Gradient Flows in the Geometry of the Sinkhorn Divergence

Mathis Hardion

10/10/2024

Introduction

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as $\tau \to 0$: ?? $\to$ **We derive the equation, analyze its structure and properties.**

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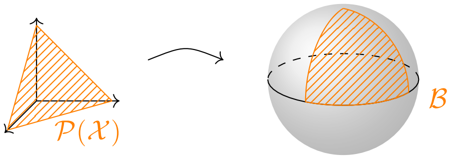
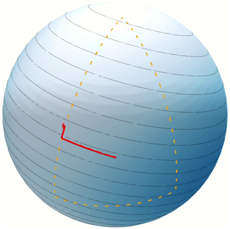
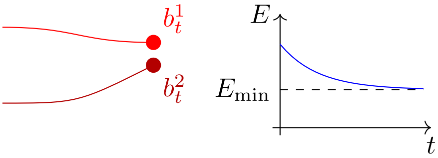


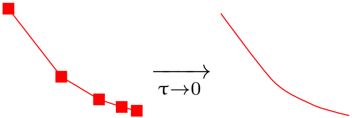
1. The Riemannian Geometry of S_ε



2. The equation and its structure



3. Well posedness and properties



4. Convergence of the SJKO scheme

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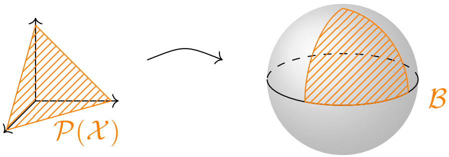

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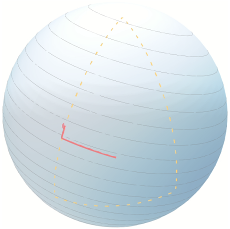

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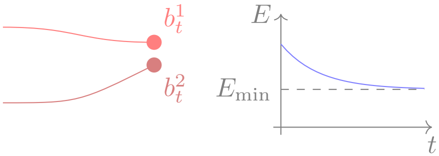

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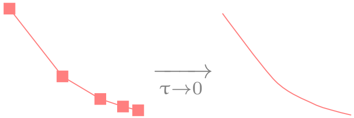

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Lavenant, Luckhardt, Mordant, Schmitzer, Tamanini. The Riemannian geometry of Sinkhorn divergences. (2024)

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↳ $\mathcal{H}_\mu$ depends on $\mu \implies$ change of variables

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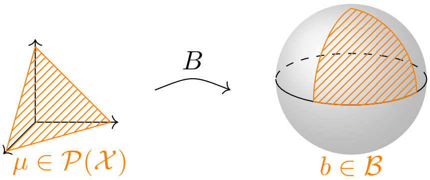

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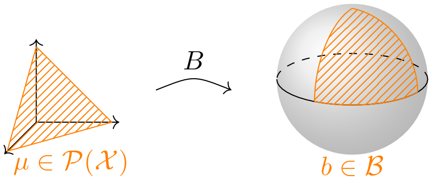

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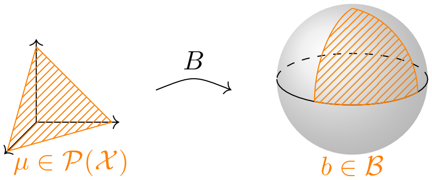

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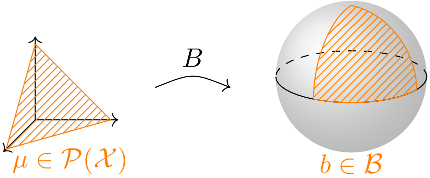

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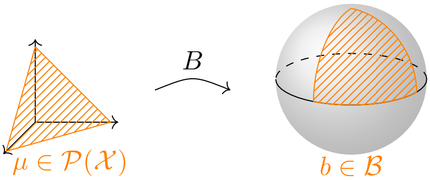

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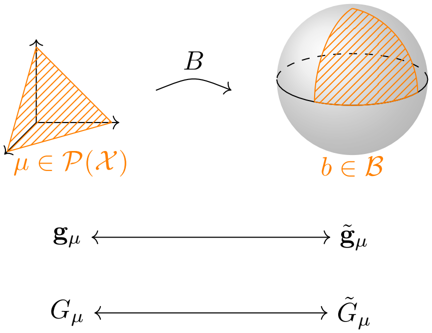
$$B(\mu) := H_c \left[\exp\left(\frac{f_\mu}{\varepsilon}\right)\mu\right] = \exp\left(-\frac{f_\mu}{\varepsilon}\right).$$

