

WASSERSTEIN GRADIENT FLOWS OF MOREAU ENVELOPES OF f -DIVERGENCES IN REPRODUCING KERNEL HILBERT SPACES

joint work with



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Goal. Recover $\nu \in \mathcal{P}(\mathbb{R}^d)$ from samples by minimizing f -divergence $D_{f,\nu}$ to ν , e.g. $\text{KL}(\cdot \mid \nu)$.

Problem. Only samples \rightsquigarrow empirical measures, but

$$\mu \not\ll \nu \implies D_{f,\nu}(\mu) = \infty.$$

weak convergence

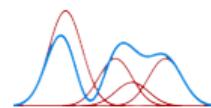
Our Solution. Regularize $D_{f,\nu}: \mathcal{M}(\mathbb{R}^d) \rightarrow [0, \infty]$.



$$m: \mathcal{M}(\mathbb{R}^d) \rightarrow \mathcal{H}_K, \quad \mu \mapsto \int_{\mathbb{R}^d} K(x, \cdot) d\mu(x)$$

pointwise convergence

$$“D_{f,\nu} \circ m^{-1}” = G_{f,\nu}: \mathcal{H}_K \rightarrow [0, \infty]$$



2. Moreau envelope regularization

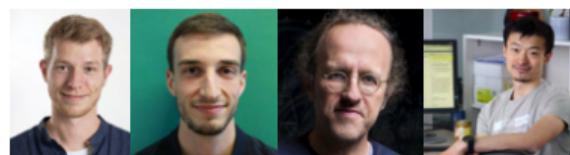
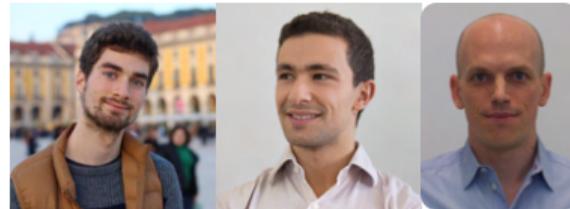
$${}^\lambda G_{f,\nu}(m(\mu)) = \min_{\sigma \in \mathcal{M}_+(\mathbb{R}^d)} D_{f,\nu}(\sigma) + \frac{1}{2\lambda} \|m(\sigma) - m(\mu)\|_{\mathcal{H}_K}^2, \quad \lambda > 0.$$

We prove existence & uniqueness of W_2 gradient flows of $({}^\lambda G_{f,\nu}) \circ m$.

Simulate particle flows = W_2 gradient flows starting at empirical measure

LITERATURE REVIEW OF PRIOR WORK

- KALE functional = MMD-regularized KL divergence
[Glaser, Arbel, Gretton. NeurIPS'21]
No Moreau envelope interpretation.
- Kernel methods of moments = f -divergence-regularized MMD
[Kremer, Nemmour, Schölkopf, Zhu. ICML'23]
Doesn't cover all f -divergences.
- (f, Γ) -divergence = Pasch-Hausdorff envelope of f -divergences
[Birrell, Dupuis, Katsoulakis, Pantazis, Rey-Bellet, JMLR'23]
Yields only Lipschitz, not differentiable functional.
- W_1 -Moreau envelope of f -divergences [Terjék. ICML'21]
No RKHS, which makes optimization finite-dimensional, hence
tractable.



1. RKHS & MMD

2. Moreau envelopes

3. f -divergences

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of f -divergences

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REPRODUCING KERNEL HILBERT SPACES

“Kernel trick”: embed data into high-dimensional Hilbert space.

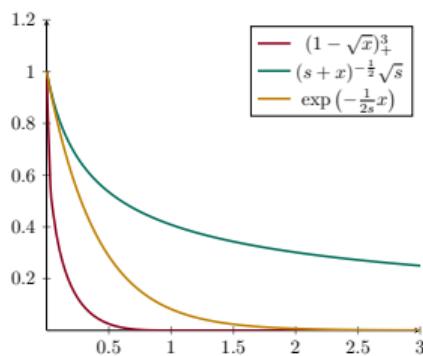
$K: \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ **symmetric, positive definite.**

We consider **radial** kernels $K(x, y) = \phi(\|x - y\|_2^2)$ with

$\phi \in \mathcal{C}^\infty((0, \infty)) \cap \mathcal{C}^2([0, \infty)), (-1)^k \phi^{(k)}(r) \geq 0, \forall k \in \mathbb{N}, r > 0.$

↪ **reproducing kernel Hilbert space (RKHS)**

$\mathcal{H}_K := \overline{\text{span}}(\{K(x, \cdot) : x \in \mathbb{R}^d\})$. Key property: $h \mapsto h(x)$ cts.



