# The Stein-log-Sobolev inequality and the exponential convergence of the Stein Variational Gradient Descent algorithm

## From non-local to local

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# The mobility equation



The following PDE denotes a general mobility equation

$$\partial_t \rho = \mathrm{div}(m(\rho)\mathcal{V}(\rho))$$

where

- $m : \mathbb{R} \to \mathbb{R}$ is some continuous mobility function,
- $\mathcal{V}(\rho)$ is some velocity that can have the form

$$\mathcal{V}(\rho_t) = \nabla U'(\rho_t) + \nabla V + \nabla(W * \rho_t).$$

# Examples [Carrillo et al., 2024b]

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- Lubrication model for thin films [Bertozzi, 1998]

$$m(\rho) = \rho^3, \quad \mathcal{V}(\rho) = -\sqrt{\mathrm{Ca}}\,\nabla\rho + \nabla\Delta\rho.$$

- Cahn-Hilliard equation for phase separation in binary alloys [Cahn, 1998]

$$m(\rho) = 1 - \rho^2, \quad \mathcal{V}(\rho) = -\nabla\frac{\delta E}{\delta\rho}, \quad E(\rho) := \int_\Omega H(\rho(x)) + \frac{\epsilon^2}{2}|\nabla\rho(x)|^2 \, \mathrm{d}x,$$

where $\rho : [0, \infty) \times \Omega \to [-1, 1]$.

- Chemotaxis with prevention of overcrowding [Burger et al., 2006]

$$m(\rho) = \rho(1 - \rho).$$

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# Stein Variational Gradient Descent [Liu and Wang, 2016]



We want to approximate $\rho_\infty \propto e^{-V}$ for a potential $V : \mathbb{R}^d \to \mathbb{R}$.

SVGD is governed by a positive definite interaction kernel $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$.

Given is some initial distribution of particles $X_0^1, \ldots, X_0^N \in \mathbb{R}^d$.

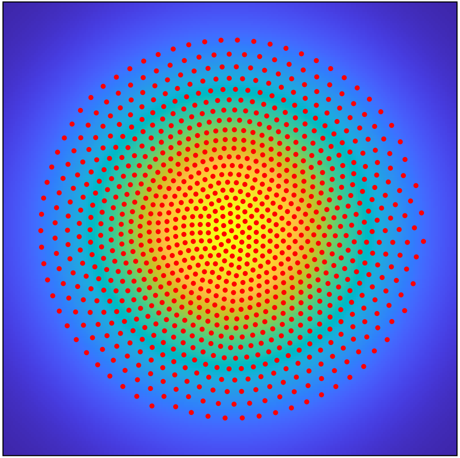
SVGD has deterministic particle dynamics

$$X_{n+1}^i := X_n^i + \varepsilon_n \sum_{j=1}^N (\nabla_y K)(X_n^i,\, X_n^j) - K(X_n^i,\, X_n^j)\nabla V(X_n^j).$$

# Computational Examples



## Normal Gaussian



# Computational Examples

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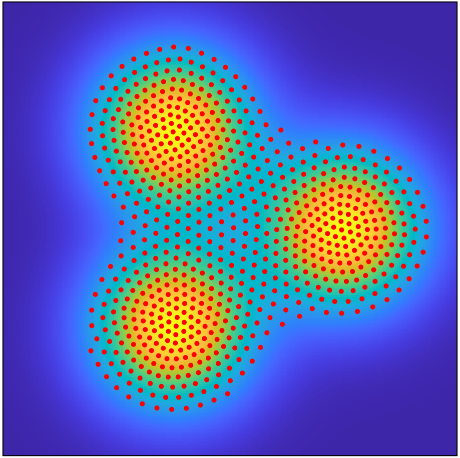
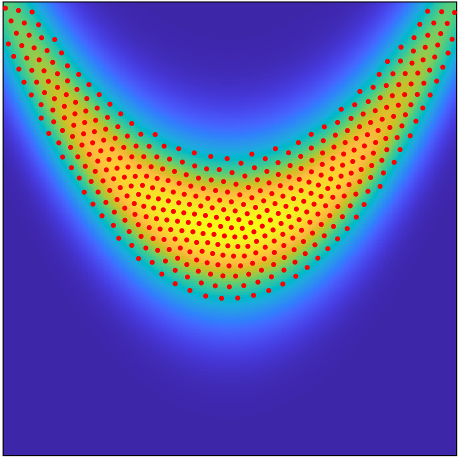
## Mixture of Gaussians



