Metric extrapolation in the Wasserstein space

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L^2-Wasserstein geodesics

__W_2 geodesics__: $\nu_0, \nu_1 \in \mathcal{P}_2(\mathbb{R}^d)$, $\exists$ curve $\nu : [0,1] \to \mathcal{P}_2(\mathbb{R}^d)$:

$$\nu(0) = \nu_0, \quad \nu(1) = \nu_1, \quad W_2(\nu(t), \nu(s)) = |t-s| W_2(\nu_0, \nu_1)\,,$$

NB *constant speed, globally length-minimizing*

- ν_0 a.c., Brenier's thm: ∇u optimal transport map (u convex)

$$\nu(t) = ((1-t)\mathrm{Id} + t\nabla u)_{\#}\nu_0$$

- $s \mapsto \nu(s)$ length-min. up to $t > 1$ iff $\boxed{u(\cdot) - \frac{t-1}{t}\frac{|\cdot|^2}{2} \text{ convex}}$

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This talk: A variational (convex) notion of extrapolation

W_2 geodesic extrapolation

Extrapolation on a metric space (X, d): given $x_0, x_1 \in X$ and $t > 1$, find $x_t \in X$ solving

$$\inf_{x \in X} \left\{ \frac{d^2(x, x_1)}{2(t-1)} - \frac{d^2(x, x_0)}{2t} \right\}$$

NB. Since d is a distance, for all $x \in X$

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If $s \in [0, t] \mapsto x(s) \in X$ is a geodesic: $x_t = x(t)$ (inequality attained)

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W_2 **extrapolation**: given $\nu_0, \nu_1 \in \mathcal{P}_2(\mathbb{R}^d)$, find $\nu_t \in \mathcal{P}_2(\mathbb{R}^d)$ solving

$$(\mathcal{P}) \qquad \inf_{\mu} \left\{ \frac{W_2^2(\mu, \nu_1)}{2(t-1)} - \frac{W_2^2(\mu, \nu_0)}{2t} \right\}$$

Related works / motivation

- Case "$t = \infty$" on $\mathcal{P}(K)$, $K \subset \mathbb{R}^d$ compact [Carlier '07] $\rightarrow$ Toland duality

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- ($d = 1$), Solve for quantile function $F_\mu^{[-1]}$, $F_\mu(x) = \mu((-\infty, x])$
- *Sticky* pressureless fluids [Grenier, Brenier, ..] in $[0, t] \times \mathbb{R}$

$$\begin{cases} \partial_t \mu + \partial_x(\mu v) = 0\,, \\ \partial_t(\mu v) + \partial_x(\mu v^2) = 0\,, \end{cases} \qquad \mu(0) = \nu_0,\;\; v(0, x) = \partial_x u(x) - x.$$

Equivalent to a gradient flow [Natile, Savaré '09] on $[1, t] \times \mathbb{R}$

$$\mathcal{E}(t, \mu) = -\frac{W_2^2(\mu, \nu_0)}{2t}\,, \quad \mu(1) = \nu_1\,.$$

($d > 1$) "free flow sol. for almost all initial data" [Bianchini, Daneri '21]

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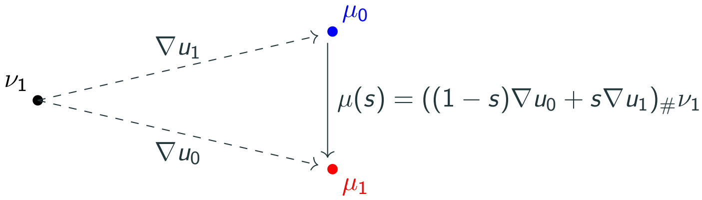
- Time discretization of W_2-gradient flows [Gallouët, N, Todeschi '23]; other variants [Turinici, Legendre '17], **BDF2** [Matthes, Plazotta '19], Runge Kutta [Han, Esedoglu, Garikipati '23]

Well-posedness/convexity

- $(\mathcal{P})$ not convex wrt linear interpolations $s \mapsto (1-s)\mu_0 + s\mu_1$
- Generalized geodesics:



