Structure Preserving Discretizations of Wasserstein Gradient Flows Part III of IV: Lagrangian scheme

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“A school on gradient flows”
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Where do we need to go today?

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Can one preserve displacement convexity by discretizing mass motion (instead of the flux)?

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Answer: Depends . . . on the space dimension!

Why a Lagrangian scheme?

'Cause mass transport is actually about transporting mass!

Continuity equation

Recall from PDE class: the solution $(\rho_t)_{t\geq 0}$ to the continuity equation

$$\partial_t \rho + \operatorname{div}(\rho\, \boldsymbol{v}_t) = 0 \tag{CE}$$

is given by $\rho_t = X_t \# \bar{\rho}$, where $X_{(\cdot)} : \mathbb{R}_{\geq 0} \times \mathbb{R}^d \to \mathbb{R}^d$ is $\boldsymbol{v}$'s flow map,

$$\partial_t X_t(x) = \boldsymbol{v}_t\big(X_t(x)\big), \quad \text{subject to} \quad X_0 \# \bar{\rho} = \rho_0.$$

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The $\mathbb{W}$-gradient flow of $\boldsymbol{E}$ has the form (CE) with

$$\boldsymbol{v}_t(x) = -\nabla_x \left(\frac{\delta \boldsymbol{E}}{\delta \rho}\bigg|_{\rho_t} \right).$$

This induces a Lagrangian picture.

Some magic happens

Idea: re-formulate $\mathbb{W}$-gradient flow consistently for flow map, i.e.,

$$\partial_t X = -\nabla_x \left(\frac{\delta \boldsymbol{E}}{\delta \rho} \bigg|_{\rho = X_t \# \bar{\rho}} \right). \qquad \text{(Lag)}$$

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$$\partial_t X = -\nabla_x \left(\frac{\delta \boldsymbol{E}}{\delta \rho} \bigg|_{\rho = X_t \# \bar{\rho}} \right). \tag{Lag}$$

(Lag) is again a gradient flow, namely

- on the manifold of diffeomorphisms $X : \mathbb{R}^d \to \mathbb{R}^d$,
- with the weighted $L^2_{\bar{\rho}}$-norm as metric tensor,

$$\|V\|^2 = \int_{\mathbb{R}^d} \big\|V(\xi)\big\|^2 \bar{\rho}(\xi)\,\mathrm{d}\xi,$$

- for the energy

$$\boldsymbol{E}_{\#}(X) := \boldsymbol{E}(X \# \bar{\rho}).$$

A simple example

Example: For the potential energy

$$\boldsymbol{E}(\rho) = \int V\rho \,\mathrm{d}x \quad \rightsquigarrow \quad \boldsymbol{E}_{\#}(X) = \int V \circ X \,\bar{\rho}\,\mathrm{d}x.$$

And indeed, $\rho_t = X_t \# \bar{\rho}$ connects the gradient flows

$$\partial_t \rho = \mathrm{div}(\rho \nabla V) \quad \rightsquigarrow \quad \partial_t X = -\nabla V \circ X.$$

A more sophisticated example

Recall: the $\mathbb{W}$-gradient flow of the internal energy

$$\boldsymbol{E}(\rho) = \int h(\rho)\,\mathrm{d}x$$

is the nonlinear diffusion equation

$$\partial_t \rho = \Delta P(\rho) \quad \text{with} \quad P(\rho) = \rho h'(\rho) - h(\rho).$$

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Theorem ([Evans+Gango+Savin'05])

The flow map $(X_t)_{t\geq 0}$ obtained from a solution to $\partial_t \rho = \Delta P(\rho)$ is a solution to the $L^2_{\bar\rho}$-gradient flow of

$$\boldsymbol{E}_\#(X) = \int h_\#\left(\frac{\det \mathrm{D}_\xi X}{\bar\rho}\right)\bar\rho(\xi)\,\mathrm{d}\xi, \quad h_\#(s) := sh(1/s).$$

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Numerical implementation [Carrillo&Ranetbauer&Wolfram'16]

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Numerical implementation [Carrillo&Ranetbauer&Wolfram'16]

Afterwards: many, many attempts to make the Lagrangian picture usable.

