Wasserstein Gradient Flows of MMD Functionals with Distance Kernel and Cauchy Problems on Quantile Functions

joint work with

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University of South Carolina, Columbia, 30.08.2024.

Joint ACM and RTG data science seminar (Changhui Tan, Siming He, Wuchen Li).

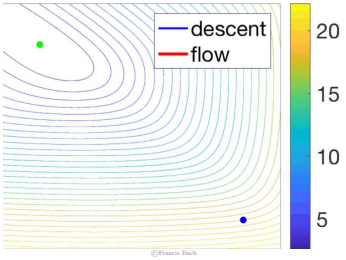
Problem: Target measure $\nu \in \mathcal{P}_2(\mathbb{R}^d)$ is unknown, only **samples** are available.

Goal: Recover ν.

Solution: *minimize* the metric **kernel discrepancy**

$$\mathcal{F}_\nu \coloneqq \mathrm{MMD}_K(\cdot, \nu)^2 \colon \mathcal{P}_2(\mathbb{R}^d) \to [0, \infty)$$

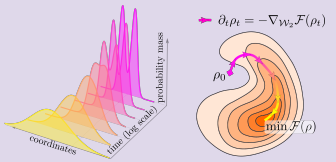
(which can be estimated using samples) to ν by finding curve of measures $(\gamma_t)_{t>0} \subset \mathcal{P}_2(\mathbb{R}^d)$ along which $\mathcal{F}_\nu$ *decreases* "the fastest".



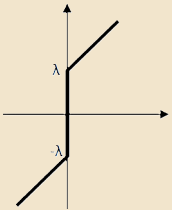
One way to construct $(\gamma_t)_{t>0}$: **Wasserstein gradient flows**.
Different kernels $K \rightsquigarrow$ very different behavior of $(\gamma_t)_{t>0}$.

Aim of this preprint: study behavior of $(\gamma_t)_{t>0}$ for irregular kernel $K(x, y) \coloneqq -|x - y|$ for $d = 1$.

1. Optimal transport and Wasserstein gradient flow

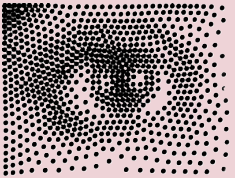


2. Maximal monotone inclusions on Hilbert spaces

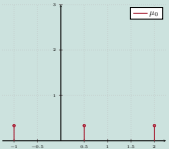


$$(I + \lambda \partial F)^{-1}$$

3. Negative distance kernel, Max. Mean Discrepancy



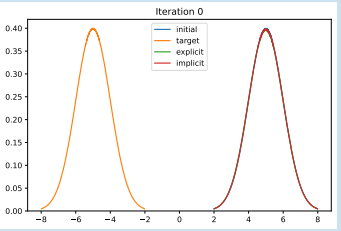
4. Wasserstein gradient flow of the MMD with negative distance kernel



5. Invariant subsets & smoothing properties

$$\gamma_0 = \delta_x,$$
$$\gamma_t \sim \mathcal{U}[a_t, b_t], \ t > 0.$$

6. Numerical results

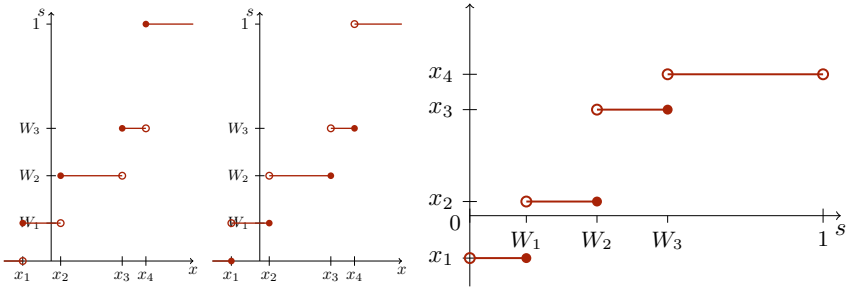


The **cumulative distribution functions** (CDFs) of $\nu \in \mathcal{P}(\mathbb{R})$ are given by

$$R_\nu^+ \colon \mathbb{R} \to [0,1], \quad R_\nu^+(x) \coloneqq \nu\big((-\infty, x]\big), \qquad R_\nu^- \colon \mathbb{R} \to [0,1], \quad R_\nu^-(x) \coloneqq \nu\big((-\infty, x)\big).$$

and its (generalized inverse, the) **quantile function** by

$$Q_\nu \colon (0,1) \to \mathbb{R}, \quad Q_\nu(s) \coloneqq \min\{x \in \mathbb{R} : R_\nu^+(x) \geq s\}.$$