- $+W_2^2(\cdot, \nu_1)$ is 2-convex along generalized geodesics based at ν_1 (*)
- $-W_2^2(\cdot, \nu_0)$ is (-2)-convex along any generalized geodesic

$$\mu \mapsto \frac{W_2^2(\mu, \nu_1)}{2(t-1)} - \frac{W_2^2(\mu, \nu_0)}{2t} \quad \text{is } \frac{1}{t(t-1)} - \text{convex along (*)}$$

$\Longrightarrow$ *existence and uniqueness minimizers*

Toland duality

Duality difference convex functions: Let V be a normed vector space, $F, G : V \to (\infty, \infty]$ convex, proper and lsc

$$\inf_{x \in V} \{F(x) - G(x)\} = \inf_{p \in V^*} \{G^*(p) - F^*(p)\}$$

In our case, F and G are given by

$$F : \mu \in \mathcal{P}_2(\mathbb{R}^d) \to \frac{W_2^2(\mu, \nu_1)}{2(t-1)} \quad \text{and} \quad G : \mu \in \mathcal{P}_2(\mathbb{R}^d) \to \frac{W_2^2(\mu, \nu_0)}{2t}$$

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Kantorovich duality:

$$\boxed{\frac{W_2^2(\mu, \nu_0)}{2t} = \sup_{\phi \in C_b} \langle \phi, \mu \rangle + \int \phi^{c_t} \mathrm{d}\nu_0}, \quad \phi^{c_t}(y) = \inf_x \frac{|x-y|^2}{2t} - \phi(x)\,.$$

$$F^*(\phi) = -\int \phi^{c_{t-1}} \mathrm{d}\nu_1\,, \quad G^*(\phi) = -\int \phi^{c_t} \mathrm{d}\nu_0$$

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$$(\mathcal{P}^*) \quad \inf \left\{ \int u^* \mathrm{d}\nu_1 + \int u \mathrm{d}\nu_0 \ : \ u - \frac{t-1}{t} \frac{|\cdot|^2}{2} \text{ is convex} \right\}$$

Equivalence with problem $(\mathcal{P})$:

$$(\mathcal{P}) = (\mathcal{P}^*) - \int \frac{|x|^2}{2} \mathrm{d}\nu_0(x) - \int \frac{|x|^2}{2} \mathrm{d}\nu_1(x)$$

Extrapolation via a balayage

Dual formulation

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- Requiring only convexity for $u \to$ Dual formulation of W_2
- Convex problem (as in [Carlier '07]) - Infimum is attainted
- Optimality conditions yield : $\overline{\nu}_0 := (\nabla u^*)_{\#}\nu_1$

$$\overline{\nu}_0 \preceq_C \nu_0 \quad \text{i.e.} \quad \int \varphi \mathrm{d}\overline{\nu}_0 \leq \int \varphi \mathrm{d}\nu_0 \,, \quad \forall \varphi \text{ convex}$$

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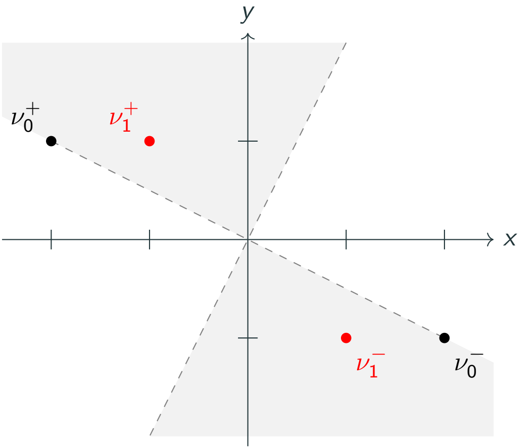
Link between minimizers

$$\nu_t \text{ solves } (\mathcal{P}) \iff \nu_t = [\nabla u^* + t(\mathrm{Id} - \nabla u^*)]_{\#}\nu_1 \,, \; u \text{ solves } (\mathcal{P}^*)$$

$$\text{NB. If } \overline{\nu}_0 \text{ a.c.,} \quad \nu_t = [\underbrace{\mathrm{Id} + t(\nabla u - \mathrm{Id})}_{\text{optimal transport map}}]_{\#}\overline{\nu}_0$$

