}(X_t)$ solves

$$\partial_t \rho = \Delta \rho + \nabla \cdot (\rho \nabla U) \text{ on } \mathbb{R}_+ \times \mathbb{R}^d$$

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$$\rho_\infty(x, v) \propto \exp\left(-U(x) - \frac{1}{2}v^2\right)$$

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So the minimizer should let $U + \log \rho = \text{constant}$, i.e. $\rho \propto \exp(-U(x))$.

Free energy as relative entropy

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Hence

$$\begin{aligned} \frac{d}{dt} H(\rho_t | \rho_\infty) &= \frac{dF(\rho_t)}{dt} = \frac{d}{dt} \int \rho_t U + \rho_t \log \rho_t \\ &= \int (U + \log \rho_t) \partial_t \rho_t \\ &= \int (U + \log \rho_t) \nabla \cdot (\rho_t \nabla (U + \log \rho_t)) \\ &= \int \rho_t |\nabla (U + \log \rho_t)|^2 = \int \left| \nabla \log \frac{\rho_t}{\rho_\infty} \right|^2 \rho_t \end{aligned}$$

Logarithmic Sobolev inequality

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Thus if ρ_∞ satisfies κ -LSI, then we have the exponential convergence of free energy (relative entropy)

$$H(\rho_t|\rho_\infty) \leq H(\rho_0|\rho_\infty) e^{-2\kappa t}.$$

Conditions for LSI

(Bakry–Émery) If $\nabla^2 U \geq \kappa > 0$, then $\rho_\infty \propto \exp(-U)$ satisfies κ -LSI.

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These conditions are all dimension-free!

Underdamped case

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Still true:

- $\rho_\infty = Z^{-1} \exp(-U - \frac{1}{2}v^2)$, $Z = \int \exp(-U - \frac{1}{2}v^2)$;
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Free energy decrease vanishes for “local equilibrium states”, that is, whose conditional law $\rho(v|x) \propto \exp(-\frac{1}{2}v^2)$.

Hypocoercivity

Nevertheless, Villani overcomes the problem by adding a term to relative entropy

$$\mathcal{E}(\rho) = H(\rho|\rho_\infty) + I_S(\rho|\rho_\infty)$$

where S is a non-degenerate $2d \times 2d$ matrix and

$$I_S(\rho|\rho_\infty) = \int \left(\nabla \log \frac{\rho}{\rho_\infty} \right)^t S \nabla \log \frac{\rho}{\rho_\infty} \rho.$$

If ρ_∞ satisfies an LSI and $\nabla^2 U$ is bounded, we can construct S such that

$$\frac{d}{dt} \mathcal{E}(\rho) \leq -\kappa' \mathcal{E}(\rho).$$

Non-linear energy functional

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- $E(\rho) = \int \rho U$;
- $E(\rho) = \int \rho U_1 + \frac{1}{2} \iint U_2(x - y) \rho(dx) \rho(dy)$;
- loss function of neural networks.

Linear functional derivative

We say that $E : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ is C^1 if there exists a continuous mapping $\delta_\rho E : \mathcal{P}_2(\mathbb{R}^d) \times \mathbb{R}^d \rightarrow \mathbb{R}$ such that for all $\rho_0, \rho_1 \in \mathcal{P}_2(\mathbb{R}^d)$, it holds

$$E(\rho_1) - E(\rho_0) = \int_0^1 \int \delta_\rho E(\rho_t, x)(\rho_1 - \rho_0)(dx) dt$$

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- $[\delta_\rho \int \rho U](\rho, x) = U(x);$
- $[\delta_\rho \frac{1}{2} \iint U_2(x - y)\rho(dx)\rho(dy)](\rho, x) = \int U_2(x - y)\rho(dy);$

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$$\begin{aligned} \frac{dX_t(x)}{dt} &= v(X_t(x)), \quad X_0(x) = x, \\ \rho_t &= (X_t)_\# \rho_0 \end{aligned}$$

Then ρ solves the continuity equation $\partial_t \rho = -\nabla \cdot (\rho v)$.