Examples (with parameter $s > 0$).

- Gaussian $\phi(r) = \exp(-\frac{1}{2s}r)$
- inverse multiquadric $\phi(r) := (s + r)^{-\frac{1}{2}}$
- spline $\phi(r) = \max(0, (1 - \sqrt{r})^{s+2})$.

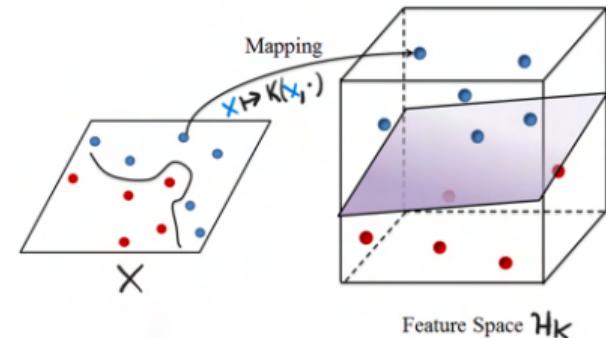


FIG. 1: “Kernel trick”.

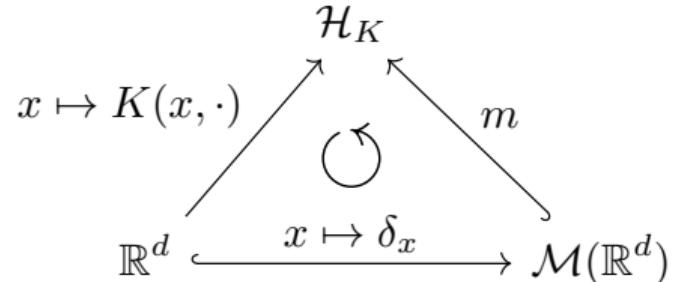
Source: songy.net/posts/story-of-basis-and-kernels-part-2/

Nonexamples.

- Laplace $\phi(r) = \exp(-\frac{1}{2s}\sqrt{r})$
(not smooth enough)
- $K(x, y) = \|x\| + \|y\| - \|x - y\|$
(not radial)

“Kernel trick for signed measures” $\mu \in \mathcal{M}(\mathbb{R}^d)$ (instead of points): **kernel mean embedding (KME)**

$$m: \mathcal{M}(\mathbb{R}^d) \rightarrow \mathcal{H}_K, \quad \mu \mapsto \int_{\mathbb{R}^d} K(x, \cdot) d\mu(x).$$



We require m to be injective (\mathcal{H}_K “characteristic”) $\iff \mathcal{H}_K \subset \mathcal{C}_0(\mathbb{R}^d)$ dense.

↔ Instead of measures, compare their embeddings in \mathcal{H}_K : **maximum mean discrepancy (MMD)**

$$d_K: \mathcal{M}(\mathbb{R}^d) \times \mathcal{M}(\mathbb{R}^d) \rightarrow [0, \infty), \quad (\mu, \nu) \mapsto \|m(\mu - \nu)\|_{\mathcal{H}_K}.$$

m injective $\implies d_K$ is a metric, but $(\mathcal{M}(\mathbb{R}^d), d_K)$ is not complete.

Easy to evaluate, e.g. for discrete measures since

$$d_K(\mu, \nu)^2 = \int_{\mathbb{R}^d \times \mathbb{R}^d} K(x, y) d(\mu - \nu)(x) d(\mu - \nu)(y) \quad \forall \mu, \nu \in \mathcal{M}(\mathbb{R}^d).$$

1. RKHS & MMD

2. Moreau envelopes

3. f -divergences

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of f -divergences

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REGULARIZATION IN CONVEX ANALYSIS - MOREAU ENVELOPES

Let $(H, \langle \cdot, \cdot \rangle, \|\cdot\|)$ Hilbert space, $f \in \Gamma_0(H)$, i.e. $f: H \rightarrow (-\infty, \infty]$ **convex**, lower semicontinuous, $\text{dom}(f) := \{x \in H : f(x) < \infty\} \neq \emptyset$.