An explicit solution



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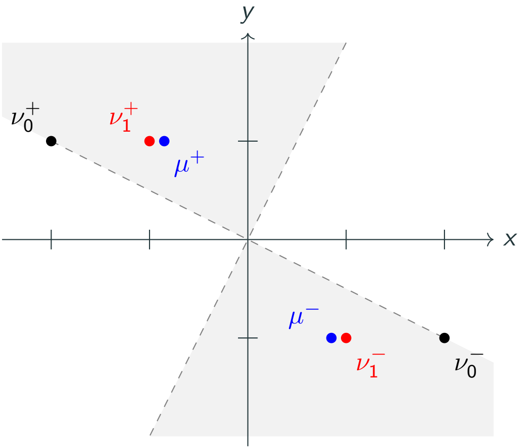

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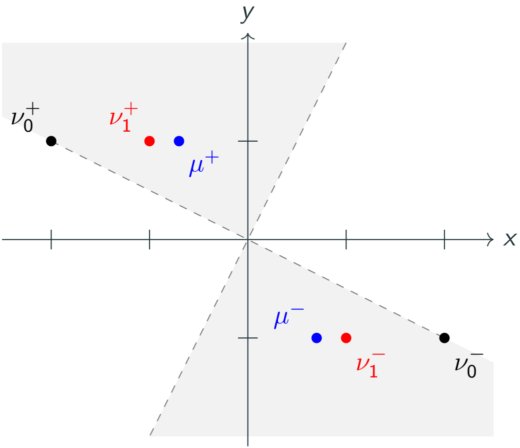

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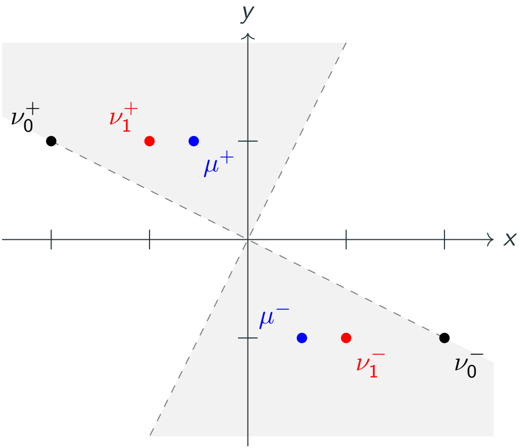

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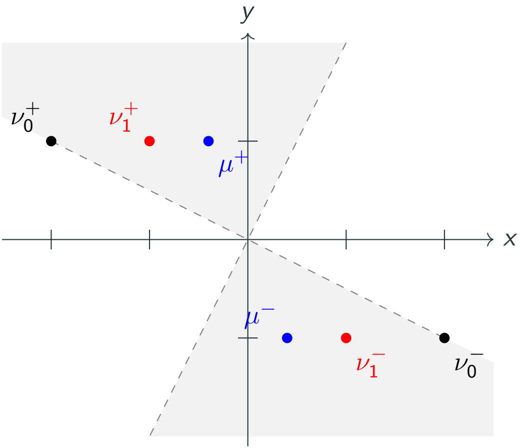

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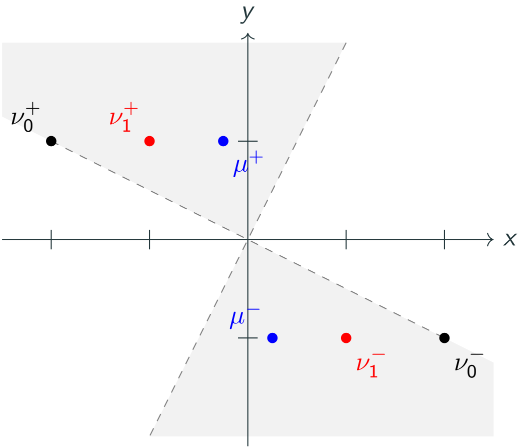

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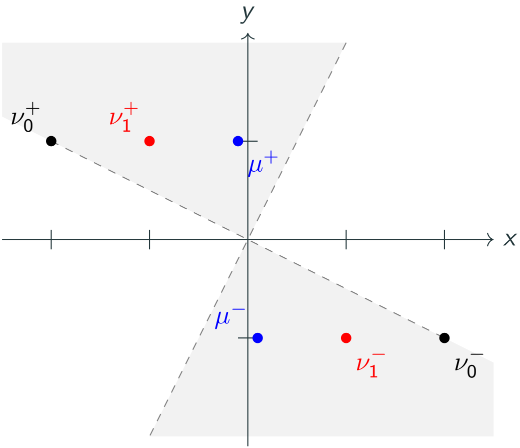