Going back to one dimension? Really?

1D-OT is a much simpler thing.

Optimal transport in 1D (1/3)

For sufficiently regular $\rho_0, \rho_1 \in \mathcal{P}_2(\mathbb{R}^d)$:

$$\mathbb{W}(\rho_0, \rho_1)^2 = \int \left\{ \int |T(x) - x|^2 \rho_0(x) \, \mathrm{d}x \,\middle|\, T \# \rho_0 = \rho_1 \right\},$$

and there is an essentially unique optimal T,
and that T is (even cyclically) monotone.

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In $d = 1$, the monotone function $T : \mathbb{R} \to \mathbb{R}$ is implicitly given by

$$\int_{-\infty}^{\xi} \rho_0(x)\,\mathrm{d}x = \int_{-\infty}^{T(\xi)} \rho_1(x)\,\mathrm{d}x \quad \forall \xi \in \mathbb{R}.$$

Optimal transport in 1D (2/3)

Definition

Define ρ's (cummulative) distribution function $F_\rho : \mathbb{R} \to [0,1]$ by

$$F_\rho(x) = \int_{(-\infty,x]} \rho(x')\,\mathrm{d}x'$$

and its inverse distribution function $X_\rho : (0,1) \to [-\infty,\infty]$ by

$$X_\rho(\xi) = \inf\left\{x \in \mathbb{R} \,|\, F_\rho(x) > \xi\right\}.$$

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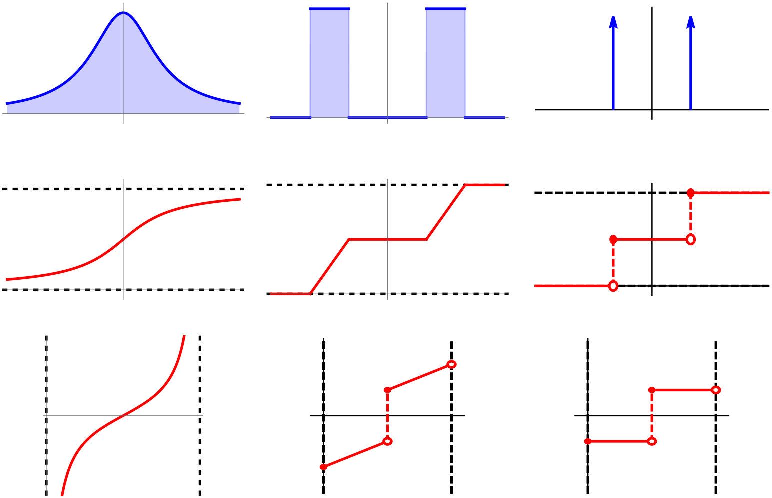
Remarks:

- $F_\rho \in D_\geq(\mathbb{R})$ und $X_\rho \in D_\geq((0,1))$ are increasing càdlàg functions.
- If $x \in \operatorname{supp}\rho$, then $X_\rho \circ F_\rho(x) = x$.
- A useful rule for change of variables:

$$\int_{\mathbb{R}} f(x)\rho(x)\,\mathrm{d}x = \int_0^1 f\big(X_\rho(\xi)\big)\,\mathrm{d}\xi.$$

- $T := X_{\rho_1} \circ F_{\rho_0}$ is a monotone map $T : \mathbb{R} \to \mathbb{R}$ with $T\#\rho_0 = \rho_1$, i.e., T is the optimal transport map from ρ_0 to ρ_1.