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The change of E is $\frac{d}{dt} E(\rho_t) = \int \delta_\rho E(\rho_t) - \nabla \cdot (\rho v) = \int D_\rho E \cdot v \rho$.

Convexity of energy functional

We say E is convex if $E(\rho_t) \leq (1-t)E(\rho_0) + tE(\rho_1)$,

$\rho_t = (1-t)\rho_0 + t\rho_1$ the functional (flat) interpolation.

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- neural networks with only one hidden layer.

Our key assumption is the functional convexity of E .

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Classical overdamped Langevin is gradient descent in sense of JKO:

$$\rho_{n+1}^h = \operatorname{argmin} \int \rho(U + \log \rho) + (2h)^{-1} W_2^2(\rho, \rho_n^h),$$

$$\lim_{nh \rightarrow t, n \rightarrow \infty} \rho_n^h = \rho_t$$

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Overdamped MFL is its generalization

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MFL energy descent (1)

Same calculus as linear shows

$$\frac{d}{dt} \left(E(\rho_t) + \int \rho_t \log \rho_t \right) = \frac{d}{dt} F(\rho_t) = -I(\rho_t | \hat{\rho}_t)$$

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Note that

$$\begin{aligned} F(\rho_t) - F(\rho_\infty) &\geq \int \delta_\rho E(\rho_\infty, \cdot)(\rho_t - \rho_\infty) + \int \rho_t \log \rho_t - \rho_\infty \log \rho_\infty \\ &= - \int \log \rho_\infty(\rho_t - \rho_\infty) + \int \rho_t \log \rho_t - \rho_\infty \log \rho_\infty \\ &= H(\rho_t | \rho_\infty). \end{aligned}$$

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For example, suppose the LFD is of form $\delta_\rho E(\rho, x) = g(x) + h(\rho, x)$, where $\nabla^2 g \geq \kappa > 0$ and $h(\rho, x)$ be uniformly bounded. Then apply Bakry–Émery and Holley–Stroock.

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Let κ' be the uniform LSI constant.

$$\begin{aligned}
 \frac{1}{2\kappa'} I(\rho_t | \hat{\rho}_t) &\geq H(\rho_t | \hat{\rho}_t) \\
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 &\geq \int \rho_t (\log \rho_t + \delta_\rho E(\rho_t, \cdot)) - \int (\delta_\rho E(\rho_t, \cdot) + \log \rho_\infty) \rho_\infty \\
 &= \int \delta_\rho E(\rho_t, \cdot) (\rho_t - \rho_\infty) + H(\rho_t) - H(\rho_\infty) \geq F(\rho_t) - F(\rho_\infty).
 \end{aligned}$$

Hypocoercivity with mean-field interaction

À la Villani, we consider the functional

$$\mathcal{E}(\rho) = E(\rho) + \frac{1}{2} \int \rho v^2 + \int \rho \log \rho + I_S(\rho|\hat{\rho}).$$

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If

- $\hat{\rho}_t$ has uniform LSI;
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we can construct non-degenerate S such that

$$\frac{d}{dt} \mathcal{E}(\rho_t) \leq -\kappa'(\mathcal{E}(\rho_t) - \mathcal{E}(\rho_\infty)).$$

Particle approximation

We consider the overdamped particle system

$$dX_t^i = -D_\rho F(\mu^{X_t}, X_t^i) dt + \sqrt{2} dW_t^i$$

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Distances between probability measure

We wish to show *uniformly* in t .

$$\frac{1}{N} W_2^2(\rho_t^N, \rho_t^{\otimes N}), \frac{1}{N} H(\rho_t^N | \rho_t^{\otimes N}) \rightarrow 0$$

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Synchronized coupling gives Grönwall-type growth estimate

$$\frac{1}{N} W_2^2(\rho_t^N, \rho_t^{\otimes N}) \leq \frac{1}{N} \exp(Ct) W_2^2(\rho_0^N, \rho_0^{\otimes N}) + \frac{C}{N} (\exp(Ct) - 1).$$

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We focus on the *long-time behavior* of the particle system.