For $\varepsilon > 0$, the **ε -Moreau envelope** of f ,

$${}^\varepsilon f: H \rightarrow \mathbb{R}, \quad x \mapsto \min \left\{ f(x') + \frac{1}{2\varepsilon} \|x - x'\|^2 : x' \in H \right\}$$

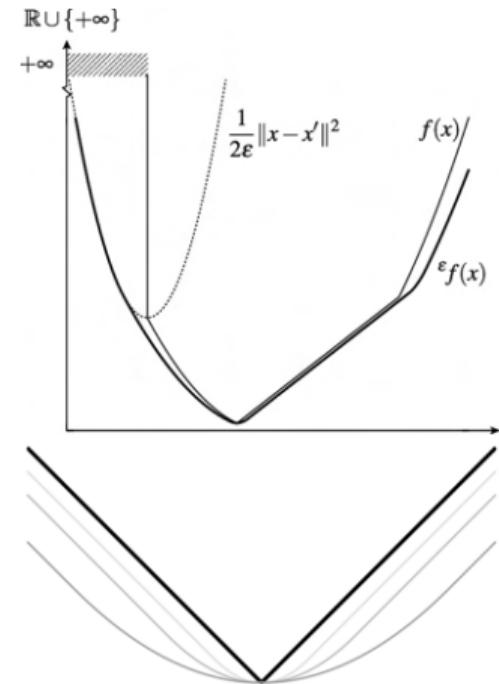
is convex, **differentiable** regularization of f **preserving its minimizers**.

Asymptotics: ${}^\varepsilon f(x) \nearrow f(x)$ for $\varepsilon \searrow 0$ and ${}^\varepsilon f(x) \searrow \inf(f)$ for $\varepsilon \rightarrow \infty$.

$(\varepsilon, x) \mapsto {}^\varepsilon f(x)$ is viscosity solution of Hamilton-Jacobi equation:

$$\begin{cases} \partial_\varepsilon({}^\varepsilon f)(x) + \frac{1}{2} \|\nabla({}^\varepsilon f)(x)\|_2^2 = 0, \\ {}^0 f(x) \rightarrow f(x). \end{cases}$$

[Osher, Heaton, Fung, PNAS 120, **14**, 2023].



Moreau envelope of an extended-real-valued non-differentiable function (top) and of $|\cdot|$ for different ε (bottom).

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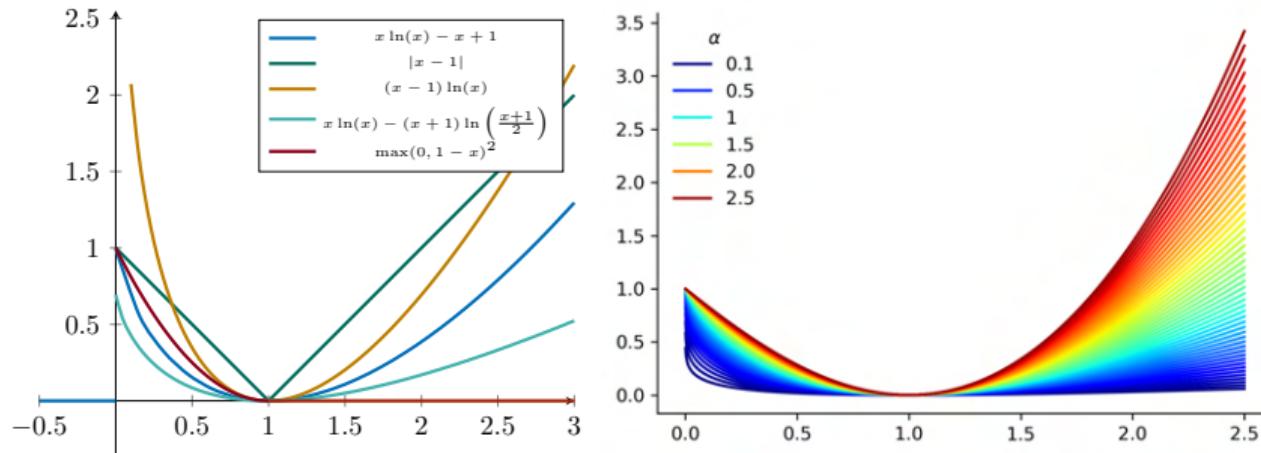
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ENTROPY FUNCTIONS

We consider $f \in \Gamma_0(\mathbb{R})$ with $f|_{(-\infty, 0)} \equiv \infty$ and with **unique minimizer at 1**: $f(1) = 0$ and positive recession constant $f'_\infty := \lim_{t \rightarrow \infty} \frac{1}{t} f(t) > 0$.