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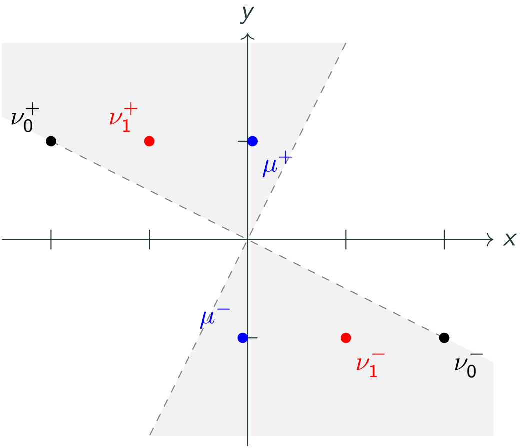

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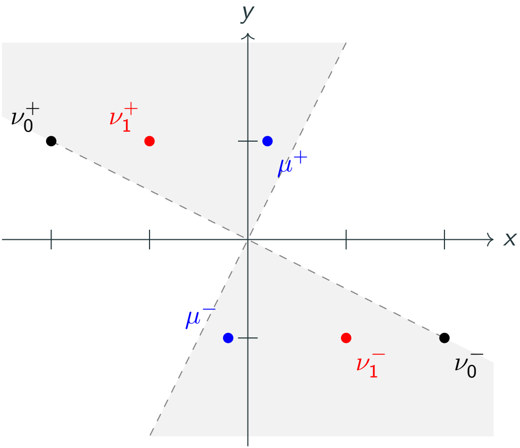

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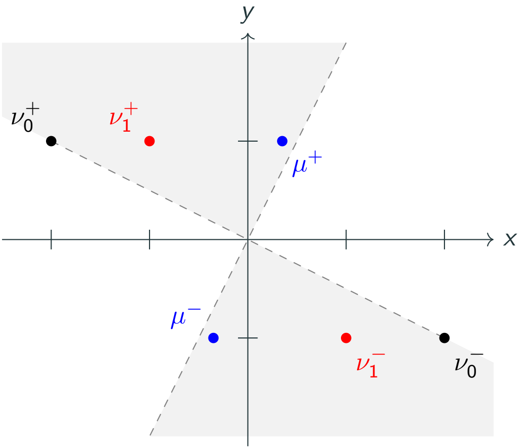

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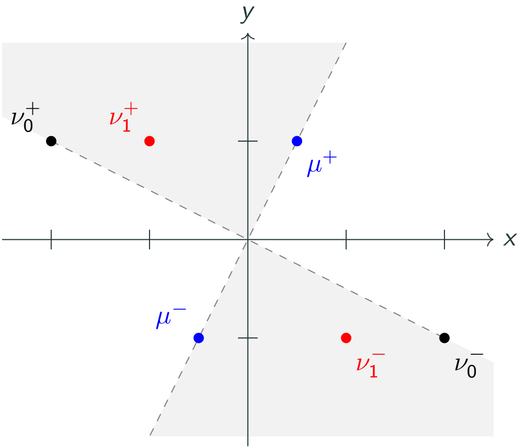

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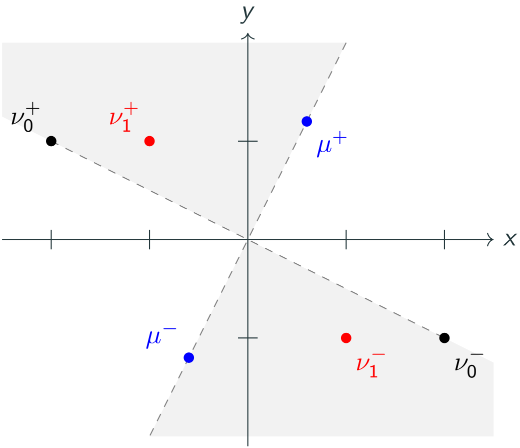