Theorem. *The map B is a homeomorphism onto its image*

$$\mathcal{B} := \boxed{H_c\left[\mathcal{M}_+(\mathcal{X})\right]} \cap \boxed{\left\{b \in \mathcal{H}_c \;\middle|\; \|b\|_{\mathcal{H}_c} = 1\right\}}$$

$\mu \geq 0$ $\qquad$ $\langle \mu, 1\rangle = 1$



Admissible paths: $(b_t)_t \in \mathscr{H}^1([0,1], \mathcal{H}_c)$ valued in $\mathcal{B}$.

Feydy, Séjourné, Vialard, Amari, Trouvé, Peyré. Interpolating between Optimal Transport and MMD using Sinkhorn Divergences. (2019)
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Change of variables

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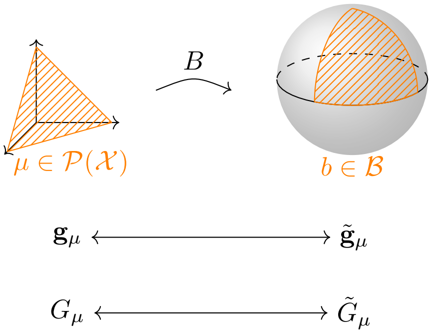

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Geodesic distance d_S defined by minimizing $\displaystyle\int_0^1 \tilde{\mathbf{g}}_{\mu_t}\left(\dot{b}_t, \dot{b}_t\right) dt$ over admissible paths.

Feydy, Séjourné, Vialard, Amari, Trouvé, Peyré. Interpolating between Optimal Transport and MMD using Sinkhorn Divergences. (2019)

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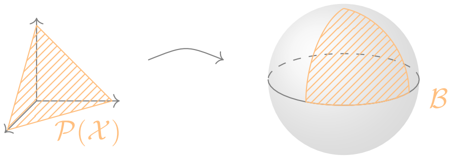
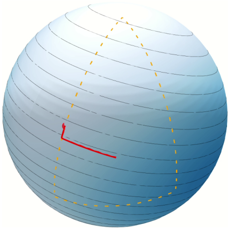
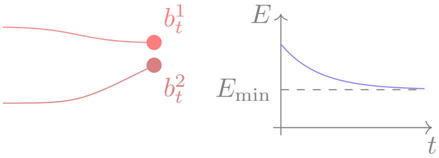
Plan



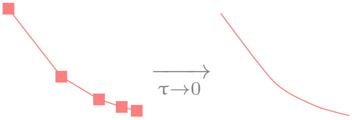
1. The Riemannian Geometry of S_ε



2. The equation and its structure



3. Well posedness and properties



4. Convergence of the SJKO scheme

Derivation of the equation

$$\mu_{k+1}^{\tau} \in \underset{\mu \in \mathcal{P}(\mathcal{X})}{\arg\min} \, \langle \mu, V \rangle + \frac{1}{2\tau} S_{\varepsilon}(\mu, \mu_k^{\tau})$$

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Intuitively: asymptotic equivalence with

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1st order conditions + formal limit:

$$\begin{cases} G_{\mu_t}[\dot{\mu}_t] + V + p_t = 0 \\ p_t \leq 0 \\ \langle \mu_t, p_t \rangle = 0 \\ \mu_t \in \mathcal{P}(\mathcal{X}) \end{cases}$$

Gradient flow of $\mu \mapsto \langle \mu, V \rangle$

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embedding in $\mathcal{B}$

Gradient flow of $\mu \mapsto \langle \mu, V \rangle$ $\longrightarrow$ Gradient flow of $b \mapsto \langle b, Vb \rangle_{\mathcal{H}_c}$