Examples. $f_{\text{KL}}(x) := x \ln(x) - x + 1$ for $x \geq 0$ yields the **Kullback-Leibler divergence** and $f_\alpha(x) := \frac{1}{\alpha-1} (x^\alpha - \alpha x + \alpha - 1)$ the **Tsallis- α divergence** T_α for $\alpha > 0$. In the limit: $T_1 = \text{KL}$.



Left: Examples of entropy functions, except the red. Right: The functions f_α for $\alpha \in [0.1, 2.5]$.

f -divergence of $\mu = \rho\nu + \mu_s \in \mathcal{M}_+(\mathbb{R}^d)$ (unique Lebesgue decomposition) to $\nu \in \mathcal{M}_+(\mathbb{R}^d)$

$$\begin{aligned} D_{f,\nu}(\rho\nu + \mu_s) &:= \int_{\mathbb{R}^d} f \circ \rho \, d\nu + f'_\infty \cdot \mu_s(\mathbb{R}^d) \quad (\infty \cdot 0 := 0) \\ &= \sup_{h \in \mathcal{C}_b(\mathbb{R}^d; \text{dom}(f^*))} \mathbb{E}_\mu[h] - \mathbb{E}_\nu[f^* \circ h], \quad \mathbb{E}_\sigma[h] := \int_{\mathbb{R}^d} h(x) \, d\sigma(x) \end{aligned}$$

The **convex conjugate** of f is $f^*: \mathbb{R} \rightarrow (-\infty, \infty]$, $s \mapsto \sup \{st - f(t) : t \geq 0\}$.

THEOREM (PROPERTIES OF $D_{f,\nu}$)

$D_{f,\nu}: \mathcal{M}_+(\mathbb{R}^d) \rightarrow [0, \infty]$ is convex, weak* lower semicontinuous. We have: $D_{f,\nu}(\mu) = 0 \iff \mu = \nu$.

We define the **MMD-regularized f -divergence** functional

$$D_{f,\nu}^\lambda(\mu) := \min \left\{ D_{f,\nu}(\sigma) + \frac{1}{2\lambda} d_K(\mu, \sigma)^2 : \sigma \in \mathcal{M}(\mathbb{R}^d) \right\}, \quad \lambda > 0, \mu \in \mathcal{M}(\mathbb{R}^d). \quad (1)$$

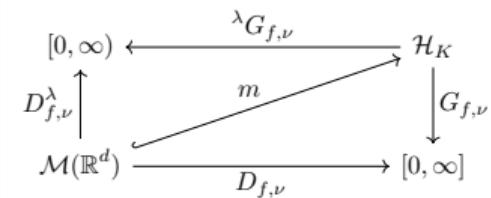
THEOREM (MOREAU ENVELOPE INTERPRETATION OF $D_{f,\nu}^\lambda$ [NSSR24])

The \mathcal{H}_K -extension of $D_{f,\nu}$,

$$G_{f,\nu}: \mathcal{H}_K \rightarrow [0, \infty], \quad h \mapsto \begin{cases} D_{f,\nu}(\mu), & \text{if } \exists \mu \in \mathcal{M}_+(\mathbb{R}^d) \text{ s.t. } h = m(\mu), \\ \infty, & \text{else.} \end{cases}$$

is convex, **lower semicontinuous** and its Moreau envelope concatenated with m is the MMD-regularized f -divergence:

$${}^\lambda G_{f,\nu} \circ m = D_{f,\nu}^\lambda$$



- Dual formulation

$$D_{f,\nu}^\lambda(\mu) = \max \left\{ \mathbb{E}_\mu[p] - \mathbb{E}_\nu[f^* \circ p] - \frac{\lambda}{2} \|p\|_{\mathcal{H}_K}^2 : p \in \mathcal{H}_K, p \leq f'_\infty \right\}. \quad (2)$$