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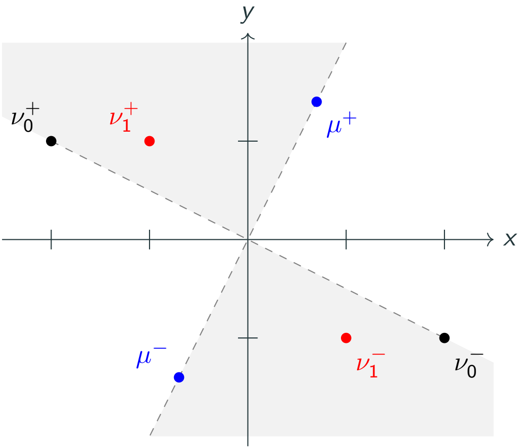

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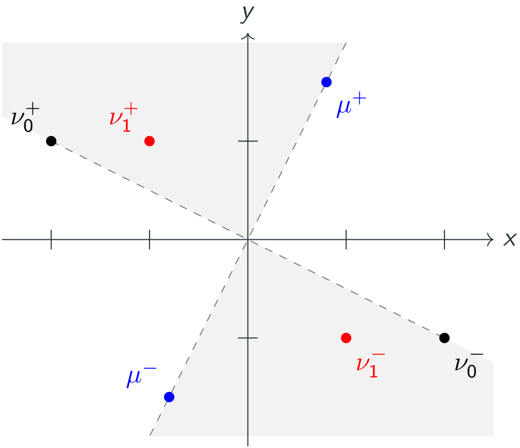

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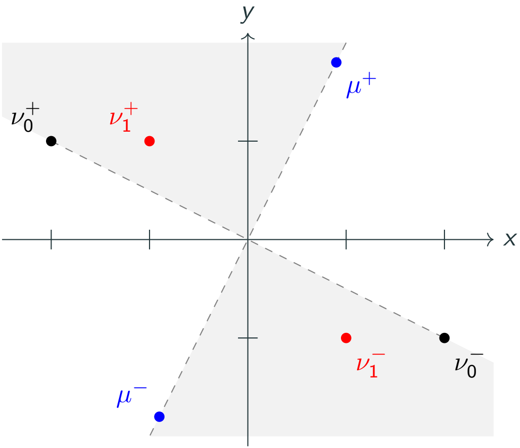

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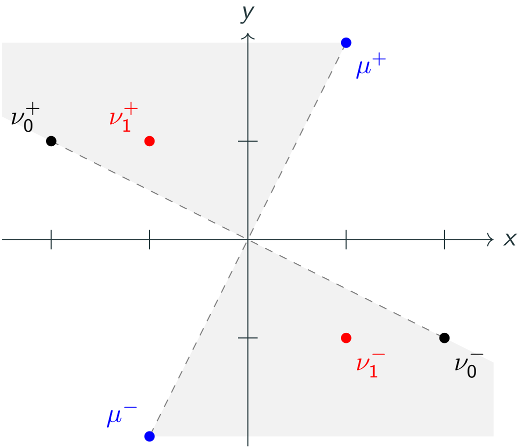

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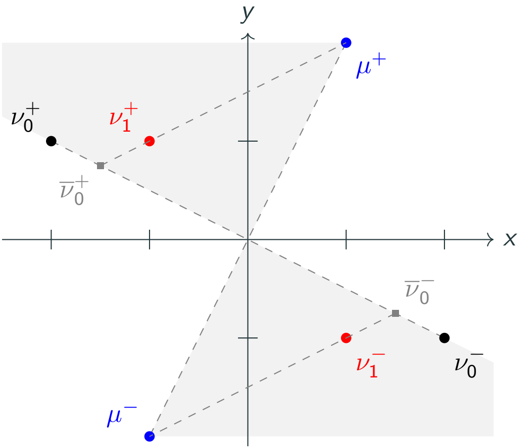

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Barycentric formulation

$$(\mathcal{B}) \quad \inf_{\gamma \in \Gamma(\nu_0, \nu_1)} \int |t x_1 - (t-1)\mathrm{bary}(\gamma_{x_1})|^2 \mathrm{d}\nu_1(x_1)$$

where $\mathrm{d}\gamma(x_0, x_1) = \mathrm{d}\gamma_{x_1}(x_0)\mathrm{d}\nu_1(x_1)\,, \quad \mathrm{bary}(\gamma_{x_1}) \coloneqq \int x_0 \mathrm{d}\gamma_{x_1}(x_0)$

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We look for η in the form $\boxed{\mathrm{d}\eta(x_0,x_1,x) = \mathrm{d}\gamma_{x_1}(x_0)\mathrm{d}\pi(x_1,x)}$,

