Nonlocal equations on discrete state space

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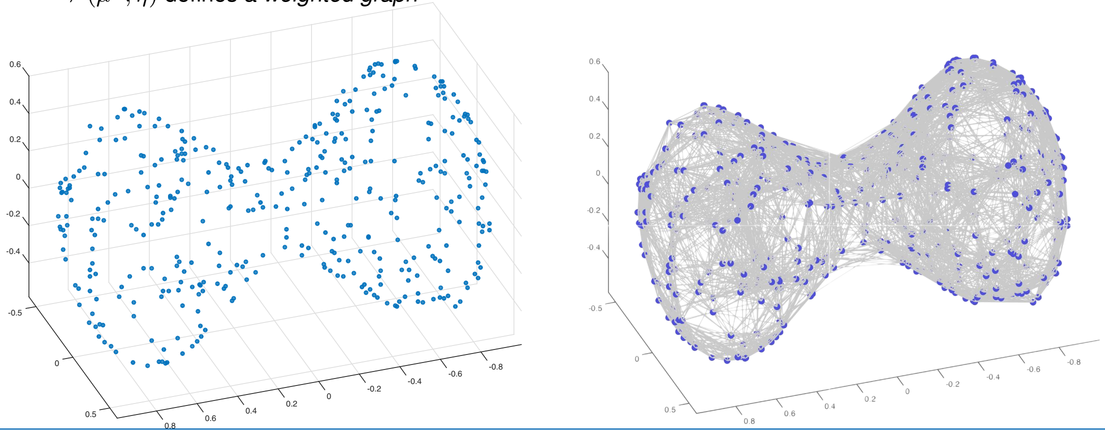
Variational modelling:
Nonlocal interaction equations on graphs

[Esposito-Patacchini-S.-Slepčev arXiv:1912.09834]

Ingredients:

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

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

Goal: *Define energy decreasing dynamic on weighted graph* (μ, η).

Subgoals:

- 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 $\eta^\delta(x,y) = \delta^{-(d+2)}\eta\big(\frac{x-y}{\delta}\big)$
  Then, the limit $\delta \to 0$ shall be the interaction/aggregation equation

$$\partial_t \rho_t = \nabla \cdot (\rho_t \nabla W * \rho_t) \qquad \text{(IE)}$$

(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)

Literature on discrete/non-local gradient flows

Recent advances in discrete/nonlocal gradient flows

- [Maas '11] / [Mielke '11] / [Chow, Huang, Li, Zhou '12] Markov chains and chemical reaction networks
- [Gigli, Maas '13; Gladbach, Kopfer, Maas, Portinale '18+] Homogenization of discrete OT
- [Erbar '14] Jump processes $-(-\Delta)^{\alpha/2}$ for $\alpha \in (0,2)$.
- [Disser, Liero '14] Passage from Markov chains to Fokker-Planck
- [Erbar, Fathi, Laschos, S. '16] Mean-field nonlinear Markov chains on graphs
- [Trillos '19] Gromov-Hausdorff convergence of random point clouds
- [Peletier, Rossi, Savaré, Tse '20+] Generalized nonlocal gradient flows

Above works are built around gradient flows for free energies/(relative) entropies:

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

Goal: Want to consider $\sigma = 0$.

Problem: The above introduced nonlocal metrics seem to not have a clear and well-defined limit for $\sigma \to 0$

Question: What is a suitable metric for gradient structure of interaction energies?

Inspiration: The numerical upwind scheme

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

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

Fluxes j_t are defined on edges $(x, y) \in G$ and the divergence is nonlocal

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

Given a nonlocal vectorfield $v_t : G \to \mathbb{R}$: *velocity of a particle going from x to y*.

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

$$j_t(x, y) = \rho(x) v_t(x, y)_+ - \rho(y) v_t(x, y)_- \ . \tag{flux}$$

Good properties: known from numerics

- positivity preserving
- stability
- entropy/energy decreasing

[Chen, Georgiou, Tannenbaum '18] use upwinding implicitly

Upwind continuity equation and upwind transportation metric

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

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

Definition of upwind transportation metric via Benamou-Brenier formulation

$$\mathcal{T}(\rho_0,\rho_1)^2 = \inf_{(\rho,v)\in \mathrm{CE}} \left\{ \int_0^1 \iint_G |v_t(x,y)_+|^2 \rho_t(x)\eta(x,y)\,\mathrm{d}\mu(x)\,\mathrm{d}\mu(y)\,\mathrm{d}t \right\}$$