$\hat{p} \in \mathcal{H}_K$ maximizes (2) $\iff \hat{g} = m(\mu) - \lambda \hat{p}$ is primal solution.

$$\frac{\lambda}{2} \|\hat{p}\|_{\mathcal{H}_K}^2 \leq D_{f,\nu}^\lambda(\mu) \leq \|\hat{p}\|_{\mathcal{H}_K} (\|m_\mu\|_{\mathcal{H}_K} + \|m_\nu\|_{\mathcal{H}_K}) \quad \text{and} \quad \|\hat{p}\|_{\mathcal{H}_K} \leq \frac{2}{\lambda} d_K(\mu, \nu).$$

- $D_{f,\nu}^\lambda$ is Fréchet differentiable on $\mathcal{M}(\mathbb{R}^d)$ and its gradient is λ -Lipschitz with respect to d_K :

$$\nabla D_{f,\nu}^\lambda(\mu) = \operatorname{argmax} (2).$$

THEOREM. (PROPERTIES OF $D_{f,\nu}^\lambda$) [NSSR24]

- **Asymptotic regimes:** Mosco resp. pointwise convergence (if $0 \in \text{int}(\text{dom}(f^*))$ resp. f^* differentiable in 0)

$$D_{f,\nu}^\lambda \rightarrow D_{f,\nu} \quad \lambda \searrow 0 \quad \text{and} \quad (1 + \lambda) D_{f,\nu}^\lambda \rightarrow \frac{1}{2} d_K(\cdot, \nu)^2 \quad \lambda \rightarrow \infty$$

	MMD metric d_K	f -divergence D_f
ingredients	characteristic kernel K	convex, lsc f , $f(1) = 0$
examples	Gaussian, IMQ, Matérn	KL, JSD, Hellinger, χ^2
positive definite	👍	👍
symmetric	👍	👎
triangle inequality	👍	👎
variational formulation	👍	👍
topology on measures	🚫	💪
geometry on measures	😐	😊

- **Divergence property:** $D_{f,\nu}^\lambda(\mu) = 0 \iff \mu = \nu$.
- If f^* is differentiable in 0, then $(\mu, \nu) \mapsto D_{f,\nu}^\lambda(\mu)$ **metrizes weak convergence** on $\mathcal{M}_+(\mathbb{R}^d)$ -balls.

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$\mathcal{P}_2(\mathbb{R}^d) := \{\mu \in \mathcal{P}(\mathbb{R}^d) : \int_{\mathbb{R}^d} \|x\|_2^2 d\mu(x) < \infty\}$, $\|\cdot\|_2$ Eucl. norm.

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

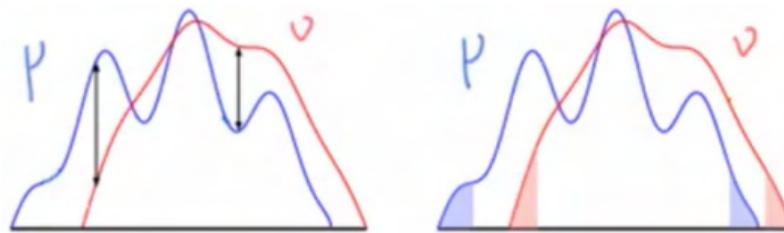


FIG. 2: Vertical (L_2) vs. horizontal (W_2) mass displacement.

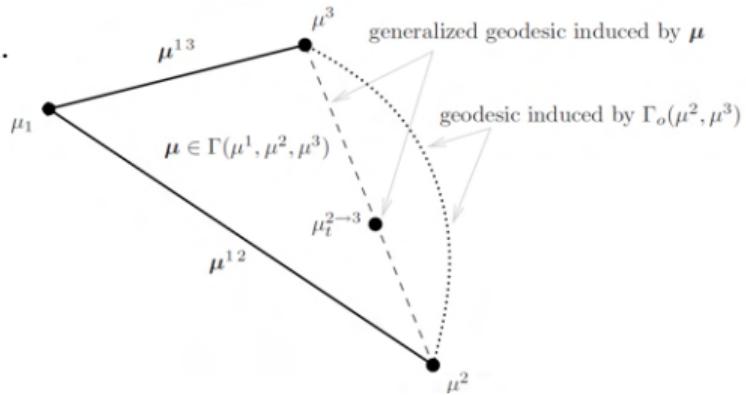


FIG. 3: Generalized geodesic from μ_2 to μ_3 with base μ_1 [AGS08].