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with $\gamma \in \Gamma(\nu_0,\nu_1)\,, \quad \mathrm{d}\gamma(x_0,x_1) = \mathrm{d}\gamma_{x_1}(x_0)\mathrm{d}\nu_1(x_1)$

$$(\mathcal{P}) \geq \sup_{\gamma\in\Gamma(\nu_0,\nu_1)} \inf_{\pi\in\Gamma(\nu_1,\mu)} \int \underbrace{\left[\frac{|x-x_1|^2}{2(t-1)} - \int \frac{|x-x_0|^2}{2t} \mathrm{d}\gamma_{x_1}(x_0) \right]}_{F(x,x_1,\gamma_{x_1})} \mathrm{d}\pi(x_1,x)$$

$$\geq \sup_{\gamma\in\Gamma(\nu_0,\nu_1)} \int \min_x F(x,x_1,\gamma_{x_1}) \mathrm{d}\nu_1(x_1)$$

Barycentric formulation

$$(\mathcal{B}) \qquad \inf_{\gamma \in \Gamma(\nu_0, \nu_1)} \int |t x_1 - (t-1)\mathrm{bary}(\gamma_{x_1})|^2 \mathrm{d}\nu_1(x_1)$$

where $\mathrm{d}\gamma(x_0, x_1) = \mathrm{d}\gamma_{x_1}(x_0)\mathrm{d}\nu_1(x_1)\,, \quad \mathrm{bary}(\gamma_{x_1}) := \int x_0 \mathrm{d}\gamma_{x_1}(x_0)$

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- Instance of WOT; "$t \to \infty$" [Gozlan et al '17][Gozlan, Juillet '20]

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- Equivalence with difference of optimal transport costs:

$$(\mathcal{P}) = -\frac{1}{t(t-1)}(\mathcal{B}) + \frac{1}{2(t-1)} \int |x|^2 \mathrm{d}\nu_1(x) - \frac{1}{2t} \int |x|^2 \mathrm{d}\nu_0(x)$$

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- ν_1 a.c., u solves $(\mathcal{P}^*)$, $\exists$ coupling $\theta \in \Gamma(\overline{\nu}_0, \nu_0)$ (law of a martingale)

$$\mathrm{d}\theta(x,y) = \mathrm{d}\theta_x(y)\mathrm{d}\overline{\nu}_0(x)\,, \quad \int y \mathrm{d}\theta_x(y) = x \quad \overline{\nu}_0\text{-a.e.}$$

$$\boxed{\mathrm{d}\gamma(x_0,x_1) = \mathrm{d}\theta_{\nabla u^*(x_1)}(x_0)\mathrm{d}\nu_1(x_1) \quad \text{solves } (\mathcal{B})}$$

A numerical scheme

$$\inf_{\gamma\in\Gamma(\nu_0,\nu_1)} \int \left[\sup_{Z\in\mathbb{R}^d} \int c(Z;x_0,x_1)\mathrm{d}\gamma_{x_1}(x_0) \right] \mathrm{d}\nu_1(x_1) + \varepsilon KL(\gamma|\nu_0\otimes\nu_1)$$

NB. Without regularization $Z(x_1)$ is the optimal transport map from ν_1 to ν_t

A two-step algorithm (*on point clouds*): Given ϕ^0, ψ^0, z^0, for $n \geq 0$

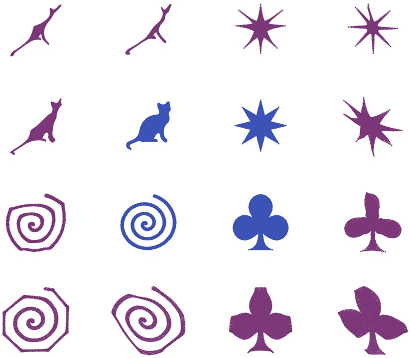
1. Compute ϕ^{n+1}, ψ^{n+1} by maximization (1 Sinkhorn cycle)
2. $Z^{n+1}(x_1) = Z^n(x_1) + \tau \int \partial_Z c(Z^n(x_1);x_0,x_1)\mathrm{d}\pi^{n+1}_{x_1}(x_0)$

- First order convergence as for Sinkhorn (see SISTA, [Carlier et al '20])