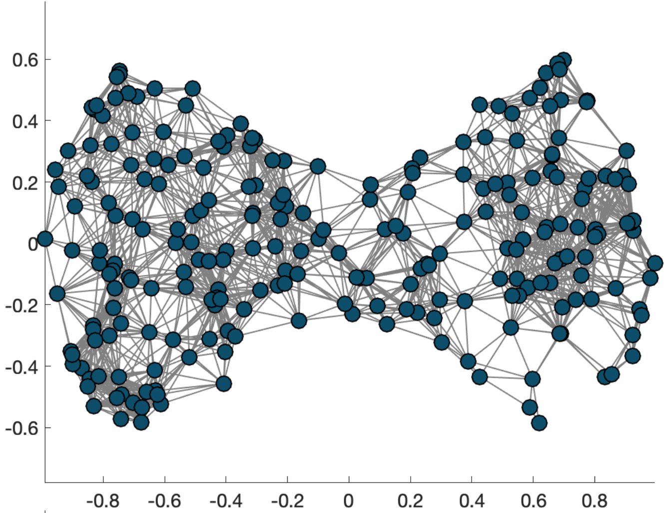
Nonlocal Otto calculus leads to the nonlocal^2 interaction equation (NL^{2}IE):

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

Main results [Esposito-Patacchini-S.-Slepčev ’20]

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

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



By previous representation: Associate to $(\rho_t)_{t\in[0,1]} \in \mathrm{AC}\big([0,1];(\mathcal{P}_2(\Omega),\mathcal{T})\big)$ an antisymmetric $(w_t)_{t\in[0,1]}$ such that $(\rho_t, \boldsymbol{j}_t)_{t\in[0,1]} \in \mathrm{CE}$ and

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

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

Finslerian upwind product

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

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

$\to$ 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.

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 $(\rho_t)_{t\in[0,1]} \in \mathrm{AC}\big([0,1];(\mathcal{P}_2(\Omega),\mathcal{T})\big)$ and $\varphi \in C_c^\infty(\Omega)$

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

- **One-sided Cauchy-Schwarz:** For all $v,w \in T_\rho\mathcal{P}_2(\Omega)$ 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 $\mathcal{E}$

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

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

(W1) $W \in C(\Omega \times \Omega)$;

(W2) W is symmetric, i.e. $W(x,y) = W(y,x)$, for all $(x,y) \in \Omega \times \Omega$;

(W3) for some $L \geq 1$ and for all $x, y, z \in \Omega$

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

local Lipschitz with at most quadratic growth

Chain rule

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

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

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

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

Variational characterization of solutions

The de Giorgi functional gives a variation characterization of solutions to

$$\partial_t \rho + \overline{\nabla} \cdot \boldsymbol{j} = 0 \qquad \text{in } C_c^\infty([0,T] \times \Omega)^* \,, \tag{NLIE}$$

where the flux $\boldsymbol{j}$ is given by

$$\mathrm{d}\boldsymbol{j}(x,y) = \overline{\nabla}(W * \rho)(x,y)_- \eta(x,y)\, \mathrm{d}\rho(x)\, \mathrm{d}\mu(y) - \overline{\nabla}(W * \rho)(x,y)_+ \eta(x,y)\, \mathrm{d}\rho(y)\, \mathrm{d}\mu(x) \,.$$

Theorem (Curves of maximal slope characterization)

Let $(\rho_t)_{t\in[0,T]} \in \mathrm{AC}([0,T];(\mathcal{P}_2(\Omega),\mathcal{T}))$ be such that $\int_0^T \mathcal{D}(\rho_t, w_t)\,\mathrm{d}t < \infty$, then

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

- 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
- Alternatively: Existence of (strong) solutions via classical fix-point argument

Stability with respect to graph approximations

Let $\mu^n \in \mathcal{M}(\Omega)$ be such that $\mu^n \rightharpoonup \mu$ and define

$$\mathcal{G}_T(\mu^n;\rho^n) = \mathcal{E}(\rho_T^n) - \mathcal{E}(\rho_0^n) + \frac{1}{2}\int_0^T \mathcal{A}(\mu^n;\rho_t^n,\boldsymbol{j}_t^n)\,\mathrm{d}t + \frac{1}{2}\int_0^T \mathcal{D}(\mu^n;\rho_t^n)\,\mathrm{d}t\,.$$

Stability of gradient flows à la Sandier-Serfaty

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

$$\rho_t^n \rightharpoonup \rho_t \quad \text{in } \mathcal{P}_2(\Omega) \text{ for a.e. } t \in [0,T]$$

$$\boldsymbol{j}^n \rightharpoonup \boldsymbol{j} \quad \text{in } \mathcal{M}_{\mathrm{loc}}(G\times[0,T])$$

$$\liminf_n \int_0^T \mathcal{A}(\mu^n;\rho_t^n,\boldsymbol{j}_t^n)\,\mathrm{d}t \ge \int_0^T \mathcal{A}(\mu;\rho_t,\boldsymbol{j}_t)\,\mathrm{d}t$$

$$\liminf_n \int_0^T \mathcal{D}(\mu^n;\rho_t^n)\,\mathrm{d}t \ge \int_0^T \mathcal{D}(\mu;\rho_t)\,\mathrm{d}t\,.$$

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.