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Structure of the equation

Sinkhorn Potential Flow:

$$(b_t)_t \in \mathscr{H}^1([0,+\infty), \mathcal{H}_c), \begin{cases} \tilde{G}_{\mu_t}\dot{b}_t + (V+V^*)b_t + p_t = 0 \\ p_t \leq 0 \\ \langle H_c^{-1} b_t, p_t \rangle = 0 \\ b_t \in \mathcal{B} \end{cases}$$

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the set of ***pressure vectors*** *at b.*

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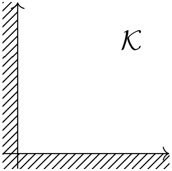

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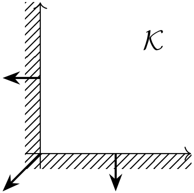

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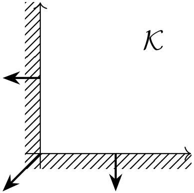

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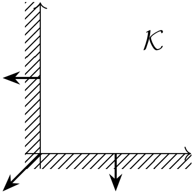

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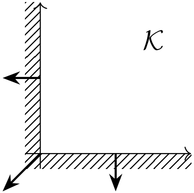

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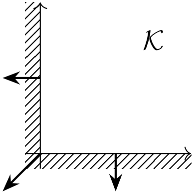

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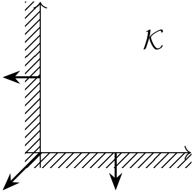

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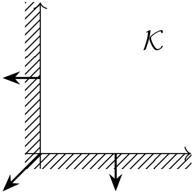

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Antisymmetric: generates rotational motion!

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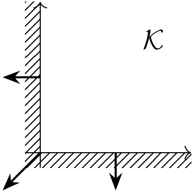

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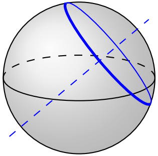

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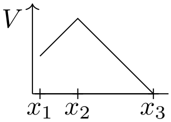
Numerics on the 3-point space

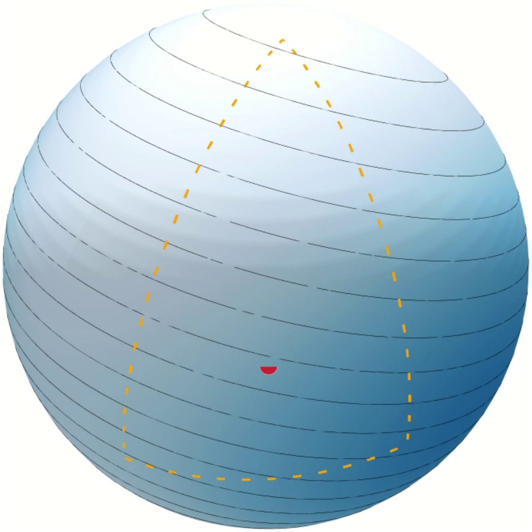


Boundary of $\mathcal{B}$

Theoretical rotation lines

SJKO Flow (embedded)

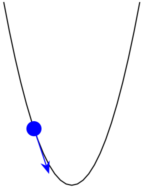
Potential energy $\langle H_c^{-1} b, V b \rangle$



Flow of a Dirac mass

Proposition. *If* $(x_t)_t \subset \mathcal{X}$ *is a smooth trajectory and* $b_t = B(\delta_{x_t})$ *then*

$$\dot{b}_t + \mathbf{W} b_t + \mathfrak{P} b_t \ni 0 \iff \dot{x}_t \in -\partial V(x_t).$$



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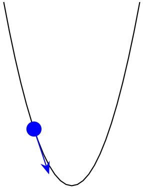
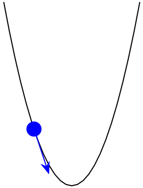


PROOF: Direct computations.

Flow of a Dirac mass

Proposition. *If* $(x_t)_t \subset \mathcal{X}$ *is a smooth trajectory and* $b_t = B(\delta_{x_t})$ *then*

$$\dot{b}_t + \mathbf{W} b_t + \mathfrak{P} b_t \ni 0 \iff \dot{x}_t \in -\partial V(x_t).$$



Proof: Direct computations.

Corollary. *For* V *convex and any* $x_0 \in \mathcal{X}$, *the Sinkhorn potential flow starting at* $b_0 = B(\delta_{x_0})$ *is given by* $B(\delta_{x_t})$ *with* $(x_t)_t$ *the subgradient flow of* V.