Optimal transport in 1D (3/3)



The magical isometry (1/3)

Theorem

For all $\rho_0, \rho_1 \in \mathcal{P}_2(\mathbb{R})$,

$$\mathbb{W}(\rho_0, \rho_1) = \left\| X_1 - X_0 \right\|_{L^2([0,1])}.$$

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Proof: with $x = X_0(\xi)$,

$$\mathbb{W}(\rho_0, \rho_1)^2 = \int_{\mathbb{R}} \big| X_1 \circ F_0(x) - x \big|^2 \rho_0(x)\,\mathrm{d}x = \int_0^1 \big| X_1(\xi) - X_0(\xi) \big|^2 \,\mathrm{d}\xi.$$

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Corollary

The Wasserstein space over $\mathbb{R}$ *is flat.*

Warning: This is not true in any dimension $d \geq 2$.

The magical isometry (2/3)

Corollary

$\boldsymbol{E}$ *is* *λ-displacement convex* *on* $\mathcal{P}_2(\mathbb{R})$ *iff*

$$\boldsymbol{E}_\# : D_\geq((0,1)) \to [0,+\infty] \quad \textit{with} \quad \boldsymbol{E}_\#(X_\rho) := \boldsymbol{E}(\rho)$$

is *λ-uniformly convex.*

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Examples:

- potential energy is λ-convex iff $V'' \geq \lambda$:

$$\boldsymbol{E}_\#(X) = \int_0^1 V \circ X \,\mathrm{d}\xi.$$

- interaction energy is (relative) λ-convex iff $W'' \geq \lambda$:

$$\boldsymbol{E}_\#(X) = \frac{1}{2}\int_0^1\int_0^1 W\big(X(\xi) - X(\eta)\big)\,\mathrm{d}\xi\,\mathrm{d}\eta.$$

- internal energy is 0-convex iff h is convex:

$$\boldsymbol{E}_\#(X) = \int_0^1 h_\#\big(\partial_\xi X(\xi)\big)\,\mathrm{d}\xi \quad \text{with} \quad h_\#(s) = s h(1/s).$$

The magical isometry (3/3)

Corollary

$(\rho_t)_{t\geq 0}$ is a solution to the $\mathbb{W}$-gradient flow

$$\partial_t \rho = \partial_x \left(\rho \, \partial_x \frac{\delta \boldsymbol{E}}{\delta \rho} \right)$$

iff $(X_t)_{t\geq 0}$ with $X_t = X_{\rho_t}$ is a solution to the L^2-gradient flow

$$\partial_t X = -\frac{\delta \boldsymbol{E}_\#}{\delta X}.$$

Example: In case of the relative entropy

$$\boldsymbol{E}(\rho) = \int \left[h(\rho) + V \rho \right] \mathrm{d}x \quad \rightsquigarrow \quad \boldsymbol{E}_\#(X) = \int \left[h_\#(\partial_\xi X) + V \circ X \right] \mathrm{d}\xi,$$

we obtain a Lagrangian form of the nonlinear Fokker-Planck equation:

$$\partial_t \rho = \partial_{xx} P(\rho) + \partial_x (V' \rho) \quad \rightsquigarrow \quad \partial_t X = -\partial_\xi P \left(\frac{1}{\partial_\xi X} \right) - V' \circ X.$$

And . . . What about DLSS?

Residual convexity survives!

Yes, you have seen this before

Recall: the rescaled DLSS equation

$$\partial_t \rho = -2\partial_x \left(\rho \, \partial_x \frac{\partial_{xx}\sqrt{\rho}}{\sqrt{\rho}} \right) + \partial_x (x\, \rho)$$

is the $\mathbb{W}$-gradient flow of the relative Fisher information

$$\boldsymbol{F}'(\rho) = 2 \int_{\mathbb{R}} \left(\partial_x \sqrt{\rho}\right)^2 \mathrm{d}x + \int_{\mathbb{R}} \frac{x^2}{2} \rho \, \mathrm{d}x,$$

which is **totally not** displacement convex, but still,

Theorem

$$\boldsymbol{H}'(\rho_t) - \boldsymbol{H}'(\rho_\infty) \leq e^{-2t} \big(\boldsymbol{H}'(\rho_0) - \boldsymbol{H}'(\rho_\infty) \big),$$
$$\boldsymbol{F}'(\rho_t) - \boldsymbol{F}'(\rho_\infty) \leq e^{-2t} \big(\boldsymbol{F}'(\rho_0) - \boldsymbol{F}'(\rho_\infty) \big).$$

