# Gradient flows in the geometry of Sinkhorn divergences

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# Joint work with

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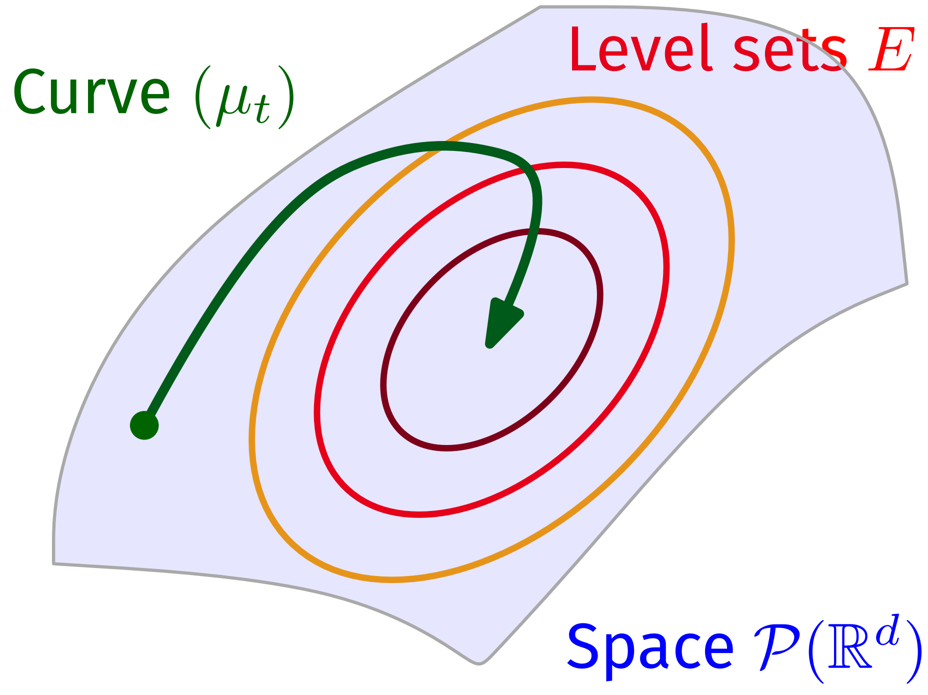
Lavenant, Luckhardt, Mordant, Schmitzer, Tamanini (2024). The Riemannian geometry of Sinkhorn divergences.
Hardion (2024). Master thesis: Gradient Flows in the Geometry of the Sinkhorn Divergence.

# Wasserstein gradient flows

$E : \mathcal{P}(\mathbb{R}^d) \to [0, +\infty]$ and $\mu_0 \in \mathcal{P}(\mathbb{R}^d)$ generate a curve $(\mu_t)_{t \geq 0}$ of **steepest descent** with respect to Wasserstein geometry.




## Examples

- $E(\mu) = \int V \, \mathrm{d}\mu$ gives the **transport equation**

$$\partial_t \mu = \mathrm{div}(\mu \nabla V).$$

- $E(\mu) = \int \mu \log \mu$ gives the **heat equation**

$$\partial_t \mu = \Delta \mu.$$

Jordan, Kinderlehrer, Otto (1998). The variational formulation of the Fokker–Planck equation.