# Computational Examples



## Banana Distribution



# Mean-field limit



Formal computations in [Liu, 2017] show that if $N \to \infty$, $\varepsilon \to 0$ and the kernel is translation invariant $K(x, y) := k(x - y)$, then the following evolution of distribution of particles holds true

$$\partial_t \rho = \mathrm{div}\left(\rho\ k * (\nabla \rho + \rho \nabla V)\right) = \mathrm{div}(\rho\ k * \nabla(\rho e^V) e^{-V}).$$

# SVGD as a gradient flow

In fact we can interpret the previous equation as a gradient flow

$$\frac{d}{dt}\mathrm{KL}(\rho_t \,||\, \rho_\infty) = -\mathbb{D}^2(\rho_t \,||\, \rho_\infty),$$

where we define the dissipation by

$$\mathbb{D}^2(\rho_t \,||\, \rho_\infty) := \int_{\mathbb{R}^d} \nabla(\rho e^V)e^{-V} \cdot k * \nabla(\rho e^V)e^{-V} \,\mathrm{d}x,$$

and the Kullback-Leibler divergence (or relative entropy)

$$\mathrm{KL}(\rho_t \,||\, \rho_\infty) := \int_{\mathbb{R}^d} \rho \ln(\rho) \,\mathrm{d}x + \int_{\mathbb{R}^d} \rho V \,\mathrm{d}x.$$

# Stein-log-Sobolev inequality



We achieve an exponential rate of decay in the Kullback-leibler divergence if the **Stein-log-Sobolev inequality** holds for some fixed $\lambda > 0$

$$\lambda \, \mathrm{KL}(\rho_t \,||\, \rho_\infty) \leq \mathbb{D}^2(\rho_t \,||\, \rho_\infty).$$

In this case we get

$$\mathrm{KL}(\rho_t \,||\, \rho_\infty) \leq e^{-\lambda t} \mathrm{KL}(\rho_0 \,||\, \rho_\infty).$$

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# From non-local to local

Take $k \in L^1(\mathbb{R}^d)$ with $k \geq 0$, $\int_{\mathbb{R}^d} k \,\mathrm{d}x = 1$ and $k$ is positive definite. Define the approximation of the identity $k_\sigma := \sigma^{-d} k(x/\sigma)$ for $\sigma \in (0,1)$. Let $\rho^\sigma$ denote the solution of

$$\partial_t \rho^\sigma = \operatorname{div}\left(\rho^\sigma \; k_\sigma * (\nabla \rho^\sigma + \rho^\sigma \nabla V)\right).$$

We observe that $k_\sigma \rightharpoonup \delta_0$ as $\sigma \to 0$ in the sense of distributions. Then, if $\rho^\sigma \rightharpoonup \rho$ as $\sigma \to 0$, then one formally derives a weak solution to the following mobility equation

$$\partial_t \rho = \operatorname{div}\left(\rho \left(\nabla \rho + \rho \nabla V\right)\right) = \operatorname{div}\left(\rho^2 \; \nabla(\ln(\rho) + V)\right).$$

# Exponential convergence rate for the continuity equation

Assume that the Stein-log-Sobolev inequality holds uniformly for all solutions $\{\rho^\sigma\}_\sigma$ with some fixed constant $\lambda > 0$. Then, we derive the uniform bound

$$\mathrm{KL}(\rho_t^\sigma \,||\, \rho_\infty) \leq e^{-\lambda t}\mathrm{KL}(\rho_0 \,||\, \rho_\infty).$$