Key: $\boldsymbol{F}'(\rho) - 1 = \frac{1}{2} \left| \partial \boldsymbol{H}'(\rho) \right|^2$ with 1-displacement convex entropy

$$\boldsymbol{H}'(\rho) = \int_{\mathbb{R}} \rho \log \rho \, \mathrm{d}x + \int_{\mathbb{R}} \frac{x^2}{2} \rho \, \mathrm{d}x.$$

Recycle!

The totally non-convex transformed relative Fisher infomation

$$\boldsymbol{F}'_{\#}(X) = \frac{1}{2}\int_0^1 \left[\left\{\partial_\xi\left(\frac{1}{\partial_\xi X}\right)\right\}^2 + X^2\right] \mathrm{d}\xi$$

is related to the 1-uniformly convex transformed relative entropy

$$\boldsymbol{H}'_{\#}(X) = \int_0^1 \left(-\log \partial_\xi X + \frac{1}{2}X^2\right) \mathrm{d}\xi,$$

by the following:

$$\boldsymbol{F}'_{\#}(X) - 1 = \frac{1}{2}\left\|\frac{\delta \boldsymbol{H}'_{\#}}{\delta X}\right\|_{L^2}^2 = \frac{1}{2}\int_0^1 \left(\frac{\delta \boldsymbol{H}'_{\#}}{\delta X}\right)^2 \mathrm{d}\xi.$$

For the L^2-gradient flow of $\boldsymbol{F}'_{\#}$, this implies:

Theorem

$$\boldsymbol{H}'_{\#}(X_t) - \boldsymbol{H}'_{\#}(X_\infty) \le e^{-2t}\big(\boldsymbol{H}'_{\#}(X_0) - \boldsymbol{H}'_{\#}(X_\infty)\big),$$
$$\boldsymbol{F}'_{\#}(X_t) - \boldsymbol{F}'_{\#}(X_\infty) \le e^{-2t}\big(\boldsymbol{F}'_{\#}(X_0) - \boldsymbol{F}'_{\#}(X_\infty)\big).$$

Finally: a Lagrangian scheme.

We have a plan!

Approximate:
$\mathbb{W}$-gradient flow of a λ-geodesically convex $\boldsymbol{E}$
on the flat "Riemannian manifold" $\mathcal{M} = \mathcal{P}_2(\mathbb{R})$

By:
Riemannian gradient flow of a λ-geodesically convex function $\mathbf{E}^{(K)}$
on a K-dimensional submanifold $\mathcal{M}^{(K)} \subset \mathcal{M}$

Construction: Choose $\mathcal{M}^{(K)}$ ...

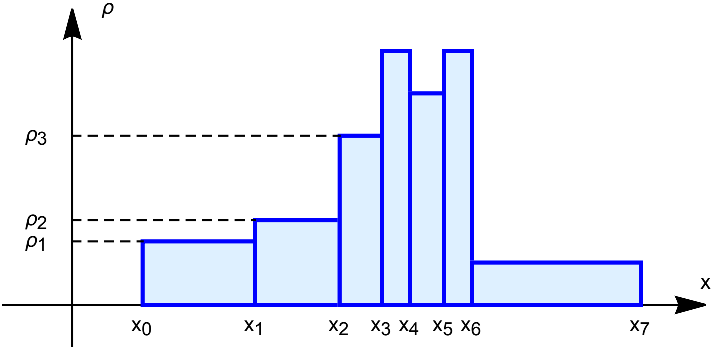
- ...corresponding to a linear cone in $L^2((0,1))$;
- ...s.t. $\boldsymbol{E}$'s restriction to $\mathcal{M}^{(K)}$ is a differentiable function.