Left to right: R_ν^+, R_ν^-, Q_ν, for $\nu = \sum_{k=1}^4 w_k \delta_{x_k}$, $W_j \coloneqq \sum_{k=1}^j w_k$.

Consider the subset of probability measures $\mathcal{P}(\mathbb{R})$,

$$\mathcal{P}_2(\mathbb{R}) := \left\{ \mu \in \mathcal{P}(\mathbb{R}) : \int_{\mathbb{R}} x^2 \, \mathrm{d}\mu(x) < \infty \right\}.$$

On $\mathcal{P}_2(\mathbb{R})$, the **Wasserstein-2 metric** is

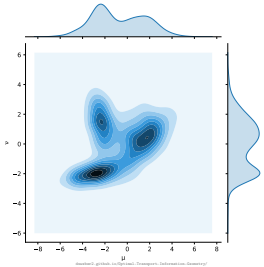
$$W_2(\mu,\nu)^2 = \min_{\pi \in \Gamma(\mu,\nu)} \int_{\mathbb{R}\times\mathbb{R}} (x-y)^2 \, \mathrm{d}\pi(x,y), \quad \mu,\nu \in \mathcal{P}_2(\mathbb{R}),$$

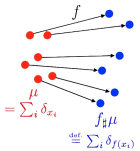
$$\Gamma(\mu,\nu) := \{\pi \in \mathcal{P}(\mathbb{R}\times\mathbb{R}) : (P_1)_{\#}\pi = \mu, (P_2)_{\#}\pi = \nu\}$$

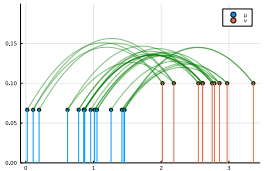
with the **projections** $P_i(x_1,x_2) := x_i$.

The **push-forward** $\#$ acts as $(f_{\#}\sigma)(A) := \sigma(f^{-1}(A))$ for all measurable sets $A \subset \mathbb{R}$.

The optimal plan $\hat{\pi}$ is unique (in 1D).



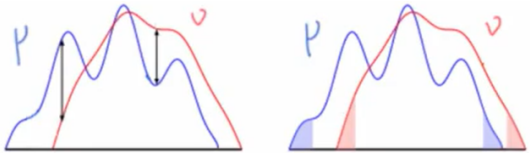




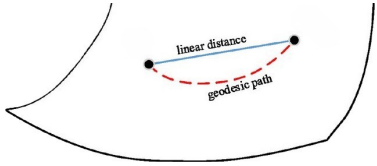
Push-forward $\hat{\pi}$ realizes monotone rearrangement.

Geodesic (= shortest constant-speed path) between μ and ν is

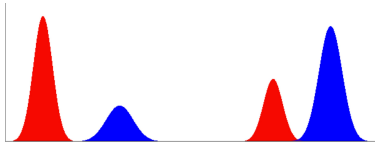
$$\gamma_t := \big((1-t)P_1 + tP_2\big)_{\#}\hat{\pi}, \quad t \in [0,1], \tag{1}$$



Vertical (L_2, $g_t := (1-t)f_\mu + tf_\nu$) vs. horizontal ($W_2$) mass displacement.



Geodesic on a manifold.



W_2 geodesic

Definition (W_2-Geodesic convexity)

$\mathcal{F}\colon \mathcal{P}_2(\mathbb{R}) \to \mathbb{R}$ is **convex along geodesics** if

$$\mathcal{F}(\gamma_t) \leq (1-t)\,\mathcal{F}(\mu) + t\,\mathcal{F}(\nu), \quad \forall \mu, \nu \in \mathcal{P}_2(\mathbb{R}),\ \gamma_t \text{ from (1)}.$$

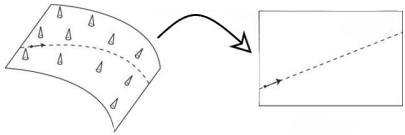
Theorem (Isometric embedding of $(\mathcal{P}_2(\mathbb{R}), W_2)$)

Let $\mathcal{C}(0,1) \coloneqq \{Q_\mu : \mu \in \mathcal{P}_2(\mathbb{R})\} \subset L_2(0,1)$ be the set of quantile functions.