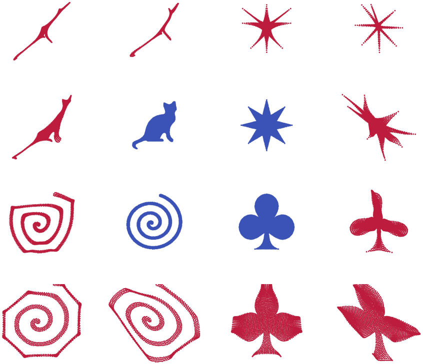
$$f(y^{n+1}) - f(y^*) \leq \eta(f(y^n) - f(y^*)), \quad \eta \leq \frac{1}{1 + C_1\exp(-C_2/\varepsilon)}$$

- Gradient step restriction: $\tau \leq K\varepsilon$ ($K = \mathcal{O}(1)$ explicit).

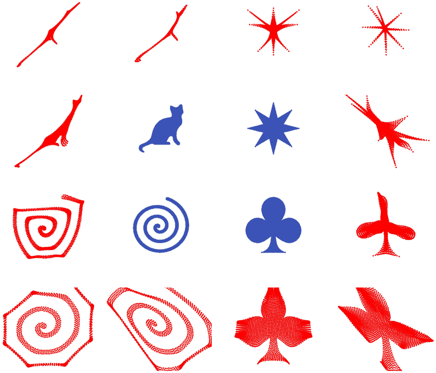
Going further...



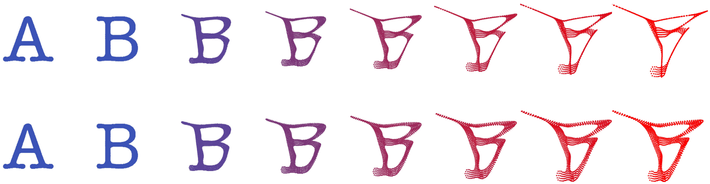
Going further...and further...



Going further...and further...and further...



Gradient flow of $-W_2^2$



Gradient flow (top) vs **Metric extrapolation** (bottom)

BDF2 scheme for W_2-gradient flows

- Let $\Omega \subset \mathbb{R}^d$ convex, $\mathcal{E}(\rho) : \mathcal{P}_2(\Omega) \to \mathbb{R} \cup \{\infty\}$ convex, lsc
- We construct a $\mathcal{O}(\tau^2)$ discretization of "$\partial_t \rho = -\nabla_{W_2} \mathcal{E}(\rho)$"

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Time discretization. Given $\rho_0, \rho_1 \in \mathcal{P}_2(\Omega)$,

$$\begin{cases} \rho^e_{n-1} = E_\alpha(\rho_{n-2}, \rho_{n-1}) \\ \rho_n \in \underset{\rho \in \mathcal{P}_2(\Omega)}{\operatorname{argmin}} \dfrac{W_2^2(\rho, \rho^e_{n-1})}{2(2-\alpha)\tau} + \mathcal{E}(\rho) \end{cases} \qquad \text{for } n \geq 2$$

NB. $\alpha = 4/3$ to get $\mathcal{O}(\tau^3)$ consistency for an ODE

Theorem. *For the metric extrap., $\mathcal{E}$ λ-convex along gen. geod., $\lambda > 0$, piecewise constant reconstruction $t \mapsto \rho_\tau(t)$ converges in W_2 to an a.c. curve $t \mapsto \rho(t)$ s.t. $\rho(0) = \rho_0$, and satisfying (EVI).*

Some more remarks

- **General costs**: $c : X \times X \to \mathbb{R}$ (*non-negative cross curvature*)
- **Multiple measures**: $\nu_i^+, \nu_j^- \in \mathcal{P}_2(\mathbb{R}^d)$, $\lambda_i^+, \lambda_j^- > 0$, $\sum_i \lambda_i^+ = \sum_i \lambda_j^-$

$$\inf_{\mu} \left\{ \sum_i \lambda_i^+ W_2^2(\mu, \nu_i^+) - \sum_j \lambda_j^- W_2^2(\mu, \nu_j^-) \right\}$$

  For only one positive coefficient $\rightsquigarrow$ multi-marginal WOT
- **Applications**: higher order JKO, reduced order models [Dalery et al 23]

Thank you!