# Wasserstein gradient flows

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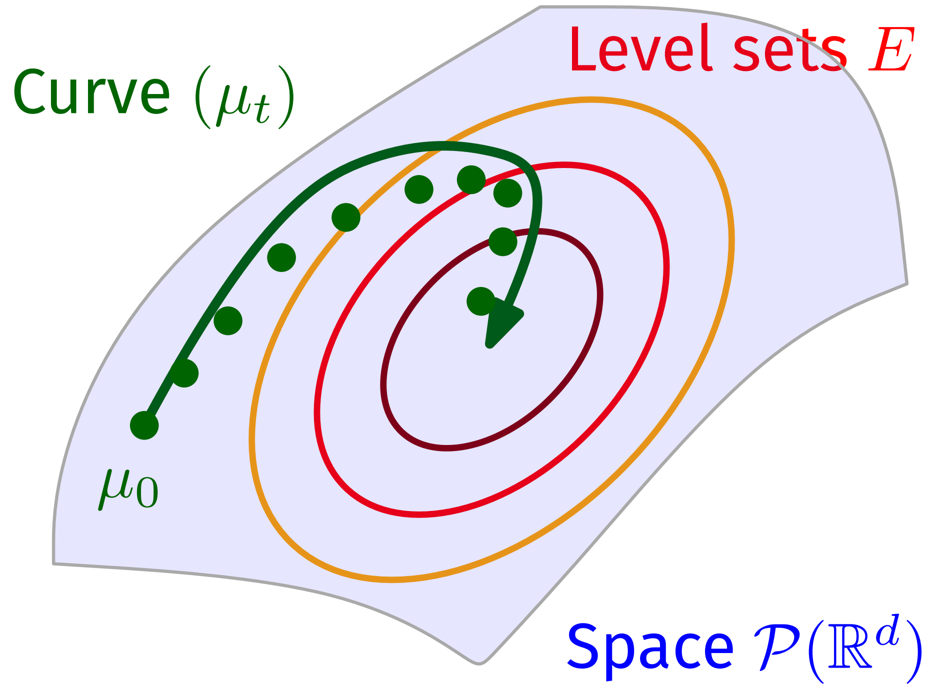



**Recall**

$$\mathrm{OT}(\mu, \nu) = \min_{\pi \in \Pi(\mu,\nu)} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |x - y|^2 \, \mathrm{d}\pi(x, y)$$

Subset of $\mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d)$, coupling between $\mu$ and $\nu$

**JKO/minimizing movement scheme.** For $\tau > 0$, define, for $k \geq 0$,

$$\mu_{k+1}^\tau \in \arg\min_{\mu} \; E(\mu) + \frac{\mathrm{OT}(\mu, \mu_k^\tau)}{2\tau}$$

Then $\mu_k^\tau \simeq \mu_{k\tau}$ as $\tau \to 0$.

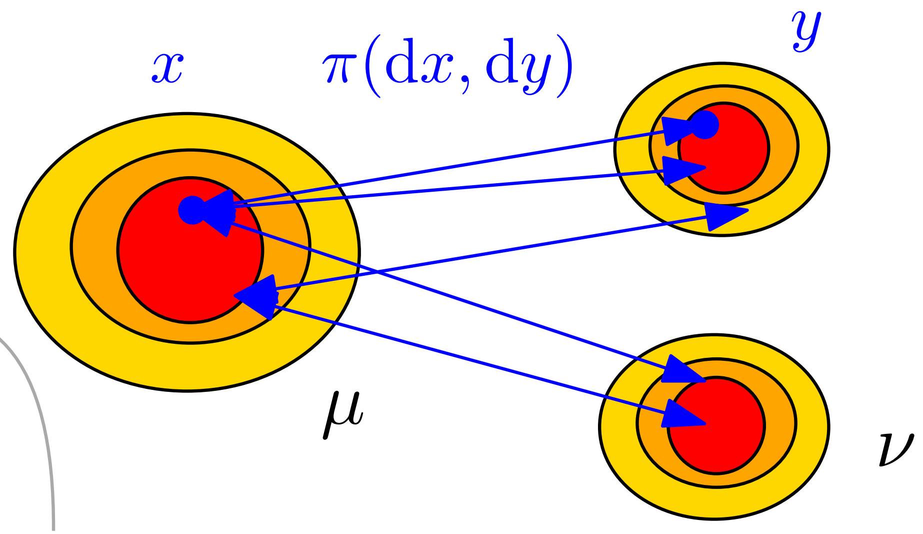
Jordan, Kinderlehrer, Otto (1998). The variational formulation of the Fokker–Planck equation.

# With entropic optimal transport?

$(X, d)$ compact metric space with symmetric cost function $c$, and $\varepsilon > 0$.

