Phase transitions and a mountain pass theorem in the space of probability measures

André Schlichting

Applied Mathematics Münster
Insitute for Analysis and Numerics

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Phase transitions in the McKean–Vlasov model

[Carrillo-Gvalani-Paviliotis-S. ARMA '20]

The McKean–Vlasov equation – Derivation

- Overdamped Langevin equation defined on $\mathbb{T}_L^d \simeq [0, L)^d$

$$\mathrm{d}X_t^i = -\frac{\kappa}{N} \sum_{j=1, j\neq i}^{N} \nabla W(X^i - X^j)dt + \sqrt{2}\,\mathrm{d}B_t^i \qquad , i = 1, \dots, N$$

- $\kappa \in [0, \infty)$ interaction strength (bifurcation parameter)
- The mean-field limit $N \to \infty$ is governed by the McKean–Vlasov equation

$$\partial_t \varrho = \Delta \varrho + \kappa \nabla \cdot (\varrho \nabla W \star \varrho) \qquad \text{in } \mathbb{T}_L^d \times (0, T]$$

- properties encoded in interaction potential $W : \mathbb{T}_L^d \to \mathbb{R}$ (coordinate-wise even)

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Some applications: Models for finite N or mean-field limit include

- Molecules of a gas (Lennard–Jones, Van-der-Waals)
- Collective motion of agents (attractive-repulsive)
- Opinions of individuals (Hegselmann–Krause)
- Liquid crystals / nanorods (anisotropic, Onsager, Maier–Saupe)
- Nonlinear synchronizing oscillators (Kuramoto)
- Chemotaxis models (Patlak–Keller–Segel)

Example: Nonlinear synchronization of oscillators

The Kuramoto model: $W(x) = -\cos x$ and $L = 2\pi$

$\kappa < \kappa_c$, no phase locking

$\kappa > \kappa_c$, phase locking

Example: 2d Gaussian attractive interaction potential

$$W(x) = -\frac{1}{2\pi\sigma^2} e^{-\frac{|x|^2}{2\sigma^2}}$$

with $\sigma^2 = \frac{1}{2}$, $L = 10$, $\kappa = \sqrt{2L} > \kappa_c$.

Transition points and types of phase transitions

Free energy functional (Lyapunov property, gradient flow)

$$\partial_t \varrho_t = \nabla \cdot (\varrho \nabla \mathcal{F}'(\varrho))$$

$$\mathcal{F}_\kappa(\varrho) = \int_{\mathbb{T}_L^d} \varrho \log \varrho \,\mathrm{d}x + \frac{\kappa}{2} \iint_{\mathbb{T}_L^d \times \mathbb{T}_L^d} W(x-y)\varrho(x)\varrho(y)\,\mathrm{d}x\,\mathrm{d}y\ .$$

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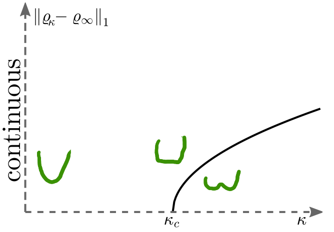
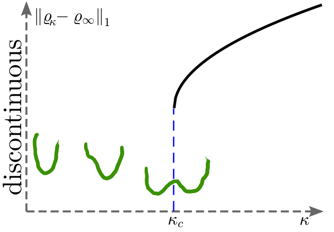
Definition: Let $\varrho_\infty \equiv L^{-d}$. κ_c is transition point, if:

- For $\kappa \le \kappa_c$ is ϱ_∞ global minimizer of $\mathcal{F}_\kappa$ and unique for $\kappa < \kappa_c$
- For $\kappa > \kappa_c$ exists another global minimizer ϱ_κ





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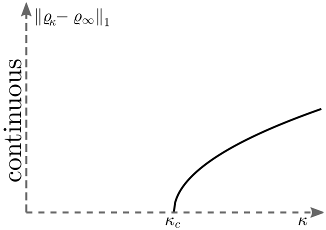
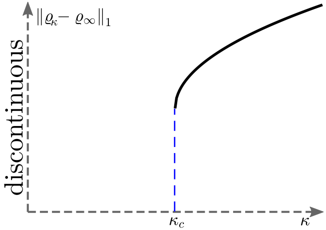


Results and Goals:

- Bifurcation analysis and local stability around $\varrho_\infty \equiv L^{-d}$
- Classification for continuous and discontinuous transitions
- Understanding of the free energy landscape
- Dynamical properties related to nucleation and coarsening



Characterization of phase transition

Theorem [Carrillo-Gvalani-Paviliotis-S. '20]

Let $\widetilde{W} : \mathbb{N}^d \to \mathbb{R}$ denote the (real) Fourier modes of W.

- If there is only one dominant unstable mode k^*: For $\alpha > 0$ small enough holds

$$\alpha \widetilde{W}(k^*) \leq \widetilde{W}(k) \qquad \text{for all } k \neq k^* : \widetilde{W}(k) < 0 \,,$$

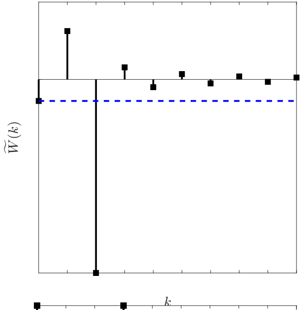
  then the transition point κ_c is continuous.

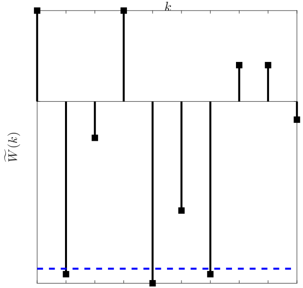
- If there exist (near)-dominant resonating modes k^a, k^b, k^c: That is for δ small enough exist

$$k^a, k^b, k^c \in \left\{ k' \in \mathbb{N}^d : \widetilde{W}(k') \leq \min_{k \in \mathbb{N}^d} \widetilde{W}(k) + \delta \right\} \quad \text{with } k^a = k^b + k^c,$$

  then the transition point κ_c is discontinuous.