The map

$$\mathcal{P}_2(\mathbb{R}) \to \mathcal{C}(0,1), \qquad \mu \mapsto Q_\mu$$

*is an **isometric isomorphism** with inverse $Q \mapsto Q_{\#}\Lambda_{(0,1)}$, where Λ is the Lebesgue measure.*

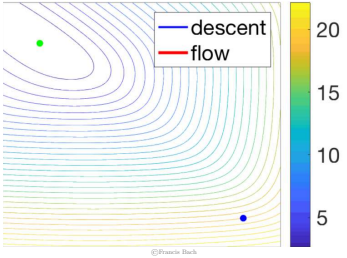


Isometric embedding.

KEY IDEA: instead of working with $\mathcal{F}\colon \mathcal{P}_2(\mathbb{R}) \to (-\infty, \infty]$, find

$$F\colon L_2(0,1) \to (-\infty, \infty] \quad \text{satisfying} \quad F(Q_\mu) = \mathcal{F}(\mu).$$

Given: Hilbert space H, energy functional $f\colon H \to (-\infty, \infty]$ (convex, bounded below).



Idea: minimize $f \rightsquigarrow$ find an *absolutely continuous* curve $t \mapsto x(t)$ such that $t \mapsto f(x(t))$ decreases "the fastest".

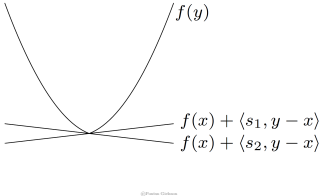
$$\frac{\mathrm{d}}{\mathrm{d}t} x(t) = -\nabla f(x(t))$$

If f is not differentiable, there might be more than one descent direction.

Definition

The **subdifferential** of a **convex** function $F\colon H \to \mathbb{R}$ is

$$\partial F(u) \coloneqq \big\{v \in H : F(w) \geq F(u) + \langle v, w - u\rangle \ \forall w \in H\big\}.$$

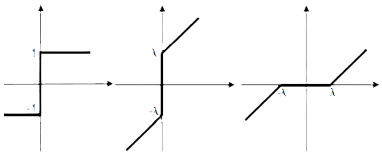


Theorem (Properties of the resolvent)

Let $F\colon H \to \mathbb{R}$ be convex and lower semicontinuous, $F \not\equiv \infty$. Then ∂F is maximal monotone, hence $\forall \varepsilon > 0$, the ***resolvent***

$$J_\varepsilon^{\partial F} \coloneqq (I + \varepsilon \partial F)^{-1} : H \to H$$

is single-valued.



∂F, $I + \lambda \partial F$, $(I + \lambda \partial F)^{-1}$, where $F \coloneqq |\cdot|$.

This theorem tells us that gradient flows in Hilbert spaces exist and are unique.

Theorem (Existence, regularity of strong solutions to Cauchy problems (Brezis '67))

Let $f\colon H \to \mathbb{R}$ s.t. $\partial f\colon H \to 2^H$ is maximal monotone and $g_0 \in \operatorname{dom}(\partial f)$. Then $\exists! g\colon [0,\infty) \to H$ s.t.

- *$g(0) = g_0$ and $\frac{\mathrm{d}g}{\mathrm{d}t}(t) \in -(\partial f)\big(g(t)\big)$ for almost all $t > 0$, and $g(t) \in \operatorname{dom}(\partial f)$ for all $t > 0$*
- *g is Lipschitz continuous on $[0,\infty)$.*
- *g is given by the exponential formula*

$$g(t) = \lim_{n\to\infty} \left(J^{\partial f}_{\frac{t}{n}}\right)^n (g_0) \qquad \text{uniformly in } t \text{ on compact intervals.}$$

For $\mathcal{P}_2(\mathbb{R})$ instead of H: what are the analogs of the tangent vector $\frac{\mathrm{d}}{\mathrm{d}t}x(t)$ and the subdifferential ∂f?