Lemma

$\boldsymbol{E}^{(K)}$ *is λ-uniformly convex on* $\mathcal{M}^{(K)}$.

Skyscrapers (1/2)

Our choice of $\mathcal{M}^{(K)}$ consists of skyscraper landscapes:



$$\boldsymbol{\rho}^{(K)}[\vec{x}] = \sum_{k=1}^{K} \rho_k \mathbf{1}_{(x_{k-1},x_k)} \quad \text{with} \quad \rho_k = \frac{1/K}{x_k - x_{k-1}}.$$

Skyscrapers (2/2)

Distance of two skyscraper landscapes with vectors $\vec{x}$ and $\vec{x}'$ is

$$\mathbb{W}\big(\boldsymbol{\rho}^{(K)}[\vec{x}], \boldsymbol{\rho}^{(K)}[\vec{x}']\big)^2 = (\vec{x}' - \vec{x})^T \mathbb{G}(\vec{x}' - \vec{x}) \quad \text{with} \quad \mathbb{G} \approx \frac{1}{K}\mathbf{1}.$$

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Linear interpolation of $\vec{x}$'s produces geodesics $(\rho_s)_{s \in [0,1]}$,

$$\rho_s = \boldsymbol{\rho}^{(K)}[(1-s)\vec{x}_0 + s\vec{x}_1].$$

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Example energies:

$$\boldsymbol{E}(\rho) = \int_{\mathbb{R}} V(x)\,\rho\,\mathrm{d}x \quad \rightsquigarrow \quad \mathbf{E}_{\#}^{(K)}(\vec{x}) = \sum_{k=1}^{K} \rho_k \int_{x_{k-1}}^{x_k} V(x)\,\mathrm{d}x,$$

$$\boldsymbol{E}(\rho) = \int_{\mathbb{R}} h(\rho)\,\mathrm{d}x \quad \rightsquigarrow \quad \mathbf{E}_{\#}^{(K)}(\vec{x}) = \sum_{k=1}^{K} (x_k - x_{k-1}) h(\rho_k),$$

$$\boldsymbol{E}(\rho) = 2\int_{\mathbb{R}} \big(\partial_x \sqrt{\rho}\big)^2\,\mathrm{d}x \quad \rightsquigarrow \quad \mathbf{E}_{\#}^{(K)} \equiv +\infty.$$

Discrete Fokker-Planck has it all (1/2)

For the entropy

$$
\begin{aligned}
\boldsymbol{H}(\rho) &= \int_{\mathbb{R}} \left[h(\rho) + V\rho\right] \mathrm{d}x \\
\rightsquigarrow \quad \mathbf{H}_{\#}^{(K)}(\vec{x}) &= \sum_{k=1}^{K} \left[(x_k - x_{k-1})h(\rho_k) + \rho_k \int_{x_{k-1}}^{x_k} V(x)\right] \mathrm{d}x \\
&= \frac{1}{K} \sum_{k=1}^{K} \left[\frac{1}{\rho_k} h(\rho_k) + \int_{x_{k-1}}^{x_k} V(x)\,\mathrm{d}x\right] \\
&\approx \frac{1}{K} \sum_{k=1}^{K} \left[h_{\#}\left(\frac{x_k - x_{k-1}}{1/K}\right) + V(x_k)\right].
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\end{aligned}
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we obtain the gradient flow

$$
\begin{aligned}
&\partial_t \rho = \partial_{xx} P(\rho) + \partial_x(V'\rho) \\
&\quad \rightsquigarrow \quad \left(\mathbb{G}\dot{\vec{x}}\right)_k = P\left(\frac{1/K}{x_{k+1} - x_k}\right) - P\left(\frac{1/K}{x_k - x_{k-1}}\right) - \frac{1}{K}V'(x_k).
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Discrete Fokker-Planck has it all (1/2)