DEFINITION (GENERALIZED GEODESIC CONVEXITY)

A function $\mathcal{F}: \mathcal{P}_2(\mathbb{R}^d) \rightarrow (-\infty, \infty]$ is *M-convex along generalized geodesics* with $M \in \mathbb{R}$ if, for every $\sigma, \mu, \nu \in \text{dom}(\mathcal{F})$, there exists a $\alpha \in \mathcal{P}_2(\mathbb{R}^{3d})$ with $(P_{1,2})_\# \alpha \in \Gamma^{\text{opt}}(\sigma, \mu)$ and $(P_{1,3})_\# \alpha \in \Gamma^{\text{opt}}(\sigma, \nu)$ s.t.

$$\mathcal{F}\left(\left((1-t)P_2 + tP_3\right)_\# \alpha\right) \leq (1-t)\mathcal{F}(\mu) + t\mathcal{F}(\nu) - \frac{M}{2}t(1-t) \int_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} \|y - z\|_2^2 d\alpha(x, y, z), \quad \forall t \in [0, 1].$$

DEFINITION (FRÉCHET SUBDIFFERENTIAL IN WASSERSTEIN SPACE)

The (reduced) Fréchet subdifferential of $\mathcal{F}: \mathcal{P}_2(\mathbb{R}^d) \rightarrow (-\infty, \infty]$ at $\mu \in \text{dom}(\mathcal{F})$ is

$$\partial \mathcal{F}(\mu) := \left\{ \xi \in L^2(\mathbb{R}^d; \mu) : \mathcal{F}(\nu) - \mathcal{F}(\mu) \geq \inf_{\pi \in \Gamma^{\text{opt}}(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} \langle \xi(x_1), x_2 - x_1 \rangle d\pi(x, y) + o(W_2(\mu, \nu)) \right\}$$

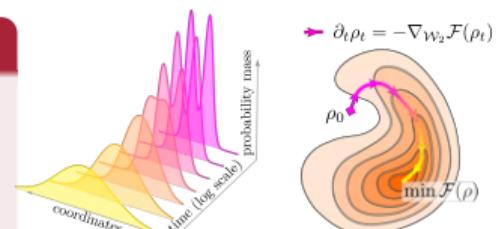
A curve $\gamma: (0, \infty) \rightarrow \mathcal{P}_2(\mathbb{R}^d)$ is *absolutely continuous* if \exists L^2 -Borel velocity field $v: \mathbb{R}^d \times (0, \infty) \rightarrow \mathbb{R}^d$ s.t.

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

DEFINITION (WASSERSTEIN GRADIENT FLOW)

A locally absolutely continuous curve $\gamma: (0, \infty) \rightarrow \mathcal{P}_2(\mathbb{R}^d)$ with velocity field $v_t \in T_{\gamma_t} \mathcal{P}_2(\mathbb{R}^d)$ is a *Wasserstein gradient flow with respect to* $\mathcal{F}: \mathcal{P}_2(\mathbb{R}^d) \rightarrow (-\infty, \infty]$ if

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



WASSERSTEIN GRADIENT FLOW WITH RESPECT TO $D_{f,\nu}^\lambda$

THEOREM (CONVEXITY AND GRADIENT OF $D_{f,\nu}^\lambda$ [NSSR24])

Since K is radial and smooth, $D_{f,\nu}^\lambda$ is M -convex along generalized geodesics with $M := -8\lambda^{-1}\sqrt{(d+2)\phi''(0)\phi(0)}$ and its (reduced) Fréchet subdifferential is $\partial D_{f,\nu}^\lambda(\mu) = \{\nabla \operatorname{argmax}(2)\}$.

Remark. M seems non-optimal, since for $\lambda \rightarrow 0$, $D_{f,\nu}^\lambda \rightarrow D_{f,\nu}$ and $D_{f,\nu}$ is 0-convex, but $M \rightarrow -\infty$.