Definition (Fréchet subdifferential in Wasserstein space)

The (reduced) Fréchet subdifferential of $\mathcal{F}\colon \mathcal{P}_2(\mathbb{R}) \to \mathbb{R}$ at μ is

$$\partial \mathcal{F}(\mu) \coloneqq \left\{ \xi \in L^2(\mathbb{R}; \mu) : \mathcal{F}(\nu) - \mathcal{F}(\mu) \geq \int_{\mathbb{R}\times\mathbb{R}} \xi(x_1)(x_2 - x_1)\, \mathrm{d}\hat{\pi}(x, y) + o\big(W_2(\mu, \nu)\big) \right\}$$

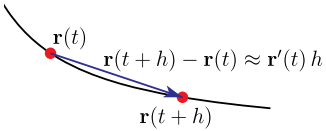
A curve $\gamma\colon (0, \infty) \to \mathcal{P}_2(\mathbb{R})$ is **absolutely continuous** if $\exists$ L^2-Borel **velocity field** $(v_t\colon \mathbb{R} \to \mathbb{R})_{t>0}$ s.t.

$$\partial_t \gamma_t + \nabla \cdot (v_t \gamma_t) = 0, \qquad (t, x) \in (0, \infty) \times \mathbb{R}, \text{ weakly.} \qquad \text{(Continuity Eq.)}$$

Definition (Wasserstein gradient flow)

A absolutely continuous curve $\gamma\colon (0, \infty) \to \mathcal{P}_2(\mathbb{R})$ with velocity field $\big(v_t \in \mathrm{T}_{\gamma_t} \mathcal{P}_2(\mathbb{R})\big)_{t>0}$ is a *Wasserstein gradient flow with respect to* $\mathcal{F}\colon \mathcal{P}_2(\mathbb{R}) \to \mathbb{R}$ if

$$v_t \in -\partial \mathcal{F}(\gamma_t), \quad \text{for a.e. } t > 0.$$



Tangent vector.

Theorem (Ambrosio, Gigli, Savaré (2005))

Let $\mathcal{F}\colon \mathcal{P}_2(\mathbb{R}) \to \mathbb{R}$ be bounded from below, lower semicontinuous, ***geodesically convex****.*

Existence and uniqueness. *Then $\exists!$* ***Wasserstein gradient flow*** *$\gamma\colon (0,\infty) \to \mathcal{P}_2(\mathbb{R})$ with respect to $\mathcal{F}$ starting at $\gamma(0+) = \mu_0 \in \mathcal{P}_2(\mathbb{R})$.*

Approximation scheme. *The piecewise constant curves constructed from the iterates*

$$\mu_{n+1} \coloneqq \operatorname*{argmin}_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \left\{ \mathcal{F}(\mu) + \frac{1}{2\tau} W_2^2(\mu_n, \mu) \right\}, \qquad \tau > 0, \tag{Minimizing movement scheme}$$

i.e., γ_τ defined by $\gamma_\tau|_{(n\tau,(n+1)\tau]} \coloneqq \mu_n$, $n \in \mathbb{N}$, converge locally uniformly to γ as $\tau \downarrow 0$.

Convergence speed. *If $\bar{\mu}$ is a minimizer of $\mathcal{F}$, then*

$$\mathcal{F}(\gamma_t) - \mathcal{F}(\bar{\mu}) \leq \frac{1}{2t} W_2^2(\mu_0, \bar{\mu}). \tag{Sublinear convergence rate}$$

We establish a correspondence between $L_2(0,1)$-gradient flows of F and Wasserstein gradient flows of $\mathcal{F}$.