Free energy descent for particle system (1)

We note that the N -particle system is subject to the potential in \mathbb{R}^{Nd}

$$U^N(x_1, \dots, x_N) = NE \left(\frac{1}{N} \sum_{i=1}^N \delta_{x^i} \right) = NE(\mu^x)$$

$$\nabla_i U^N(x_1, \dots, x_N) = D_\rho E \left(\frac{1}{N} \sum_{j=1}^N \delta_{x^j}, x^i \right) = D_\rho E(\mu^x, x^i).$$

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Define free energy $F^N(\rho^N) = N \int E(\mu^x) \rho^N(dx) + \int \rho^N \log \rho^N$ and the invariant measure $\rho_\infty^N \propto \exp(-NE(\mu^x))$. We know by classical results

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However, under our conditions the LSI constant for ρ_∞^N vanishes when $N \rightarrow \infty$.

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- the marginal distribution by $\rho_{i_1, \dots, i_k}^N(x_{i_1}, \dots, x_{i_k})$;
- the conditional distribution by

$$\rho_{i|-i}^N(x_i | x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n) = \rho_{i|-i}^N(x_i | x_{-i}).$$

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Fisher information decomposes

$$\begin{aligned} I(\rho_t^N | \rho_\infty^N) &= \sum_{i=1}^N \int \left| \nabla_i \log \frac{\rho_{i| -i, t}^N \rho_{-i, t}^N}{\rho_{i| -i, \infty}^N \rho_{-i, \infty}^N} \right|^2 \rho_{i| -i, t}^N \rho_{-i}^N \\ &= \sum_{i=1}^N \mathbb{E}^{-i} \left[\int \left| D_\rho E(\mu^x, x^i) + \nabla_i \log \rho_{i| -i}^N \right|^2 \rho_{i| -i}^N \right] \end{aligned}$$

Modulo an $o(1)$ error, we may replace μ^x by $\mu^{x^{-i}} = \frac{1}{N-1} \sum_{j \neq i} \delta_{x_j}$.

Free energy descent for particle system (3)

Hence $I(\rho_t^N | \rho_\infty^N) = \sum_{i=1}^N \mathbb{E}^{-i} I(\rho_{i|-i}^N | \hat{\rho}_{i|-i}^N) + o(N)$, with

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Applying LSI and use Jensen's inequality as before

$$\begin{aligned} \frac{1}{2\kappa'} \sum_{i=1}^N \mathbb{E}^{-i} I(\rho_{i|-i,t}^N | \hat{\rho}_{i|-i}^N) &= \sum_{i=1}^N \mathbb{E}^{-i} H(\rho_{i|-i,t}^N | \hat{\rho}_{i|-i}^N) \\ &= \sum_{i=1}^N \mathbb{E}^{-i} \int (\rho_{i|-i,t}^N (\delta_\rho E(\mu^{x^{-i}} \cdot x_i) + \log \rho_{i|-i,t}^N) + \log \int \exp(-\delta_\rho E(\mu^{x^i}, \cdot))) \\ &\geq \sum_{i=1}^N \mathbb{E}^{-i} \int (\rho_{i|-i,t}^N - \rho_\infty) \delta_\rho E(\mu^{x^{-i}} \cdot x_i) + \int \rho_{i|-i}^N \log \rho_{i|-i}^N - \rho_\infty \log \rho_\infty \end{aligned}$$

Free energy descent for particle system (4)