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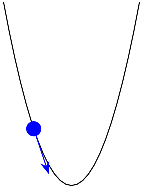

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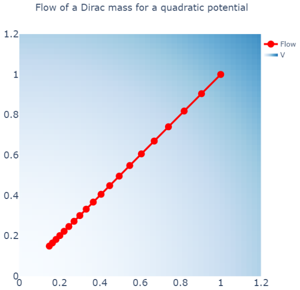
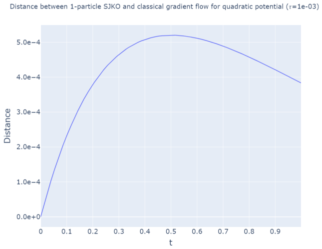
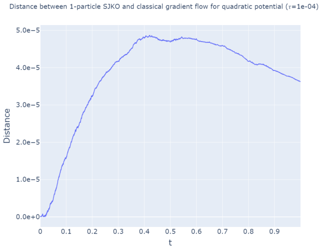
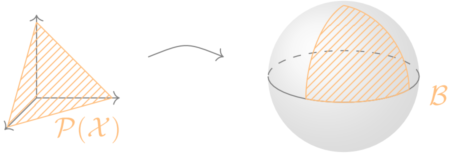






Plan



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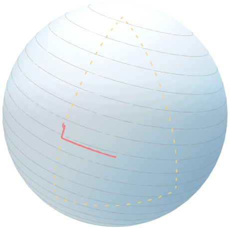

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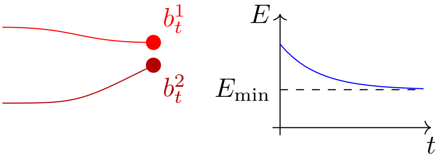

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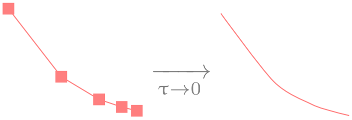

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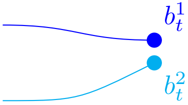

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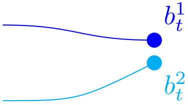
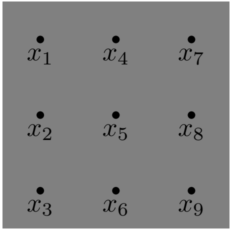


Sketch of proof: Discretize the space to utilize the structure of $\mathcal{H}_c$:

For $\mathcal{X} = \{x_1, \ldots, x_n\}$, $\mathcal{C}(\mathcal{X}) = \mathcal{H}_c = \mathbb{R}^n$



$\mathcal{X}$

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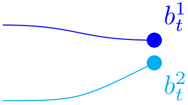

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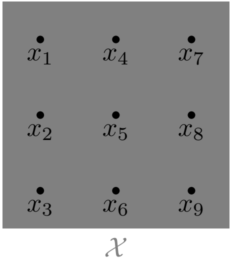

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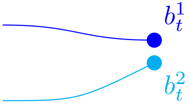

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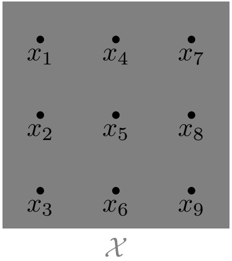

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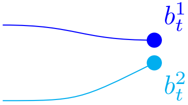

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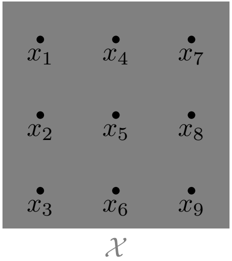

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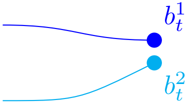

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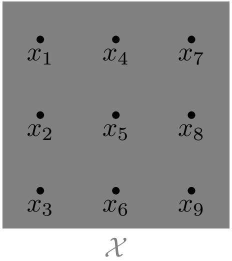

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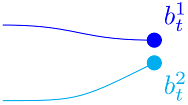

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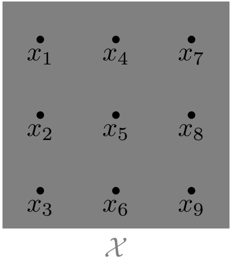