Theorem (Quantile function reformulation [DSBHS24])

Let $F\colon L_2(0,1) \to (-\infty, \infty]$ be convex and lsc, $F \not\equiv \infty$ with $F(Q_\mu) = \mathcal{F}(\mu)$ for all $\mu \in \mathcal{P}_2(\mathbb{R})$. Assume $J_\varepsilon^{\partial F}$ maps $\mathcal{C}(0,1)$ into itself $\forall \varepsilon > 0$. Then, $\forall$ initial datum $g_0 \in \mathcal{C}(0,1) \cap \operatorname{dom}(\partial F)$,

$$\begin{cases} \partial_t g(t) + \partial F(g(t)) \ \ni \ 0, \quad t \in (0,\infty), \\ g(0) = g_0, \end{cases} \tag{Cauchy Problem}$$

has a unique strong solution g.

*The curve $\gamma_t \coloneqq (g(t))_\# \Lambda_{(0,1)}$ has quantile functions $Q_{\gamma_t} = g(t)$ and is a **Wasserstein gradient flow of** $\mathcal{F}$ with $\gamma(0+) = (g_0)_\# \Lambda_{(0,1)}$.*

Consider the **negative distance kernel** $K(x, y) \coloneqq -|x - y|$.

K is only **conditionally positive definite**.

Motivation: electrostatic principles, interacting species, dithering.

Definition (MMD)

The **maximum mean discrepancy** of with respect to K is

$$\mathcal{P}_2(\mathbb{R}) \times \mathcal{P}_2(\mathbb{R}) \to [0, \infty),$$
$$(\mu, \nu) \mapsto \frac{1}{2} \operatorname{MMD}_K(\mu, \nu)^2 = \int_{\mathbb{R} \times \mathbb{R}} K(x, y) \, \mathrm{d}(\mu - \nu)(x) \, \mathrm{d}(\mu - \nu)(y).$$

Dithering

$$\mathcal{F}_\nu(\mu) \coloneqq -\frac{1}{2} \underbrace{\int_{\mathbb{R} \times \mathbb{R}} |x - y| \, \mathrm{d}\mu(x) \, \mathrm{d}\mu(y)}_{\text{interaction}} + \underbrace{\int_{\mathbb{R}^d \times \mathbb{R}^d} |x - y| \, \mathrm{d}\mu(x) \, \mathrm{d}\nu(y)}_{\text{potential}}. \tag{2}$$

We now apply this theorem to the MMD with the negative distance kernel, i.e. to

$$\mathcal{F}_\nu \coloneqq \frac{1}{2}\,\mathrm{MMD}_K(\cdot,\nu).$$

Lemma (Properties of F_ν)

The functional

$$F_\nu\colon L_2(0,1)\to\mathbb{R},\qquad u\mapsto \int_0^1 \Big((1-2s)\big(u(s)-Q_\nu(s)\big)+\int_0^1 |u(s)-Q_\nu(t)|\,\mathrm{d}t\Big)\,\mathrm{d}s$$

is convex and continuous, we have $F_\nu(Q_\mu)=\mathcal{F}_\nu(\mu)\ \forall \mu\in\mathcal{P}_2(\mathbb{R})$, and

$$\partial F_\nu(u)=\Big\{f\in L_2(0,1): f(s)\in 2\big[R_\nu^-\big(u(s)\big),R_\nu^+\big(u(s)\big)\big]-2s \text{ for a.e. } s\in(0,1)\Big\},\quad u\in L_2(0,1)$$

and $J_\varepsilon^{\partial F_\nu}$ maps $\mathcal{C}(0,1)$ into itself $\forall\varepsilon>0$.

Proof. By elementary means, nothing fancy happens here.

The lower Lipschitz constant of $g \in \mathcal{C}(0,1)$ is

$$L_{\text{low}}(g) := \max\left\{ L \geq 0 : \frac{g(s_1) - g(s_2)}{s_1 - s_2} \geq L \ \forall s_1, s_2 \in (0,1) \right\} \geq 0,$$

If $\mu = \delta_x$, then $Q_\mu \equiv x$ and $L_{\text{low}}(Q_\mu) = 0$.