$\Rightarrow$ local attractive potentials lead to discontinuous phase transitions





A mountain pass theorem

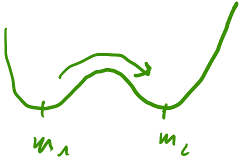
[Gvalani-S. JFA '20]

Noise-induced transitions in $\mathbb{R}^d$

Start form deterministic gradient flow in $\mathbb{R}^d$

$$\dot{x}(t) = -\nabla F(x) \quad \text{with} \quad x(0) = x_0 \in \mathbb{R}^d$$

- F has two global minima $m_1, m_2 \in \mathbb{R}^d$.



Describe the particle transition from m_1 to m_2 under the influence of noise.

Modelproblem: Add Brownian motion

$$dX_t = -\nabla F(X_t)\,\mathrm{d}t + \sqrt{2\sigma} dB_t\,,$$

Question: Given $X(0) = m_1$, what is the probability that in some finite time $T > 0$, we have that $X(T) = m_2$ in the regime $\sigma \ll 1$?

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Theorem (Freidlin–Wentzell)

The family of processes $\{X_t^\sigma\} \in C([0,T];\mathbb{R}^2)$ satisfy a LDP with good rate function $I : C([0,T];\mathbb{R}^d) \to \mathbb{R} \cup \{+\infty\}$

$$I(\gamma) = \frac{1}{4}\int_0^T |\dot{\gamma}(t) + \nabla F(\gamma(t))|^2\,\mathrm{d}t.$$

and it holds

$$\mathbb{P}(X_t^\sigma \in \Gamma) \approx \exp\left(-\sigma^{-1} \inf_{\gamma\in\Gamma} I(\gamma)\right) \qquad \sigma \ll 1,$$

for any $\Gamma \subset C([0,T];\mathbb{R}^d)$.

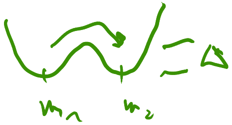
Noise-induced transitions in $\mathbb{R}^d$

For $\gamma \in \Gamma = \{f \in C^1([0,T];\mathbb{R}^d) : \gamma(0) = m_1, \gamma(T) = m_2\}$ let $T^* = \arg\max_{t\in[0,T]}(F(\gamma(t)) - F(\gamma(0)))$:

$$\begin{aligned} I(\gamma) &\geq \frac{1}{4}\int_0^{T^*} |\dot\gamma(t) + \nabla F(\gamma(t))|^2 \,\mathrm{d}t = \frac{1}{4}\int_0^{T^*} |\dot\gamma(t) - \nabla F(\gamma(t))|^2 \,\mathrm{d}t + \int_0^{T^*} \dot\gamma(t)\cdot\nabla F(\gamma(t))\,\mathrm{d}t \\ &\geq F(\gamma(T^*)) - F(\gamma(0)) \geq \inf_{\gamma\in\Gamma}(F(\gamma(T^*)) - F(\gamma(0))) =: c - F(\gamma(0))\,, \end{aligned}$$

By classical mountain pass theorem: c a critical value of F, i.e., $\exists s \in \mathbb{R}^d : \nabla F(s) = 0, F(s) = c$.

$$\Rightarrow \qquad \mathbb{P}(X_t^\sigma \in \Gamma) \lesssim \exp(-\sigma^{-1}\Delta F) \qquad \text{where} \quad \Delta F = F(s) - F(m_1).$$



LDP for McKean-Vlasov interaction particle system

- Apply argument to the McKean–Vlasov N-particle system for $N \gg 1$

$$\mathrm{d}X_t^i = -\frac{\kappa}{N} \sum_{j=1, j\neq i}^{N} \nabla W(X^i - X^j)dt + \sqrt{2}\,\mathrm{d}B_t^i, \qquad i = 1, \dots, N$$

- [Dawson-Gärtner 1987] proved LDP with rate function for $\mu \in AC^2([0,T], \mathcal{P}_2(\mathbb{T}_L^d))$ given by

$$I_\kappa(\mu(\cdot)) := \frac{1}{4}\int_0^T \|\partial_t \mu_t - \nabla \cdot (\mu_t \nabla(\log \mu_t + \kappa W \star \mu_t))\|_{-1,\mu_t}^2 \,\mathrm{d}t$$

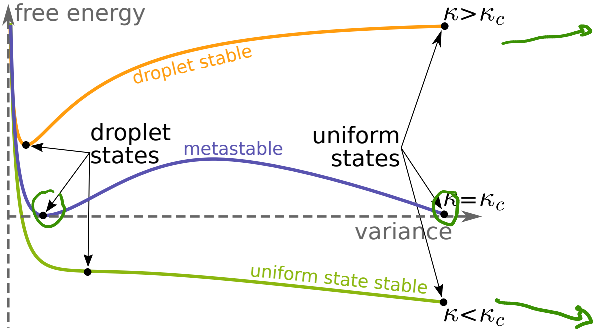
- Associated quasipotential to LDP is $\mathcal{F}_\kappa$!