Open questions

- local limit $\delta \to 0$ to obtain interaction equation (IE)
- diagonal limits: $N \to \infty$ and $\delta \to 0$ to obtain even different PDEs
- Dynamic phenomena: waiting phenomena, stationary states, coarsening, metastability, coarsening
- Homogenization of upwind optimal transport
- Back to free energies including entropies

$$\mathcal{F}^\kappa(\rho) = \kappa \int \log \rho(x) \, \mathrm{d}\rho(x) + \frac{1}{2} \iint W(x,y) \, \mathrm{d}\rho(x) \, \mathrm{d}\rho(y)$$

For $\kappa > 0$ expect a Scharfetter-Gummel gradient structure with flux

$$j^\kappa(x,y) = v(x,y) \frac{\rho(x) e^{\frac{v(x,y)}{2\kappa}} - \rho(y) e^{-\frac{v(x,y)}{2\kappa}}}{e^{\frac{v(x,y)}{2\kappa}} - e^{-\frac{v(x,y)}{2\kappa}}} \overset{\kappa \to 0}{\to} \rho(x) v(x,y)_+ - \rho(y) v(x,y)_- \; .$$

- [S.-Seis arXiv: 2004.13981] Scharfetter-Gummel scheme for diffusion-aggregation equation:
  - free energy decreasing
  - consistent thermodynamic equilibrium (longtime behavior of the scheme)
  - convergence to local (IE)

Scharfetter-Gummel scheme for diffusion-aggregation equation

[S.-Seis arXiv: 2004.13981]

Motivation: Structure preserving discretization

Goal: Consistent discretization of

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

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}

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

and discrete potential gradient

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

Desired properties:

$\Rightarrow$ mass and positivity preserving

$\Rightarrow$ Free energy

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

dissipation principle

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

$\Rightarrow$ thermodynamic consistent stationary states

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

$\Rightarrow$ Fixed point property

$$\rho^* = T(\rho^*) = \frac{e^{-\kappa^{-1} W * \rho^*(x)}}{\int e^{-\kappa^{-1} W * \rho^*(y)} \,\mathrm{d}y}.$$

Cell problem: The normal flux solves

Results

Theorem [S.-Seis '20]

Given a Voronoi tesselation $\mathcal{T}^h$ with $\sup_K \operatorname{diam} K \leq h$.

$$\frac{|\partial K|}{|K|} \leq \frac{C_{\text{iso}}}{h} \qquad \text{and} \qquad \delta t \leq \frac{h}{6 C_{\text{iso}} \operatorname{Lip} W}.$$

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

$\Rightarrow$ Free energy dissipation principle

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

$\Rightarrow$ Characterization of stationary states of scheme as:

- critical point of $\mathcal{F}^h$
- vanishing dissipation $\mathcal{D}^h = 0$
- fixed point of T^h

$\Rightarrow$ Longtime behavior of scheme to stationary states

$\Rightarrow$ convergence of scheme as $h \to 0$ to agg-diff.

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

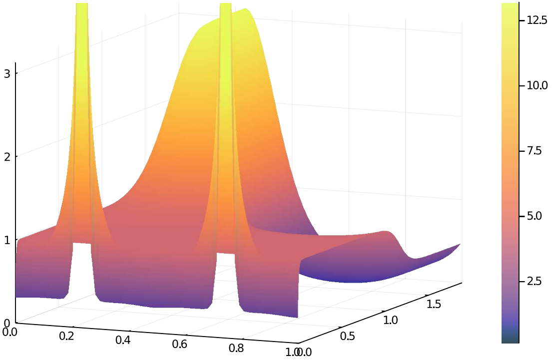
$$\mathcal{S}^h(\rho) = \sum_K |K| \rho_K \log \rho_K$$

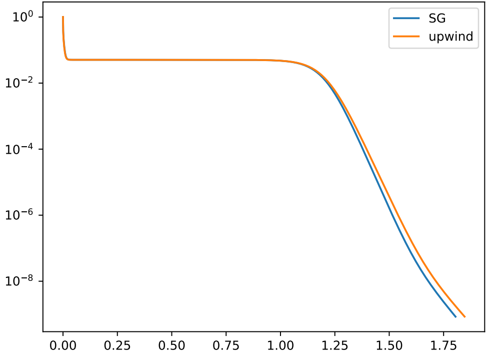
$$\mathcal{E}^h(\rho) = \frac{1}{2} \sum_{K,L} |K||L| W(x_K - x_L) \rho_K \rho_L$$

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

$$T^h(\rho)_K = \frac{\exp\left(-\kappa^{-1} \sum_J |J| \rho_J W(x_K - x_J)\right)}{Z^h(\rho)},$$

Numerical examples: Time evolution and free energy decay





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

Question: Scharfetter-Gummel gradent flow structure?

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

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

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

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

to arrive at

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

Questions:

- Convergence in variational structure? $\rightarrow$ talk by A. Hraivoronska joint with O. Tse
- Contractivity of scheme based on variational structure?