**Definition**

$$\mathrm{OT}_\varepsilon(\mu,\nu) = \min_{\pi \in \Pi(\mu,\nu)} \iint_{X \times X} c(x,y)\,\mathrm{d}\pi(x,y) + \varepsilon \mathrm{KL}(\pi | \mu \otimes \nu)$$




Kullback-Leibler divergence, a.k.a relative entropy

**Why?**

1. easier to compute (**Sinkhorn algorithm**),
2. better statistical complexity,
3. smoother dependence in $(\mu, \nu)$.

Peyré & Cuturi (2018). Computational Optimal Transport.

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If $c$ quadratic cost on $\mathbb{R}^d$, **Entropic JKO scheme:**

$$\mu_{k+1}^\tau \in \arg\min_\mu \; E(\mu) + \frac{\mathrm{OT}_\varepsilon(\mu,\mu_k^\tau)}{2\tau}$$

Peyré (2015). Entropic approximation of Wasserstein gradient flows.

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Conforti & Tamanini (2021). A formula for the time derivative of the entropic cost and applications.

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- $\varepsilon \ll \tau$: convergence to the Wasserstein GF of $E$.
- $\varepsilon \sim \tau$: convergence to a new flow.
- $\varepsilon \gg \tau$: the bias dominates, no evolution.

Conforti & Tamanini (2021). A formula for the time derivative of the entropic cost and applications.
Carlier, Duval, Peyré, Schmitzer (2017). Convergence of entropic schemes for optimal transport and gradient flows.
Baradat, Hraivoronska, Santambrogio (2024+). Using Sinkhorn in JKO adds diffusion in the limiting PDE.

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**Today: I will keep $\varepsilon$ fixed.**

# Using Sinkhorn divergences

As $\mathrm{OT}_\varepsilon(\mu, \mu) > 0$, **debias** by defining **Sinkhorn divergence**

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

Genevay, Peyré, & Cuturi (2018). Learning generative models with Sinkhorn divergences.

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Assumption until the end of the talk

**Theorem** Assume $\exp(-c/\varepsilon)$ positive definite universal kernel.

1. $S_\varepsilon(\mu,\nu) \geq 0$ with equality iff $\mu = \nu$, and $S_\varepsilon$ "metrizes" weak convergence.
2. $S_\varepsilon$ convex in each of its inputs.

but $\sqrt{S_\varepsilon}$ not a distance

Genevay, Peyré, & Cuturi (2018). Learning generative models with Sinkhorn divergences.
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If $\quad S_\varepsilon(\mu_t,\mu_{t+\tau}) \sim \tau^2 \mathbf{g}_{\mu_t}(\dot\mu_t,\dot\mu_t)$,

we expect the equation when $\tau \to 0$:

$$\dot\mu_t \in \arg\min_\sigma \; DE(\mu_t)[\sigma] + \frac{\mathbf{g}_{\mu_t}(\sigma,\sigma)}{2}.$$

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**Metric tensor** $\mathbf{g}_\mu(\dot\mu,\dot\mu)$, defining the geometry of Sinkhorn divergences

**Sinkhorn JKO:**

$$\mu^\tau_{k+1} \in \arg\min_\mu \; E(\mu) + \frac{S_\varepsilon(\mu,\mu_k)}{2\tau}$$

… distance

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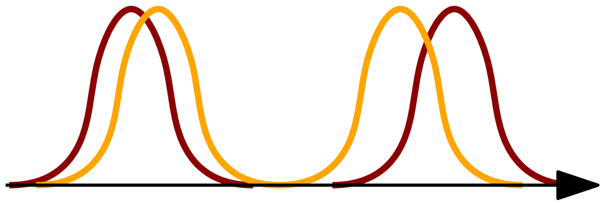
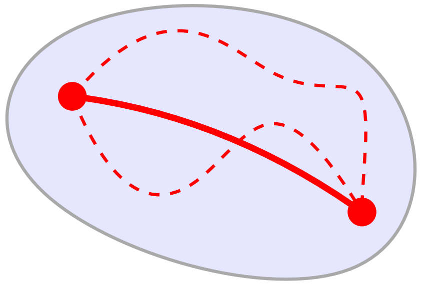
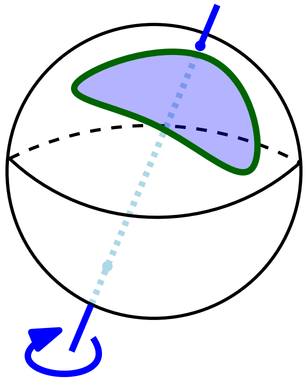