Theorem (Time evolution of CDF's lower Lipschitz constants)

Let $\nu \in \mathcal{P}_2(\mathbb{R})$ with $L_{\text{low}}(Q_\nu) > 0$, and $g_0 = Q_{\mu_0} \in \mathcal{C}(0,1)$. We have

$$\text{Lip}(R_{\gamma_t}) \leq \left(L_{\text{low}}(g_0) \cdot e^{-\frac{2t}{L_{\text{low}}(Q_\nu)}} + L_{\text{low}}(Q_\nu) \cdot (1 - e^{-\frac{2t}{L_{\text{low}}(Q_\nu)}}) \right)^{-1} < \infty.$$

Theorem (Continuity is preserved & monotonicity of the support)

Let $\nu \in \mathcal{P}_2(\mathbb{R})$, g_0 be continuous and g the solution of the Cauchy problem starting in g_0.

- *$g(t)$ is continuous for all $t \geq 0$.*
- *The ranges fulfill $\overline{g(t_1)(0,1)} \subseteq \overline{g(t_2)(0,1)}$ for all $0 \leq t_1 \leq t_2$.*

Corollary (Point measure target)

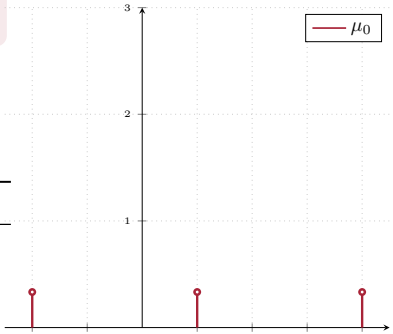
Let $\nu \coloneqq \sum_{j=1}^{n} w_j \delta_{x_j}$. Then F_ν flow is given by

$$[g(t)](s) \coloneqq \begin{cases} Q_{\mu_0}(s) + 2\,(s - R_{s,0})\,t, & t \in [t_{s,0}, t_{s,1}), \\ x_{s,j} + 2\,(s - R_{s,j})\,(t - t_{s,j}), & t \in [t_{s,j}, t_{s,j+1}), \\ Q_\nu(s), & t \geq t_{s,|\ell_s - k_s|}, \end{cases}$$

where

$$t_{s,0} \coloneqq 0, \quad t_{s,1} \coloneqq \frac{x_{s,1} - Q_{\mu_0}(s)}{2(s - R_{s,0})}, \quad t_{s,j+1} \coloneqq t_{s,j} + \frac{x_{s,j+1} - x_{s,j}}{2(s - R_{s,j})},$$

	$Q_{\mu_0}(s) \leq Q_\nu(s)$	$Q_{\mu_0}(s) \geq Q_\nu(s)$	
ℓ_s	$W_{\ell_s - 1} < s < W_{\ell_s}$	$W_{\ell_s - 1} < s < W_{\ell_s}$	
k_s	$x_{k_s} \leq Q_{\mu_0}(s) < x_{k_s + 1}$	$x_{k_s - 1} < Q_{\mu_0}(s) \leq x_{k_s}$	
$x_{s,j}$	$x_{k_s + j}$	$x_{k_s - j}$	$j \leq \lvert \ell_s - k_s \rvert$
$R_{s,j}$	$W_{k_s + j}$	$W_{k_s - j - 1}$	$j \leq \lvert \ell_s - k_s \rvert - 1$



Let $\tau > 0$. The minimizing movement (or JKO) scheme,

$$\mu_{n+1} \coloneqq \operatorname*{argmin}_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \Big\{ \mathcal{F}_\nu(\mu) + \frac{1}{2\tau} W_2^2(\mu_n, \mu) \Big\},$$

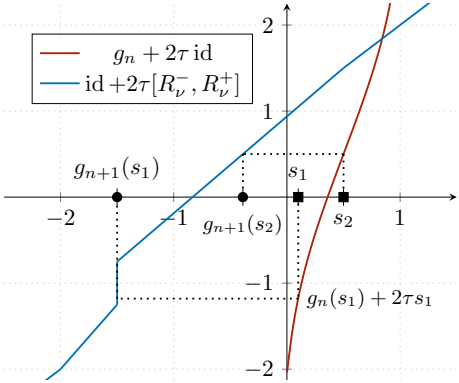
can be rewritten using the isometry $\mathcal{P}_2(\mathbb{R}) \to \mathcal{C}(0,1)$ as

$$g_{n+1} = \operatorname*{argmin}_{g \in \mathcal{C}(0,1)} \Big\{ F_\nu(g) + \frac{1}{2\tau} \int_0^1 |g - g_n|^2 \, \mathrm{d}s \Big\}$$
$$\overset{F_\nu \in \Gamma_0(L_2(0,1))}{=} (I + \tau \partial F_\nu)^{-1}(g_n),$$

which is equivalent to

$$g_n(s) + 2\tau s \in g_{n+1}(s) + 2\tau \big[R_\nu^-(g_{n+1}(s)), R_\nu^+(g_{n+1}(s)) \big] \quad (3)$$

for all $s \in (0,1)$.