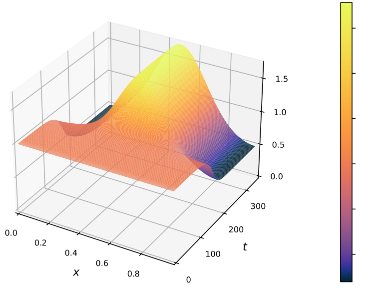
$$\mathbb{P}(\text{transition: } \varrho_\infty \to \varrho_{\kappa_c}) \lesssim \exp\Big(-N \inf\{I_\kappa(\mu(\cdot)) : \mu(0) = \varrho_\infty, \mu(T) = \varrho_{\kappa_c}\}\Big)$$

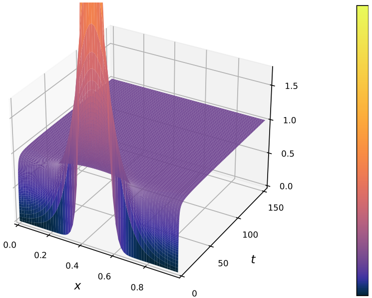
$$\leq \exp\left(-N \inf_\mu \left\{ \sup_{T^* \in [0,T]} (\mathcal{F}_\kappa(\mu(T^*)) - \mathcal{F}_\kappa(\mu(0))) : \mu(0) = \varrho_\infty, \mu(T) = \varrho_{\kappa_c} \right\}\right).$$

Discontinuous phase transitions and metastability

- N-particle system is metastable at disc. phase transition
- By [Dawson-Gärtner 1989] need to understand free energy .







- Missing ingredient: mountain pass theorem for $\mathcal{F}_\kappa$
  Difficulties:
  - $(\mathcal{P}(\mathbb{T}_L^d), W_2)$ only metric space
  - $\mathcal{F}_\kappa$ only lower semicontinuous

A mountain pass theorem

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Theorem [Gvalani-S. '20]

If $\mathcal{F}_{\kappa_c}$ has two distinct minimizers $\varrho_\infty \equiv 1/L^d$ and $\varrho_{\kappa_c} \in \mathcal{P}(\mathbb{T}_L^d)$, then there exists $\varrho^* \in \mathcal{P}(\mathbb{T}_L^d)$ distinct from ϱ_∞ and ϱ_{κ_c} such that $|\partial \mathcal{F}_{\kappa_c}|(\varrho^*) = 0$.

Moreover: $\mathcal{F}_{\kappa_c}(\varrho^*) = c$ with $c = \inf_{\gamma \in \Gamma} \max_{t \in [0,Ts]} \mathcal{F}(\gamma(t))$,

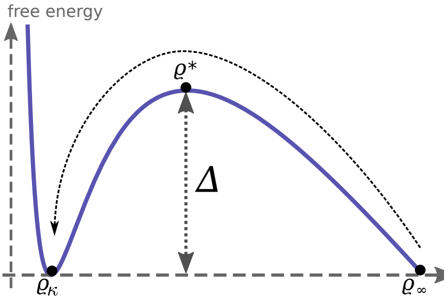
where $\Gamma = \{C([0,T];\mathcal{P}(\mathbb{T}_L^d)) : \gamma(0) = \varrho_\infty, \gamma(T) = \varrho_{\kappa_c}\}$.

Corollary (Arrhenius law)

The empirical McKean-Vlasov process $\varrho^{(N)}$ satisfies

$$\mathbb{P}\left[\varrho^N(T) \in \overline{B}_\varepsilon^{W_2}(\varrho_{\kappa_c}), \varrho^{(N)}(0) = \varrho_0^{(N)}\right] \lesssim e^{-N\Delta}$$

for N sufficiently large with $\mathbb{E}(W_2(\varrho_0^{(N)}, \varrho_\infty)) \to 0$ and $\Delta := \mathcal{F}_{\kappa_c}(\varrho^*) - \mathcal{F}_{\kappa_c}(\varrho_\infty)$ with ϱ^* the mountain pass point.



A structure preserving disretization of the McKean-Vlasov model

[S-Seis arXiv: 2004.13981]

Motivation: Structure preserving discretization

Goal: Consistent discretization of

$$\partial_t \rho = \nabla \cdot (\sigma \nabla \rho + \rho \nabla W * \rho)$$

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Desired properties:

⇒ mass and positivity preserving

⇒ Free energy

$$\mathcal{F}(\rho) = \sigma \int \rho \log \rho + \frac{1}{2} \iint W(x-y)\rho(x)\rho(y)$$

dissipation principle

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(\rho) = -\int_\Omega \rho |\nabla(\sigma \log \rho + W * \rho)|^2 \, \mathrm{d}x = -\mathcal{D}(\rho)$$

⇒ consistent stationary states

$$D\mathcal{F}(\rho^*) = 0 \qquad \text{and} \qquad \mathcal{D}(\rho^*) = 0.$$

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$$\partial_t \rho = \nabla \cdot (\sigma \nabla \rho + \rho \nabla W * \rho)$$

Finite volume SG-scheme:

$$|K| \frac{\rho_K^{n+1} - \rho_K^n}{\delta t} + \sum_{L \sim K} \frac{|K|L|}{d_{KL}} f_{KL}^{n+1} = 0$$

with normal flux f_{KL}^{n+1}

$$f_{KL}^{n+1} = q_{KL}^{n+1} \frac{\rho_K^{n+1} e^{\frac{q_{KL}^{n+1}}{2\sigma}} - \rho_L^{n+1} e^{-\frac{q_{KL}^{n+1}}{2\sigma}}}{e^{\frac{q_{KL}^{n+1}}{2\sigma}} - e^{-\frac{q_{KL}^{n+1}}{2\sigma}}}$$

and discrete potential gradient

$$q_{KL}^{n+1} = \sum_{J \in \mathcal{T}} |J| \frac{\rho_J^{n+1} + \rho_J^n}{2} (W(x_K - x_J) - W(x_L - x_J)).$$

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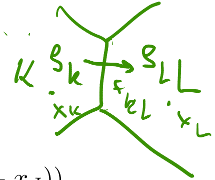
Cell problem: The normal flux solves

$$f_{KL} = -\sigma \partial_x \rho(\cdot) + q_{KL} \rho(\cdot) \quad \text{on } (0,1),$$
$$\rho(0) = \rho_K \quad \text{and} \quad \rho(1) = \rho_L.$$

- f_{KL} and $\rho : [0,1] \to \mathbb{R}$ are unknown
- first-order boundary value problem

Connection to Upwind:

$$f_{KL} \overset{\sigma \to 0}{\to} \rho_K (q_{KL})_+ + \rho_L (q_{KL})_-$$



Results

Theorem [S.-Seis arXiv:2004.13981]

Given Voronoi tesselation $\mathcal{T}^h$ with $\sup_K \operatorname{diam} K \leq h$ and $h|\partial K| \leq C_{\text{iso}}|K|$ for all $K \in \mathcal{T}^h$.