COROLLARY

There exists a unique Wasserstein gradient flow $(\gamma_t)_{t>0}$ of $D_{f,\nu}^\lambda$ starting at $\mu_0 \in \mathcal{P}_2(\mathbb{R}^d)$, fulfilling the continuity equation $\partial_t \gamma_t = \nabla \cdot (\gamma_t(\partial D_{f,\nu}^\lambda(\gamma_t)))$, $\gamma_0 = \mu_0$.

LEMMA (PARTICLE FLOWS ARE W_2 GRADIENT FLOWS)

If μ_0 is empirical, then so is γ_t for all $t > 0$.

NUMERICAL EXPERIMENTS - PARTICLE DESCENT ALGORITHM

Take i.i.d. samples $(x_j^{(0)})_{j=1}^N \sim \mu_0$ and $(y_j)_{j=1}^M \sim \nu$. Forward Euler discretization in time with step size $\tau > 0$ yields

$$\gamma_{n+1} := (\text{id} - \tau \nabla \hat{p}_n)_\# \gamma_n, \quad \hat{p}_n = \text{argmax in } D_{f,\nu}^\lambda(\gamma_n)$$

so $(\gamma_n)_{n \in \mathbb{N}} = \frac{1}{N} \sum_{j=1}^N \delta_{x_j^{(n)}}$ with gradient step

$$x_j^{(n+1)} = x_j^{(n)} - \tau \nabla \hat{p}_n(x_j^{(n)}), \quad j \in \{1, \dots, N\}, n \in \mathbb{N}.$$

THEOREM (REPRESENTER-TYPE THEOREM [NSSR24])

If $f'_\infty = \infty$ or if $\lambda > 2d_K(\gamma_n, \nu) \sqrt{\phi(0)} \frac{1}{f'_\infty}$, then finding \hat{p}_n is a **finite-dimensional strongly convex** problem.

To find \hat{p}_n , we use **L-BFGS-B**, a quasi-Newton method. We use annealing strategy for λ if $f'_\infty < \infty$.

NUMERICAL EXPERIMENTS

FIG. 4: IMQ kernel, $\lambda = \frac{1}{100}$, $\tau = \frac{1}{1000}$, Top: Tsallis-3 divergence, Bottom: Tsallis- $\frac{1}{2}$ divergence, with annealing.

FIG. 5: Number of starting particles N , less than number of samples of target, $M \rightsquigarrow$ quantization

- **Non-differentiable** (e.g. Laplace = $\frac{1}{2}$ -Matérn) and unbounded (e.g. Riesz, Coulomb) kernels.
- **Convergence rates** in suitable metric.
- Prove consistency bounds [Leclerc, Mérigot, Santambrogio, Stra. 2020] and **better M -convexity estimates**.
- Convergence for annealing strategy?
- Different domains, e.g. compact subsets of \mathbb{R}^d (manifolds like sphere, torus), groups, infinite-dimensional spaces.
- Regularize other divergences, e.g. Rényi divergences, Bregman divergences.
- Gradient flow of $D_{f,\nu}^\lambda$ with respect to other metrics, like Kantorovich-Hellinger (related to unbalanced OT), MMD, Fisher-Rao or Wasserstein- p for $p \in [1, \infty]$.
- More elaborate time discretizations, variable step sizes.

- We created novel objective. Minimizing it allows sampling from a target measure of which only samples are known.
- Clear, rigorous interpretation using Convex Analysis and RKHS.
- Theory covers (almost) all f -divergences.
- Best of both worlds: $D_{f,\nu}^\lambda$ interpolates between $D_{f,\nu}$ and $d_K(\cdot, \nu)^2$.
- Effective algorithms due to (modified) representer theorem & GPU / PyTorch.

Thank you for your attention!

I am happy to take any questions.

Paper link: arxiv.org/abs/2402.04613

My website: viktorajstein.github.io

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Interpolating between OT and KL regularized OT using Rényi Divergences

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

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

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

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

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

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

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

W_2 gradient flows of $d_K(\cdot, \nu)^2$ with
 $K(x, y) := -|x - y|$ in 1D.

Reformulation as **maximal monotone** inclusion Cauchy problem in $L_2(0, 1)$ via **quantile functions**.

Comprehensive description of solutions' behavior, **instantaneous measure-to- L^∞ regularization**, implicit Euler is simple.