By taking the limit $\sigma \to 0$ and using the lower semicontinuity of the Kullback-Leibler divergence, we see that the continuity equation would possess an exponential convergence rate

$$\mathrm{KL}(\rho_t \,||\, \rho_\infty) \leq e^{-\lambda t}\mathrm{KL}(\rho_0 \,||\, \rho_\infty).$$

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# Main Theorem [Carrillo et al., 2024a]

We were inspired by [Duncan et al., 2023] to use the following ansatz form

$$K(x,y) = e^{V(x)-\frac{V_0(x)}{2}}k(x-y)e^{V(y)-\frac{V_0(y)}{2}}.$$

A sufficient criteria for the Stein-log-Sobolev inequality is

- $V \geq \mathbb{V}_0$ for $\mathbb{V}_0(x) = \alpha|x|^2 + \beta$,
- $k \in L^1(\mathbb{R}^d) + L^2(\mathbb{R}^d)$,
- There exists two constants $C_0, C_1 \geq 1$ such that

$$\frac{1}{C_0}\frac{1}{1+|\xi|^2} \leq \hat{k}(\xi) \leq C_1\frac{1}{1+|\xi|^2}.$$

# Existence of weak solution [Carrillo et al., 2024a]

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If additionally $V \in C^1(\mathbb{R}^d) \cap H^m_{\mathrm{loc}}(\mathbb{R}^d)$ for some $m > \frac{d}{2}$, then there exists a solution $\rho \in C^0([0,\infty), \mathcal{P}(\mathbb{R}^d))$ in the distributional sense to the non-local continuity equation

$$\partial_t \rho_t = \mathrm{div}\left(\rho_t e^{V - \frac{V_0}{2}} \; k * \left[(\nabla \rho_t + \rho_t \nabla V) e^{V - \frac{V_0}{2}}\right]\right). \tag{$*$}$$

Moreover, we have exponential decay in Kullback-Leibler divergence and the energy dissipation inequality

$$\mathrm{KL}(\rho_t \,||\, \rho_\infty) \leq e^{-\lambda t} \mathrm{KL}(\rho_0 \,||\, \rho_\infty),$$

$$\mathrm{KL}(\rho_t \,||\, \rho_\infty) + \int_0^t \mathbb{D}^2(\rho_s \,||\, \rho_\infty)\, \mathrm{d}s \leq \mathrm{KL}(\rho_0 \,||\, \rho_\infty).$$

# Stein-log-Sobolev constant [Carrillo et al., 2024a]

The Stein-log-Sobolev constant has the form

$$\lambda = \lambda_0 \, (\alpha \wedge 1) \, e^{\beta} \, \frac{1}{C_0^2} \, \frac{1}{\|e^{-V}\|_{L^1}},$$

where $\lambda_0 > 0$ is some constant independent of dimension $d$, and we recall that $\alpha$ and $\beta$ determine $\mathbb{V}_0$, and $C_0$ is used for the lower bound of $\hat{k}$.

If we only vary $k$, then we see that the Stein-log-Sobolev constant only depends on $C_0$.

# Application of result

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Let $\rho^\sigma$ be the weak solution to $(*)$ with kernel $k_\sigma(x) := \sigma^{-d} k(x/\sigma)$.

We observe a uniform lower bound

$$\hat{k}_\sigma(x) = \hat{k}(\sigma x) \geq \frac{1}{C_0} \frac{1}{1 + |\sigma \xi|^2} \geq \frac{1}{C_0} \frac{1}{1 + |\xi|^2}.$$

Thus we see that the Stein-log-Sobolev inequality holds uniformly for all $\{k_\sigma\}_\sigma$.

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# Passing to the limit

Let $\{\rho^\sigma\}_\sigma$ be the weak solutions to $(*)$.