For the entropy

$$\boldsymbol{H}(\rho) = \int_{\mathbb{R}} \left[h(\rho) + V\rho\right] \mathrm{d}x$$

$$\rightsquigarrow \quad \mathbf{H}_{\#}^{(K)}(\vec{x}) = \sum_{k=1}^{K} \left[(x_k - x_{k-1}) h(\rho_k) + \rho_k \int_{x_{k-1}}^{x_k} V(x) \right] \mathrm{d}x$$

$$= \frac{1}{K} \sum_{k=1}^{K} \left[\frac{1}{\rho_k} h(\rho_k) + \int_{x_{k-1}}^{x_k} V(x)\, \mathrm{d}x \right]$$

$$\approx \frac{1}{K} \sum_{k=1}^{K} \left[h_{\#}\left(\frac{x_k - x_{k-1}}{1/K} \right) + V(x_k) \right].$$

we obtain the gradient flow

$$\partial_t \rho = \partial_{xx} P(\rho) + \partial_x (V'\rho)$$

$$\rightsquigarrow \quad \dot{x}_k = K \left[P\left(\frac{1/K}{x_{k+1} - x_k} \right) - P\left(\frac{1/K}{x_k - x_{k-1}} \right) \right] - V'(x_k).$$

Discrete Fokker-Planck has it all (2/2)

$$\dot{x}_k = K\left[P\left(\frac{1/K}{x_{k+1}-x_k}\right) - P\left(\frac{1/K}{x_k - x_{k-1}}\right)\right] - V'(x_k)$$

Theorem

If h is convex and $V'' \geq \lambda > 0$, then

- $\mathbf{H}_{\#}^{(K)}$ *has a unique minimizer* $\vec{x}_\infty$;
- *the entropy decays exponentially,*

$$\mathbf{H}_{\#}^{(K)}(\vec{x}_t) - \mathbf{H}_{\#}^{(K)}(\vec{x}_\infty) \leq e^{-2\lambda t}\big(\mathbf{H}_{\#}^{(K)}(\vec{x}_0) - \mathbf{H}_{\#}^{(K)}(\vec{x}_\infty)\big).$$

  and so do dissipation, metric velocity, and $\mathbb{W}(\boldsymbol{\rho}[\vec{x}_t], \boldsymbol{\rho}[\vec{x}_\infty])^2$
- *the flow is* λ*-contractive:*

$$\mathbb{W}\big(\boldsymbol{\rho}[\hat{\vec{x}}_t], \boldsymbol{\rho}[\check{\vec{x}}_t]\big)^2 \leq e^{-2\lambda t}\,\mathbb{W}\big(\boldsymbol{\rho}[\hat{\vec{x}}_0], \boldsymbol{\rho}[\check{\vec{x}}_0]\big)^2.$$

And . . . what about DLSS?

Residual convexity survives!

What a persistent idea! (1/2)

Recall: Discretizing $\boldsymbol{F}'$ directly using skyscrapers is no good.

What a persistent idea! (1/2)

Recall: Discretizing $\boldsymbol{F}'$ directly using skyscrapers is no good. Instead, take $\boldsymbol{F}' - 1 = \frac{1}{2}|\partial \boldsymbol{H}'|^2$ as starting point. With

$$\mathbf{H}_{\#}^{(K)'}(\vec{x}) = \frac{1}{K}\sum_{k=1}^{K}\left[-\log\left(\frac{x_k - x_{k-1}}{1/K}\right) + \frac{x_k^2}{2}\right],$$

we define

$$\begin{aligned}
\boldsymbol{F}_{\#}^{(K)'}(\vec{x}) &:= \frac{1}{2K}\sum_{k=1}^{K}\left(\frac{\partial \mathbf{H}_{\#}^{(K)}}{\partial x_k}\right)^2 + 1 \\
&= \ldots \text{see computations on board} \ldots \\
&= \frac{1}{2K}\sum_{k=1}^{K}\left[K^2\left(\frac{x_{k+1} - 2x_k + x_{k-1}}{(x_{k+1} - x_k)(x_k - x_{k-1})}\right)^2 + x_k^2\right].
\end{aligned}$$