Then $\exists!\{\rho^n\}_{n\in N}$ solution of SG-scheme.

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$\Rightarrow$ Free energy dissipation principle

$$\frac{\mathcal{F}^h(\rho^{n+1}) - \mathcal{F}^h(\rho^n)}{\delta t} + \sigma \frac{\mathcal{H}(\rho^n \mid \rho^{n+1})}{\delta t} = -\mathcal{D}^h(\rho^{n+1}).$$

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$\Rightarrow$ Longtime behavior of scheme to stationary states

$\Rightarrow$ convergence of scheme as $\delta t, h \to 0$.

Discrete scheme has a formal generalized gradient structure (upto implicit time discretization)

$$\mathcal{F}^h(\rho) = \sigma\mathcal{S}^h(\rho) + \mathcal{E}^h(\rho),$$

$$\mathcal{S}^h(\rho) = \sum_K |K|\rho_K \log \rho_K$$

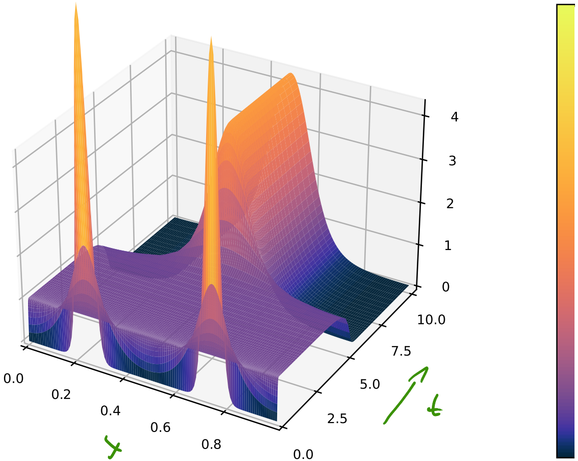
$$\mathcal{E}^h(\rho) = \frac{1}{2}\sum_{K,L}|K||L|W(x_K - x_L)\rho_K\rho_L$$

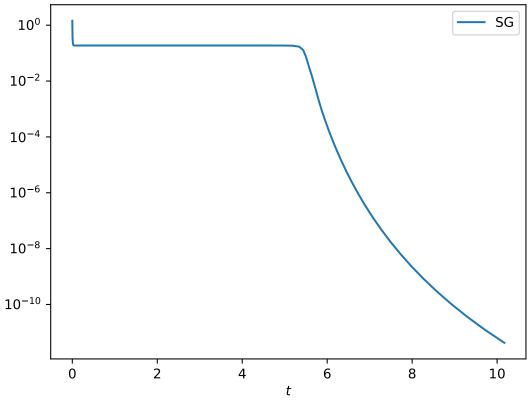
$$\mathcal{H}(\rho \mid \tilde\rho) = \sum_K |K|\rho_K \log\frac{\rho_K}{\tilde\rho_K}$$

Need: for stability/convergence

$\delta t, h \lesssim \frac{\sigma}{\mathrm{Lip} W}$

Numerics: Metastability and free energy decay





Scheme resolves near-metastable states at high accuracy

⇒ implement a string method [E, Ren, Vanden-Eijnden '02 & '07]

String method for McKean-Vlasov gradient flow

Algorithm to approximate saddle point following [E-Ren-Vanden-Eijnden '02 & '07]:

Scharfetter-Gummel gradient flow structure

The SG-scheme defines a potential difference q_{KL} to flux relation f_{KL}

$$f_{KL}(\rho_K, \rho_L; q_{KL}) = q_{KL} \frac{\rho_K e^{\frac{q_{KL}}{2\sigma}} - \rho_L e^{-\frac{q_{KL}}{2\sigma}}}{e^{\frac{q_{KL}}{2\sigma}} - e^{-\frac{q_{KL}}{2\sigma}}}.$$

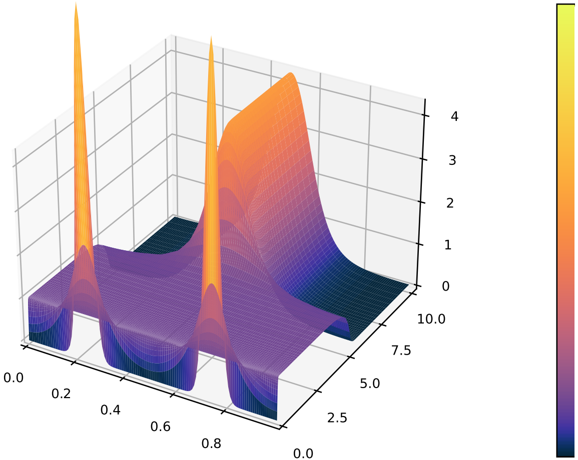
Turn into a free-energy difference to flux relation by setting