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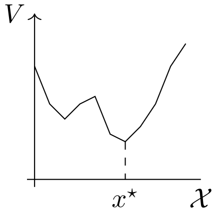

Theorem. *Assume V has a unique minimizer $x^\star$ on $\mathcal{X}$. Then,*

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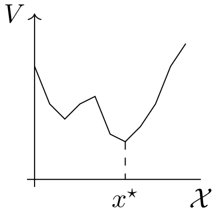

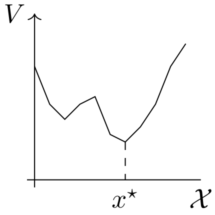

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Asymptotics

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- $\mathcal{B}$ compact $\implies$ convergent subsequences exist
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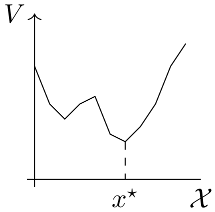

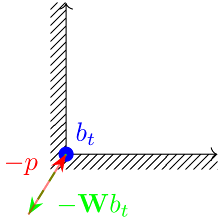

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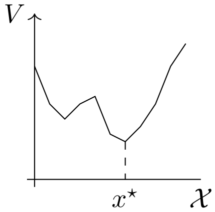

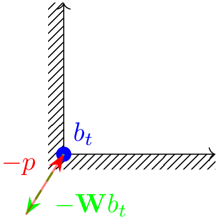

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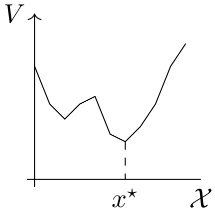

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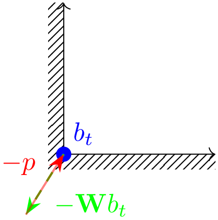
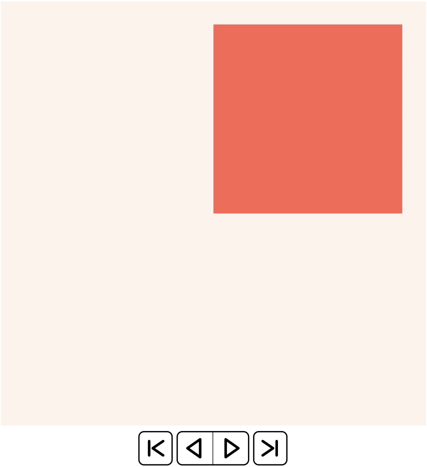
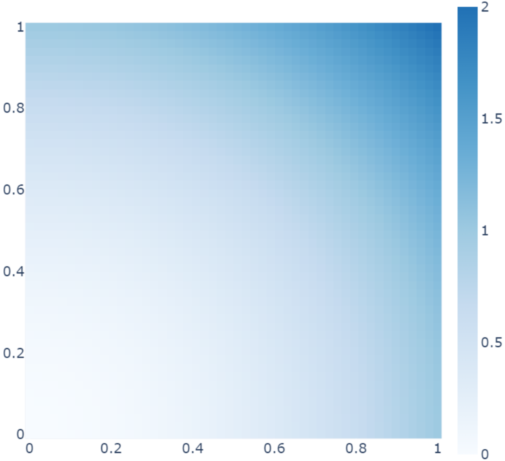


Because vertical perturbations are admissible for Sinkhorn!

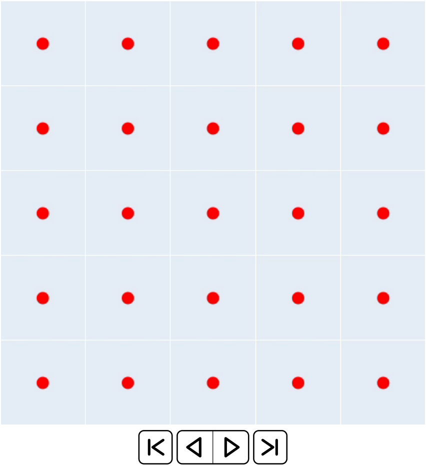


Sinkhorn flow ($\varepsilon = 0.2$)