Implicit Euler step visualized.

$(g_n)_{\#}\Lambda_{(0,1)}$ approximates WGF for $t \in (n\tau, (n+1)\tau]$.

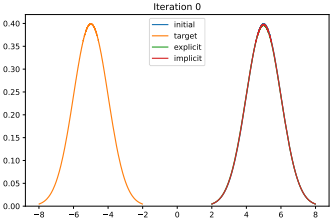
$(g_n)_{n \in \mathbb{N}} \to Q_\nu$ weakly in $L_2(0,1)$ and $\mu_n \coloneqq (g_n)_{\#}\Lambda_{(0,1)} \to \nu$ narrowly for fixed $\tau > 0$.

If $R_\nu^+ = R_\nu^- =: R_\nu$, we can also use explicit Euler discretization

$$g_{n+1} = g_n - \tau \nabla F_\nu(g_n) = g_n - 2\tau(R_\nu \circ g_n - \mathrm{id}),$$

Advantage: we don't have to solve an inclusion in each step.

Disadvantage: weaker convergence guarantees, might not preserve $\mathcal{C}(0,1)$ (iterates not monotone).



$\mu_0 = \mathcal{N}(-5,1)$, $\nu = \mathcal{N}(5,1)$.

- Extension to higher dimensions. Lagrangian reformulation now involves flow map.
- Deterministic particle approximations and mean field limits.
- Convergence of explicit scheme, distance of implicit and explicit iterates.
- Generalize Lipschitz properties to Hölder properties.
- Applying similar techniques to non-convex functional and then regularize.

- Reformulation as **maximal monotone** inclusion Cauchy problem in $L_2(0,1)$ via **quantile functions**.
- Comprehensive description of solutions' behavior, qualitative description of **instantaneous measure-to-L^∞ regularization**.
- Implicit Euler is simple.

Thank you for your attention!

I am happy to take any questions.

Paper link: `https://arxiv.org/abs/2408.07498`

My website: `viktorajstein.github.io`

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Interpolating between OT and KL regularized OT using Rényi Divergences

Rényi divergence $\notin \{f\text{-div.}, \text{Bregman div.}\}$, $\alpha \in (0,1)$

$$R_\alpha(\mu \mid \nu) \coloneqq \frac{1}{\alpha - 1} \ln \left[\int_X \left(\frac{\mathrm{d}\mu}{\mathrm{d}\tau} \right)^\alpha \left(\frac{\mathrm{d}\nu}{\mathrm{d}\tau} \right)^{1-\alpha} \mathrm{d}\tau \right],$$

$$\mathrm{OT}_{\varepsilon,\alpha}(\mu,\nu) \coloneqq \min_{\pi \in \Pi(\mu,\nu)} \langle c, \pi \rangle + \varepsilon R_\alpha(\pi \mid \mu \otimes \nu)$$

is a metric, where $\varepsilon > 0$, $\mu, \nu \in \mathcal{P}(X)$, X compact.

$$\mathrm{OT}(\mu,\nu) \xleftarrow[\text{or } \varepsilon \to 0]{\alpha \searrow 0} \mathrm{OT}_{\varepsilon,\alpha}(\mu,\nu) \xrightarrow{\alpha \nearrow 1} \mathrm{OT}_\varepsilon^{\mathrm{KL}}(\mu,\nu).$$

In the works: **debiased** Rényi-Sinkhorn divergence

$$\mathrm{OT}_{\varepsilon,\alpha}(\mu,\nu) - \frac{1}{2}\mathrm{OT}_{\varepsilon,\alpha}(\mu,\mu) - \frac{1}{2}\mathrm{OT}_{\varepsilon,\alpha}(\nu,\nu).$$