What a persistent idea! (2/2)

With that definition of $\boldsymbol{F}_{\#}^{(K)'}$, the respective gradient flow satisfies:

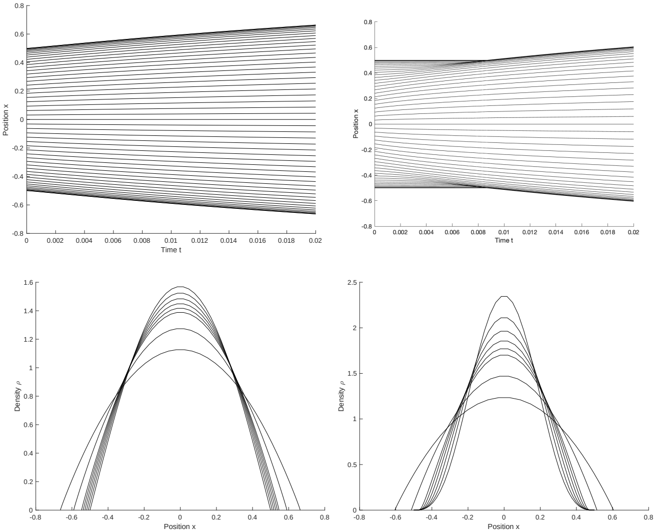
Theorem

$$\mathbf{H}_{\#}^{(K)'}(X_t) - \mathbf{H}_{\#}^{(K)'}(X_\infty) \leq e^{-2t}\big(\mathbf{H}_{\#}^{(K)'}(X_0) - \mathbf{H}_{\#}^{(K)'}(X_\infty)\big),$$
$$\boldsymbol{F}_{\#}^{(K)'}(X_t) - \boldsymbol{F}_{\#}^{(K)'}(X_\infty) \leq e^{-2t}\big(\boldsymbol{F}_{\#}^{(K)'}(X_0) - \boldsymbol{F}_{\#}^{(K)'}(X_\infty)\big).$$

Sometimes the flow perspective pays off!

Waiting time phenomenon (1/2)

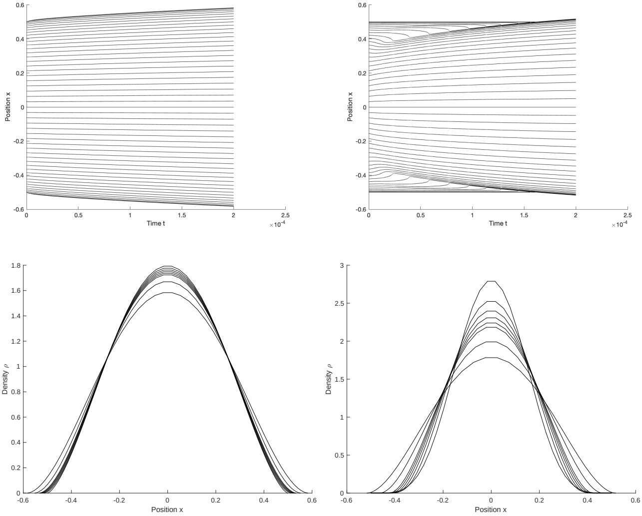
Numerics for PME $\partial_t u = \partial_{xx}(u^2)$ with data $u_0(x) = [\cos(\pi x)]_+^q$.



$q = 1.0$ (left) vs. $q = 3.0$ (right).

Waiting time phenomenon (2/2)

Numerics for TFE $\partial_t u = -\partial_x \big(u\, \partial_{xxx} u\big)$ with data $u_0(x) = [\cos(\pi x)]_+^q$.



$q = 1.5$ (left) vs. $q = 4.5$ (right).

That's all for today

Thank you, and see you tomorrow!