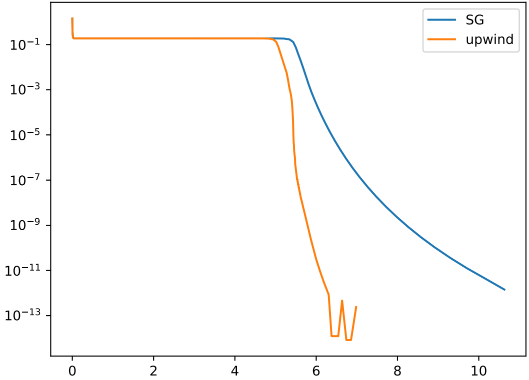
$$x = \xi_L - \xi_K = \sigma \log \frac{\rho_K}{\rho_L} + q_{KL}$$

to arrive at

$$D_\xi \mathcal{R}^*(\rho, \xi)|_{KL} = f_{KL}\left(\rho_K, \rho_L; x - \sigma \log \frac{\rho_K}{\rho_L}\right) = 2\sigma \sinh\left(\frac{x}{2\sigma}\right) \frac{\log \frac{e^{\frac{x}{2\sigma}}}{\rho_K} - \log \frac{e^{-\frac{x}{2\sigma}}}{\rho_L}}{\frac{e^{\frac{x}{2\sigma}}}{\rho_K} - \frac{e^{-\frac{x}{2\sigma}}}{\rho_L}}.$$

Numerics: Metastability and free energy decay





Upwind-scheme from [Bailo, Carrillo, Hu arXiv:1811.11502]

Converges earlier in physical time at higher computational cost.

Nonlocal interaction equations on graphs

Motivation: Graph approximation of data sets

Ingredients:

- n points $\{x_i\}_{i=1}^n$ sampled from $\mu \in \mathcal{M}(\mathbb{R}^d) \Rightarrow$ empirical measure $\mu^n = \frac{1}{n}\sum_{i=1}^n \delta_{x_i}$

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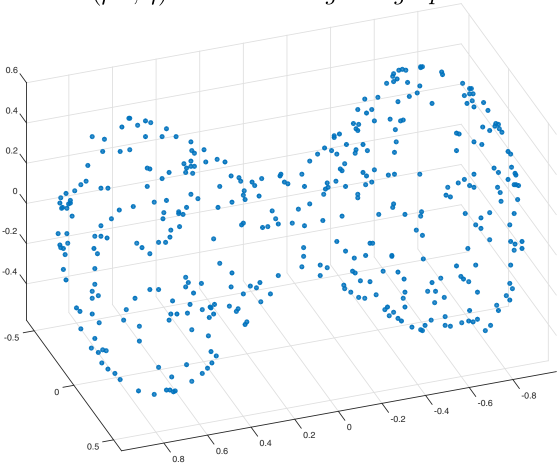
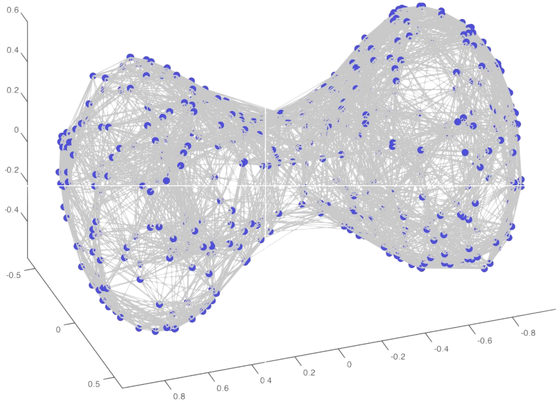
- n points $\{x_i\}_{i=1}^n$ sampled from $\mu \in \mathcal{M}(\mathbb{R}^d) \Rightarrow$ empirical measure $\mu^n = \frac{1}{n}\sum_{i=1}^n \delta_{x_i}$
- a symmetric *weight function* $\eta : G \to [0,\infty)$ with $G = \{(x,y) \in \mathbb{R}^d \times \mathbb{R}^d : x \neq y, \eta(x,y) > 0\}$

  $\Rightarrow (\mu^n, \eta)$ defines a *weighted graph*





Goal: Evolution equations on graphs

For $\rho \in \mathcal{P}(\mathbb{R}^d)$ and symmetric $W \in C(\mathbb{R}^d \times \mathbb{R}^d)$ define the *interaction energy*

$$\mathcal{E}(\rho) = \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} W(x, y) \, \mathrm{d}\rho(x) \, \mathrm{d}\rho(y)$$

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- Dynamic is stable under graph limit $n \to \infty$ such that $\mu^n \rightharpoonup \mu$
  (μ^n, η) becomes a continuous graph/graphon (μ, η)
- Dynamic is stable for local limit: Let $\mu = \mathrm{Leb}(\mathbb{R}^d)$ and $\eta^\delta(x,y) = \delta^{-(d+2)} \eta\left(\frac{x-y}{\delta}\right)$
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(IE) is Wasserstein gradient flow for $\mathcal{E}$ [Carrillo-DiFrancesco-Figalli-Laurent-Slepčev]

Strategy: Find suitable nonlocal metric $\mathcal{T}$ on (μ, η)

$\Rightarrow$ Construct gradient flow of $\mathcal{E}$ wrt $\mathcal{T}$ as *nonlocal interaction equation* (μ, η)

Inspiration: The numerical upwind scheme

What is the nonlocal analog of the continuity equation on $\mathbb{R}^d$:

$$\partial_t \rho_t + \nabla \cdot \boldsymbol{j}_t = 0 \qquad \text{with flux} \qquad j_t(x) = \rho_t(x)\boldsymbol{v}_t(x) \text{ ?}$$

Fluxes j_t are defined on edges $(x, y) \in G = \{\eta > 0\}$ and the divergence is nonlocal

$$\partial_t \rho_t(x) + (\overline{\nabla} \cdot \boldsymbol{j}_t)(x) = \partial_t \rho_t(x) + \int_{\mathbb{R}^d} \eta(x, y)\, \boldsymbol{j}_t(x, \mathrm{d}y) = 0 \,. \tag{div}$$