By convexity of E , we have

$$\begin{aligned}
 E^N(\rho_t^N) - NE(\rho_\infty) &= N\mathbb{E}[E(\mu^X) - E(\rho_\infty)] \\
 &\leq N\mathbb{E}\left[\int \delta_\rho E(\mu^X, x)(\mu^X - \rho_\infty)(dx)\right] \\
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Again changing μ^X to μ^{X-i} and use the information inequality

$$\sum_{i=1}^N \mathbb{E}^{-i} \int \rho_{i| -i}^N \log \rho_{i| -i}^N \geq \int \rho^N \log \rho^N,$$

we derive

$$\frac{d}{dt} F^N(\rho_t^N) \leq -2\kappa'(F^N(\rho_t^N) - NF(\rho_\infty)) + o(N).$$

Free energy descent for particle system (5)

Previous differential inequality gives bound on energy of one side

$$\frac{1}{N}F^N(\rho_t^N) - F(\rho_\infty) \leq \left(\frac{1}{N}F^N(\rho_0^N) - F(\rho_\infty) \right) e^{-2\kappa' t} + o(1).$$

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The other bound is obtained by convexity

$$\begin{aligned} \frac{1}{N}F^N(\rho_t^N) - F(\rho_\infty) &= \mathbb{E}[E(\mu^{X_t}) - E(\rho_\infty)] + \frac{1}{N} \int \rho_t^N \log \rho_t^N - \int \rho_\infty \log \rho_\infty \\ &\geq \mathbb{E} \left[\int \delta_\rho E(\rho_\infty, \cdot) (\mu^{X_t} - \rho_\infty) \right] + \frac{1}{N} \int \rho_t^N \log \rho_t^N - \int \rho_\infty \log \rho_\infty \\ &= \frac{1}{N} \int (\rho_t^N - \rho_\infty^{\otimes N}) \sum_{i=1}^N \delta_\rho E(\rho_\infty, x^i) + \frac{1}{N} \int \rho_t^N \log \rho_t^N - \rho_\infty^{\otimes N} \log \rho_\infty^{\otimes N} \\ &= \frac{1}{N} H(\rho_t^N | \rho_\infty^{\otimes N}) \geq 0. \end{aligned}$$

Propagation of chaos in long time

From previous computations, $\frac{1}{N}H(\rho_t^N | \rho_\infty^{\otimes N}) \leq C_0 e^{-2\kappa' t} + o(1)$.

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If E is regular enough, $o(1)$ -term is actually $O(N^{-1})$.

Propagation of chaos in long time

From previous computations, $\frac{1}{N}H(\rho_t^N|\rho_\infty^{\otimes N}) \leq C_0 e^{-2\kappa't} + o(1)$.

Tensorizing MFL $H(\rho_t|\rho_\infty)$, we have $\frac{1}{N}H(\rho_t^{\otimes N}|\rho_\infty^{\otimes N}) \leq C_0 e^{-2\kappa't}$.

Since $\rho_\infty \propto \exp(-\delta_\rho E(\rho_\infty, \cdot))$ satisfies a LSI, $\rho_\infty^{\otimes N}$ too with the same constant.

LSI implies Talagrand's T_2 inequality, $\frac{\kappa'}{2} W_2^2(\rho, \rho_\infty^{\otimes N}) \leq H(\rho|\rho_\infty^{\otimes N})$

Hence

$$\begin{aligned} \frac{1}{N} W_2^2(\rho_t^N, \rho_t^{\otimes N}) &\leq \frac{1}{N} W_2^2(\rho_t^N, \rho_\infty^{\otimes N}) + \frac{1}{N} W_2^2(\rho_t^{\otimes N}, \rho_\infty^{\otimes N}) \\ &\leq \frac{2}{\kappa'} \frac{1}{N} (H(\rho_t^N|\rho_\infty^{\otimes N}) + H(\rho_t^{\otimes N}|\rho_\infty^{\otimes N})) \leq \frac{C_0}{\kappa'} e^{-2\kappa't} + o(1) \end{aligned}$$

If E is regular enough, $o(1)$ -term is actually $O(N^{-1})$.

Convergence of relative entropy requires uniform LSI for ρ_t .

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The method for relative entropy's and *relative Fisher information's* convergence is different, and we lose some exponents in N .