V

Some numerics



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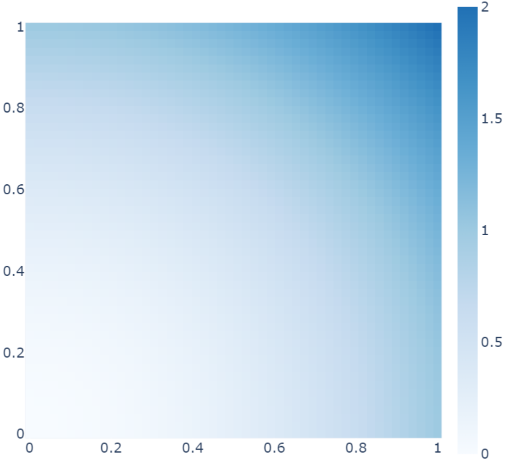

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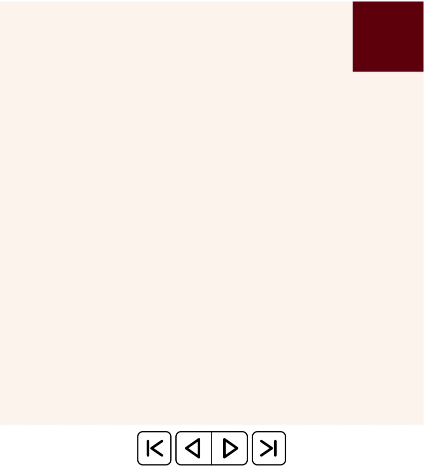
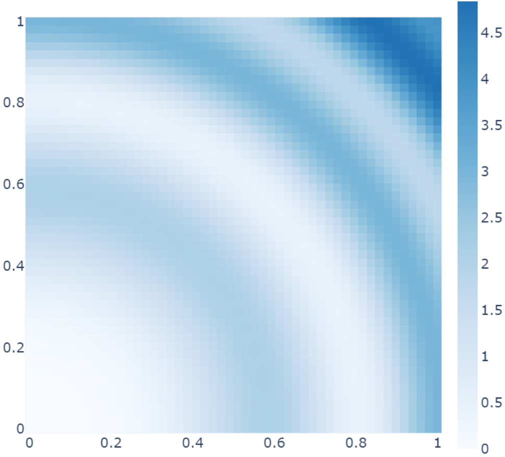


Sinkhorn flow ($\varepsilon = 5$)



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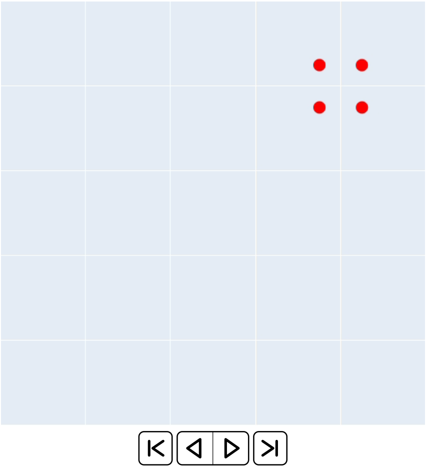

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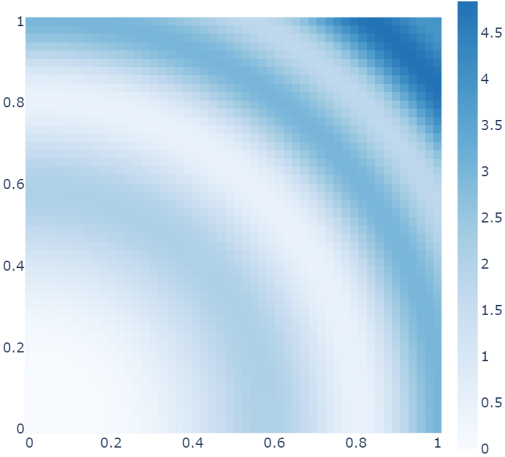
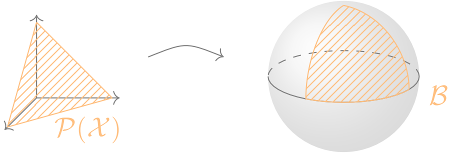


V

Plan



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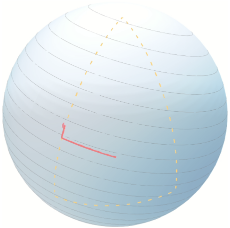