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Upwind flux: Set $(a)_+ = \max\{0, a\}$ and $(a)_- = \max\{0, -a\}$ and define

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Good properties: known from numerics

- positivity preserving
- stability, monotonicity
- energy decreasing

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Ingredients for abstract setup:

$$\overline{K}_\rho[v](x) = -\left(\overline{\nabla} \cdot \boldsymbol{J}_{\mathrm{up}}[v]\right)(x) = D_v \overline{\mathcal{R}}(\varrho, v)$$

$$\overline{\mathcal{R}}(\varrho, v) = \frac{1}{2} \iint |v|^2 \Big(\chi_{\{v>0\}}(x, y)\, \mathrm{d}\rho(x)\, \mathrm{d}\mu(y) + \chi_{\{v<0\}}(x, y)\, \mathrm{d}\mu(x)\, \mathrm{d}\rho(y) \Big)$$

Upwind transportation metric

$\Rightarrow$ Nonlocal upwind continuity equation (div)+(flux):

$$\partial_t \rho_t(x) + \int_{\mathbb{R}^d} \eta(x,y)\Big(v_t(x,y)_+ \rho_t(x)\,\mathrm{d}\mu(y) - v_t(x,y)_- \mu(x)\rho_t(y)\Big) = 0\ . \tag{CE}$$

Definition of upwind transportation metric via Benamou-Brenier formulation

$$\mathcal{T}(\rho_0,\rho_1)^2 = \inf_{(\rho,v)\in \mathrm{CE}} \left\{ \int_0^1 \overline{\mathcal{R}}(\rho_t, v_t)\,\mathrm{d}t \right\}.$$

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Driving vector-field $v_t = -\overline{\nabla}\frac{\delta\mathcal{E}}{\delta\rho} = -\overline{\nabla}(W*\rho_t)$ with $\overline{\nabla}V(x,y) = V(y)-V(x)$ leads to

$$\partial_t \rho_t(x) + \int_{\mathbb{R}^d} \eta(x,y)\Big(\overline{\nabla}(W*\rho_t)(x,y)_- \rho_t(x)\,\mathrm{d}\mu(y) - \rho_t(y)\overline{\nabla}(W*\rho_t)(x,y)_+ \mu(x)\,\mathrm{d}\rho(y)\Big) = 0,$$

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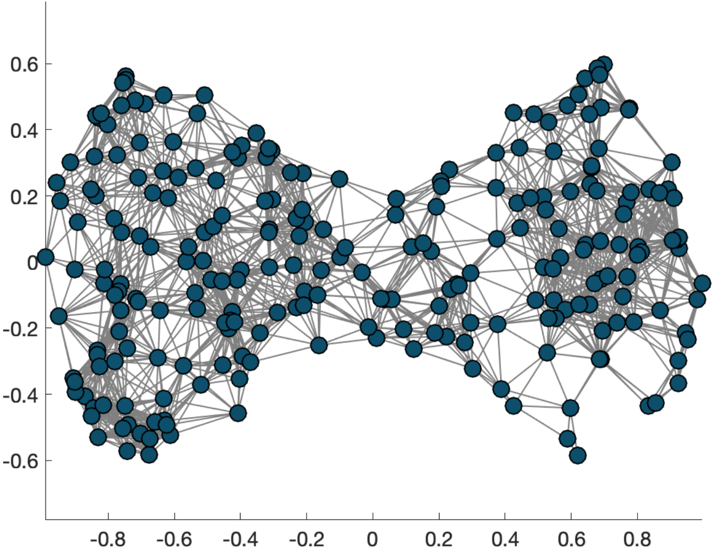
Main results [Esposito-Patacchini-S.-Slepčev '21]

- Properties of nonlocal upwind transportation quasi-metric (non-symmetric)
- Gradient flows in Finsler geometry
- Variational framework for ($\mathrm{NL}^2\mathrm{IE}$)
- Stability of ($\mathrm{NL}^2\mathrm{IE}$) under graph limit $\mu^n \rightharpoonup \mu$

Numerical example: Dumpbell shape

Evolution on random geometric graph based on 240 sample points in 2D:



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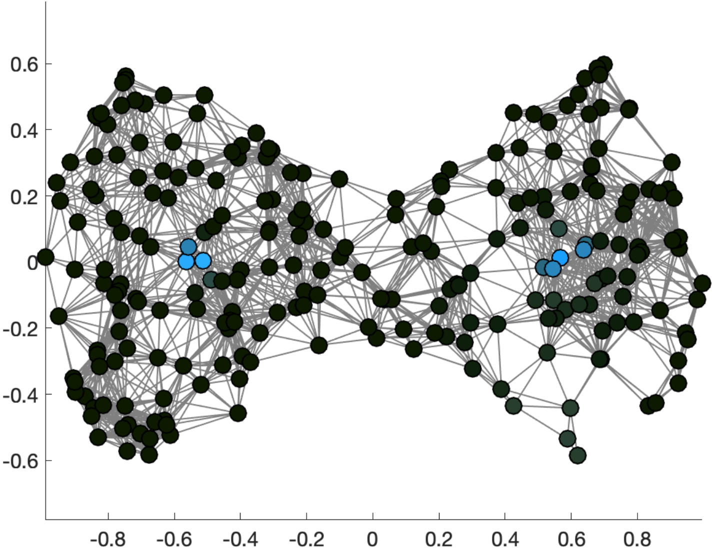