If we assume $k = \omega * \omega$ for some measurable function $\omega : \mathbb{R}^d \to \mathbb{R}$ that satisfies certain constraints, and $\omega_\sigma(x) = \sigma^{-d}\omega(x/\sigma)$, then we need to pass to the limit in the following PDE

$$\partial_t \rho_t^\sigma = \mathrm{div}\left( \left(\rho_t^\sigma e^{V - \frac{V_0}{2}}\right)\ \omega_\sigma * \left[ (\nabla \rho_t^\sigma + \rho_t^\sigma \nabla V) e^{V - \frac{V_0}{2}} \right] * \omega_\sigma \right).$$

# Passing to the limit

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$$\partial_t \rho_t^\sigma = \mathrm{div}\left( (\rho_t^\sigma e^{V - \frac{V_0}{2}}) \ \omega_\sigma * \left[ (\nabla \rho_t^\sigma + \rho_t^\sigma \nabla V) e^{V - \frac{V_0}{2}} \right] * \omega_\sigma \right)$$

We restrict ourselves to the domain $[0, T] \times B_R$. A commutator argument shows that the above limit coincides with the one below

$$\partial_t \rho_t^\sigma = \mathrm{div}\left( (\rho_t^\sigma e^{V - \frac{V_0}{2}} \chi) * \omega_\sigma \ \left[ (\nabla \rho_t^\sigma + \rho_t^\sigma \nabla V) e^{V - \frac{V_0}{2}} \right] * \omega_\sigma \right)$$

where $\chi \in C_c^\infty(\mathbb{R}^d)$ satisfies $0 \leq \chi \leq 1$, $\chi = 1$ on $B_R$ and $\chi = 0$ outside $B_{2R}$.

# Passing to the limit

$$\partial_t \rho_t^\sigma = \operatorname{div}\left( (\rho_t^\sigma e^{V - \frac{V_0}{2}} \chi) * \omega_\sigma \ \ \left[ (\nabla \rho_t^\sigma + \rho_t^\sigma \nabla V) e^{V - \frac{V_0}{2}} \right] * \omega_\sigma \right)$$

The energy dissipation gives us weak compactness in $L^2([0,T] \times \mathbb{R}^d)$.

# Passing to the limit

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$$\partial_t \rho_t^\sigma = \mathrm{div}\left( (\rho_t^\sigma e^{V-\frac{V_0}{2}} \chi) * \omega_\sigma \quad \left[ (\nabla \rho_t^\sigma + \rho_t^\sigma \nabla V) e^{V-\frac{V_0}{2}} \right] * \omega_\sigma \right)$$

Using the Aubin-Lions lemma we show compactness in $L^2([0,T] \times \mathbb{R}^d)$.

# Passing to the limit



$$\color{red}{\partial_t \rho_t^\sigma} = \operatorname{div}\left( \left(\rho_t^\sigma e^{V - \frac{V_0}{2}} \chi\right) * \omega_\sigma \quad \left[ (\nabla \rho_t^\sigma + \rho_t^\sigma \nabla V) e^{V - \frac{V_0}{2}} \right] * \omega_\sigma \right)$$

We show weak compactness in $L^{2\frac{q+2}{q+1}}(0, T; H^{-m}(B_R))$ to derive uniform convergence in $C^0([0, T]; \mathcal{P}(\mathbb{R}^d))$ for $q := d \vee 3$ and some fixed $m > \frac{d}{2}$.

Combining everything allows us to pass to the limit.

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# Summary

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We've shown the existence of a solution $\rho \in C^0([0,\infty);\mathcal{P}(\mathbb{R}^d))$ in the sense of distributions to the following mobility equation

$$\partial_t \rho = \mathrm{div}(\rho^2 \nabla(\ln(\rho) + V)).$$

Moreover, we have shown that this equation possess an exponential decay in the Kullback-Leibler divergence (or relative entropy), for some $\lambda > 0$ depending only on $V$,

$$\mathrm{KL}(\rho_t \,||\, \rho_\infty) \leq e^{-\lambda t}\mathrm{KL}(\rho_0 \,||\, \rho_\infty).$$

# Thank you for your attention

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