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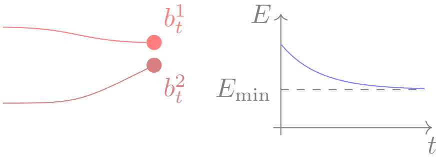

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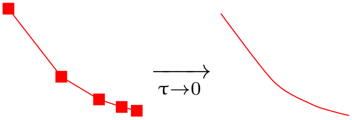

4. Convergence of the SJKO scheme

Limit of the SJKO scheme as $\tau \to 0$ (finite $\mathcal{X}$)

Theorem. *On a finite space, with $(b_k^\tau)_k$ given by the SJKO scheme after embedding, $\left(\bar{b}_t^\tau\right)_t$ the piecewise constant interpolation, $(b_t^\tau)_t$ the piecewise geodesic interpolation, then*

$$b^\tau, \bar{b}^\tau \xrightarrow[\tau \to 0]{} b \text{ uniformly on } [0, T]$$

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- Classical estimates and compactness yields a limit

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Theorem. *On a finite space, with $(b_k^\tau)_k$ given by the SJKO scheme after embedding, $\left(\bar{b}_t^\tau\right)_t$ the piecewise constant interpolation, $(b_t^\tau)_t$ the piecewise geodesic interpolation, then*

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Hope:

$$\begin{array}{ccc} \mathrm{SJKO}_n & \xrightarrow[\tau \to 0]{} & \mathrm{Flow}_n \\ & & \downarrow n \to \infty \\ & & \mathrm{Flow} \end{array}$$

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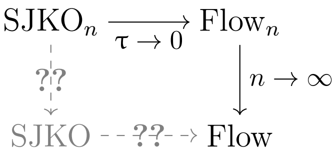

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Thank you for listening!

Appendix

Challenges in the general case

$$\frac{\partial f_{t,s}}{\partial s} = -\varepsilon \left(\mathrm{Id} - K_{t,s} K_{s,t}\right)^{-1} H_{t,s}\left[\dot{\mu}_s\right]$$

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$$\frac{\partial f_{t,s}}{\partial s} = -\varepsilon \left(\mathrm{Id} - K_{t,s}K_{s,t}\right)^{-1} H_{t,s} \boxed{\dot{\mu}_s} \in \mathcal{H}^*_{\mu_s,0}$$

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$$\mathcal{H}^*_{\mu_t,\mu_s} \to \mathcal{H}_{\mu_t,\mu_s}$$

$$\text{where } \mathcal{H}_{\mu,\nu} := \exp\left(\frac{f_{\mu,\nu}}{\varepsilon}\right)\mathcal{H}_c$$

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But generally speaking $\mathcal{H}^*_{\mu_s,0} \not\subset \mathcal{H}^*_{\mu_t,\mu_s}$!

$$\mathcal{H}^*_{\mu_t,\mu_s} \to \mathcal{H}_{\mu_t,\mu_s}$$

where $\mathcal{H}_{\mu,\nu} \coloneqq \exp\left(\frac{f_{\mu,\nu}}{\varepsilon}\right)\mathcal{H}_c$

Finite space case

Theorem. *On a finite space, the differential inclusion*

$$\begin{cases} \dot{b}_t + \mathbf{W} b_t + p_t = 0 \\ p_t \in \partial \iota_{\mathcal{K}}(b_t) \\ b_t \in \mathcal{B} \end{cases}$$

has a solution that additionally verifies

(a) $p_t = \underset{p \in \partial \iota_{\mathcal{K}}(b_t)}{\arg\min} \|\mathbf{W} b_t + p\|_{\mathcal{H}_c}$

(b) $\frac{d}{dt} E(b_t) = -\tilde{\mathbf{g}}_{\mu_t}\left(\dot{b}_t, \dot{b}_t\right) \implies \begin{cases} (E(b_t))_t \text{ decreases} \\ \int_0^T \left\|\dot{b}_t\right\|_{\mathcal{H}_c}^2 dt \text{ bounded} \end{cases}$

(c) $\left\|\dot{b}_t\right\|_{\mathcal{H}_c}$ *decreases.*

The flow is contractive.