Finslerian geometry and gradient flows

For any $(\rho_t)_{t\in[0,1]} \in \mathrm{AC}\big([0,1];(\mathcal{P}_2(\mathbb{R}^d),\mathcal{T}_\mu)\big)$ exists an antisymmetric $(v_t)_{t\in[0,1]}$ such that $(\rho_t,\boldsymbol{j}_t)_{t\in[0,1]} \in \mathrm{CE}$ and

$$\mathrm{d}\boldsymbol{j}_t(x,y) = v_t(x,y)_+ \,\mathrm{d}\rho(x)\,\mathrm{d}\mu(y) - v_t(x,y)_- \,\mathrm{d}\mu(x)\,\mathrm{d}\rho(y)\ .$$

The geometry induced by $\mathcal{T}$ is Finslerian:
$\Rightarrow$ *inner product in tangent space depends on* ρ *and* $w \in T_\rho\mathcal{P}_2(\mathbb{R}^d)$*!*

Finslerian upwind product

For $\rho \in \mathcal{P}_2(\mathbb{R}^d)$ and $w \in T_\rho\mathcal{P}_2(\mathbb{R}^d)$ define $g_{\rho,w} \colon T_\rho\mathcal{P}_2(\mathbb{R}^d) \times T_\rho\mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}$ by

$$g_{\rho,w}(u,v) = \iint_G u(x,y)v(x,y)\,\eta(x,y)\times$$
$$\times\big(\chi_{\{w>0\}}(x,y)\,\mathrm{d}\rho(x)\,\mathrm{d}\mu(y) + \chi_{\{w<0\}}(x,y)\,\mathrm{d}\mu(x)\,\mathrm{d}\rho(y)\big)\ .$$

$\rightarrow$ define gradient flow for interaction energy $\mathcal{E}$ in terms of curves of maximal slope

See also [Ohta-Sturm ’09, ’12] and [Agueh ’12] for gradient flows in Finslerian setting.

Variational characterization of solutions

The de Giorgi functional gives a variation characterization of solutions to

$$\partial_t \rho_t = K_{\rho_t}(-\overline{\nabla} W * \rho_t) \qquad \text{in } C_c^\infty([0,T]\times\mathbb{R}^d)^* \ , \tag{NLIE}$$

Theorem (Curves of maximal slope characterization)

For $(\rho_t)_{t\in[0,T]} \in \mathrm{AC}([0,T];(\mathcal{P}_2(\mathbb{R}^d),\mathcal{T}_\mu))$ take $(\rho_t, \boldsymbol{j}_t)_{t\in[0,T]} \in \mathrm{CE}$ with

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and define

$$\mathcal{J}_T(\rho) = \mathcal{E}(\rho_T) - \mathcal{E}(\rho_0) + \int_0^T \left(\overline{\mathcal{R}}(\rho_t, v_t) + \overline{\mathcal{R}}(\rho_t, -\overline{\nabla} W * \rho_t)\right) \mathrm{d}t.$$

Then $\mathcal{J}_T(\rho) \geq 0$ and $\mathcal{J}_T(\rho) = 0$ iff $(\rho_t)_{t\in[0,T]}$ is a weak solution to (NLIE).

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- Minimizers exist by direct method, however not necessarily global!
- Possibility: Redo the minimizing movement scheme in the quasimetric setting
- Instead: Show existence via finite dimensional approximation and stability

Stability with respect to graph approximations

Let $\mu^n \in \mathcal{M}_+(\mathbb{R}^d)$ be such that $\mu^n \rightharpoonup \mu$ and define

$$\mathcal{J}_T(\mu^n;\rho^n) = \mathcal{E}(\rho_T^n) - \mathcal{E}(\rho_0^n) + \int_0^T \Big(\overline{\mathcal{R}}(\mu^n;\rho_t^n, v_t^n) + \overline{\mathcal{R}}(\mu^n;\rho_t^n, -\overline{\nabla} W * \rho_t^n)\Big)\,\mathrm{d}t\ .$$

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Stability of gradient flows à la Sandier-Serfaty

Let $\rho^n \in \mathrm{AC}([0,T];(\mathcal{P}_2(\mathbb{R}^d),\mathcal{T}_{\mu^n}))$ such that $\sup_n \mathcal{G}_T(\mu^n;\rho^n) < \infty$.
Then, there exists $\rho \in \mathrm{AC}([0,T];(\mathcal{P}(\mathbb{R}^d),\mathcal{T}_\mu))$ such that

$$\rho^n_t \rightharpoonup \rho_t \qquad \text{in } \mathcal{P}_2(\mathbb{R}^d) \text{ for a.e. } t\in[0,T];$$

$$\boldsymbol{J}_{\mathrm{up}}[v^n] = \boldsymbol{j}^n \rightharpoonup \boldsymbol{j} = \boldsymbol{J}_{\mathrm{up}}[v] \qquad \text{in } \mathcal{M}_{\mathrm{loc}}(G\times[0,T]);$$

$$\liminf_n \int_0^T \overline{\mathcal{R}}(\mu^n;\rho^n_t,v^n_t)\,\mathrm{d}t \geq \int_0^T \overline{\mathcal{R}}(\mu;\rho_t,v_t)\,\mathrm{d}t;$$

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In particular weak solutions of (NLIE) on graph (μ^n,η) converge to ones on (μ,η).

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In particular weak solutions of (NLIE) on graph (μ^n,η) converge to ones on (μ,η).

Corollary: Existence of weak solution to (NLIE) via finite-dimensional approximation.

Finslerian product: two basic properties

$$g_{\rho,w}(u,v) = \iint_G u(x,y)v(x,y)\,\eta(x,y)\times$$
$$\times\left(\chi_{\{w>0\}}(x,y)\,\mathrm{d}\rho(x)\,\mathrm{d}\mu(y) + \chi_{\{w<0\}}(x,y)\,\mathrm{d}\mu(x)\,\mathrm{d}\rho(y)\right).$$

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- **Chain-rule:** For $(\rho_t)_{t\in[0,1]} \in \mathrm{AC}\big([0,1];(\mathcal{P}_2(\mathbb{R}^d),\mathcal{T})\big)$ and $\varphi \in C_c^\infty(\mathbb{R}^d)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int \varphi\,\mathrm{d}\rho_t = \iint \overline{\nabla}\varphi(x,y)\eta(x,y)\,\mathrm{d}\boldsymbol{j}_t(x,y) = g_{\rho_t,w_t}\big(w_t,\overline{\nabla}\varphi\big)\ .$$

Finslerian product: two basic properties

$$g_{\rho,w}(u,v) = \iint_G u(x,y)v(x,y)\,\eta(x,y)\times$$
$$\times\left(\chi_{\{w>0\}}(x,y)\,\mathrm{d}\rho(x)\,\mathrm{d}\mu(y) + \chi_{\{w<0\}}(x,y)\,\mathrm{d}\mu(x)\,\mathrm{d}\rho(y)\right)\,.$$

- **Chain-rule:** For $(\rho_t)_{t\in[0,1]} \in \mathrm{AC}\big([0,1];(\mathcal{P}_2(\mathbb{R}^d),\mathcal{T})\big)$ and $\varphi \in C_c^\infty(\mathbb{R}^d)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int \varphi\,\mathrm{d}\rho_t = \iint \overline{\nabla}\varphi(x,y)\eta(x,y)\,\mathrm{d}\boldsymbol{j}_t(x,y) = g_{\rho_t,w_t}\big(w_t,\overline{\nabla}\varphi\big)\,.$$

- **One-sided Cauchy-Schwarz:** For all $v,w \in T_\rho\mathcal{P}_2(\mathbb{R}^d)$ holds

$$\begin{aligned} g_{\rho,w}(w,v) &= \iint_G v(x,y)\eta(x,y)\big(w(x,y)_+\,\mathrm{d}\rho(x)\,\mathrm{d}\mu(y) - w(x,y)_-\,\mathrm{d}\mu(x)\,\mathrm{d}\rho(y)\big) \\ &\le \iint_G v(x,y)_+ w(x,y)_+ \eta(x,y)\,\mathrm{d}\rho(x)\,\mathrm{d}\mu(y) + \iint_G v(x,y)_- w(x,y)_- \eta(x,y)\,\mathrm{d}\mu(x)\,\mathrm{d}\rho(y) \\ &\le \sqrt{g_{\rho,v}(v,v)\,g_{\rho,w}(w,w)}\,. \end{aligned}$$

Chain rule and curves of maximal slope

Recall: interaction energy $\mathcal{E}$

$$\mathcal{E}(\rho) = \frac{1}{2}\iint W(x,y)\,\mathrm{d}\rho(x)\,\mathrm{d}\rho(y)\ .$$

Assumption: The potential $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ satisfies

(W1) $W \in C(\mathbb{R}^d \times \mathbb{R}^d)$;

(W2) W is symmetric, i.e. $W(x,y) = W(y,x)$, for all $(x,y) \in \mathbb{R}^d \times \mathbb{R}^d$;

(W3) for some $L \geq 1$ and for all $x, y, z \in \mathbb{R}^d$

$$|W(x,z) - W(y,z)| \leq L\left(|x-y| \vee |x-y|^2\right)$$

local Lipschitz with at most quadratic growth

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Chain rule

Let $\rho \in \mathrm{AC}([0,T];(\mathcal{P}_2(\mathbb{R}^d),\mathcal{T}))$, then $\forall\; 0 \leq s \leq t \leq T$

$$\mathcal{E}(\rho_t) - \mathcal{E}(\rho_s) = \int_s^t \iint_G \overline{\nabla}\frac{\delta\mathcal{E}}{\delta\rho}(x,y)\eta(x,y)\,\mathrm{d}\boldsymbol{j}_\tau(x,y)\,\mathrm{d}\tau = \int_s^t g_{\rho_\tau,w_\tau}\left(w_\tau, \overline{\nabla}\frac{\delta\mathcal{E}}{\delta\rho}\right)\mathrm{d}\tau$$

Chain rule and curves of maximal slope

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Curves of maximal slope: For any $\rho \in \mathrm{AC}([0,T];(\mathcal{P}_2(\mathbb{R}^d),\mathcal{T}))$ holds

$$\mathcal{E}(\rho_T) - \mathcal{E}(\rho_0) \ge -\frac{1}{2}\int_0^T g_{\rho_t,-\overline{\nabla}\frac{\delta\mathcal{E}(\rho_t)}{\delta\rho}}\left(-\overline{\nabla}\frac{\delta \mathcal{E}}{\delta \rho}, -\overline{\nabla}\frac{\delta \mathcal{E}}{\delta \rho}\right)\mathrm{d}t - \frac{1}{2}\int_0^T g_{\rho_t,w_t}(w_t,w_t)\,\mathrm{d}t\ .$$

with equality iff $w_t = -\overline{\nabla}\frac{\delta\mathcal{E}(\rho_t)}{\delta\rho} = -\overline{\nabla}W * \rho_t$

$\Rightarrow$ Define the nonnegative de Giorgi functional by

$$\mathcal{G}_T(\rho) = \mathcal{E}(\rho_T) - \mathcal{E}(\rho_0) + \frac{1}{2}\int_0^T \mathcal{D}(\rho_t)\,\mathrm{d}t + \frac{1}{2}\int_0^T \mathcal{A}(\rho_t,w_t)\,\mathrm{d}t \ge 0\ ,$$

where

$$\mathcal{D}(\rho_t) = 2\int_G \left|\overline{\nabla}\frac{\delta\mathcal{E}(\rho_t)}{\delta\rho}(x,y)_-\right|^2 \eta(x,y)\,\mathrm{d}\rho(x)\,\mathrm{d}\mu(y)\ .$$