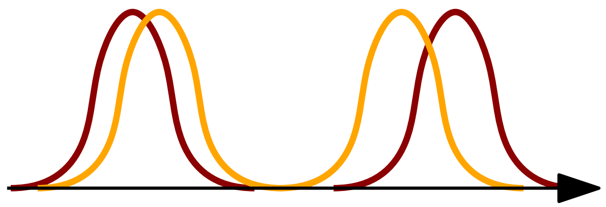
**1 - Optimal transport: metric tensor, geometry, gradient flows**

**2 - Building a Riemannian geometry out of Sinkhorn divergences**





**3 - Gradient flows of potential energies for the Sinkhorn geometry**



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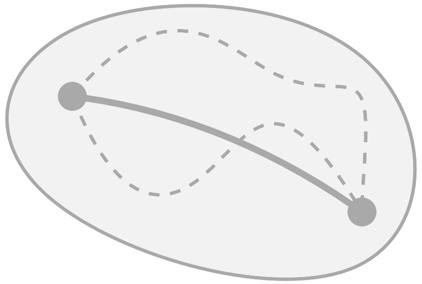

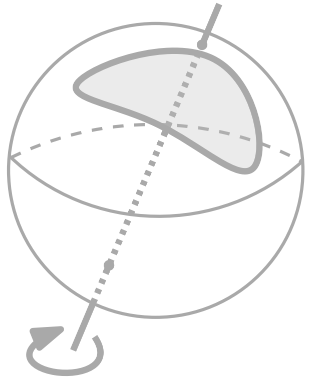

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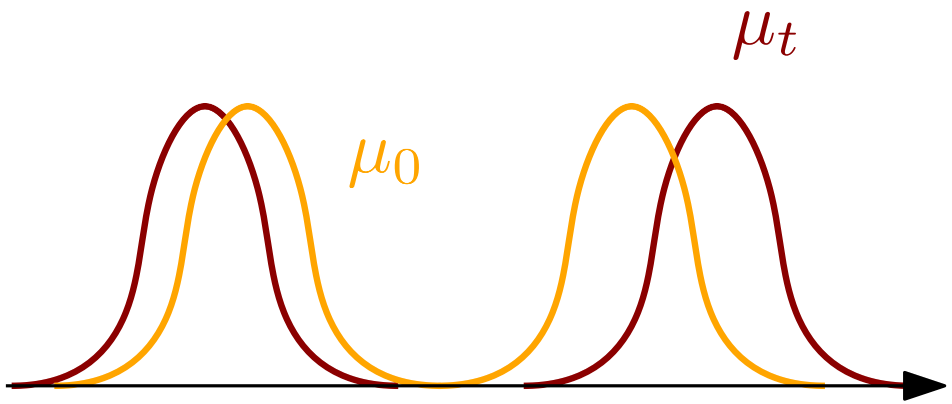
# The linearization of optimal transport

On $\mathbb{R}^d$, what happens to $\mathrm{OT}(\mu, \nu)$ if $\mu \simeq \nu$?

$\rightsquigarrow$ $(\mu_t)_t$ curve in $\mathcal{P}(\mathbb{R}^d)$, we look at $\mathrm{OT}(\mu_0, \mu_t)$.




Ambrosio, Gigli & Savaré (2008). Gradient flows: in metric spaces and in the space of probability measures.

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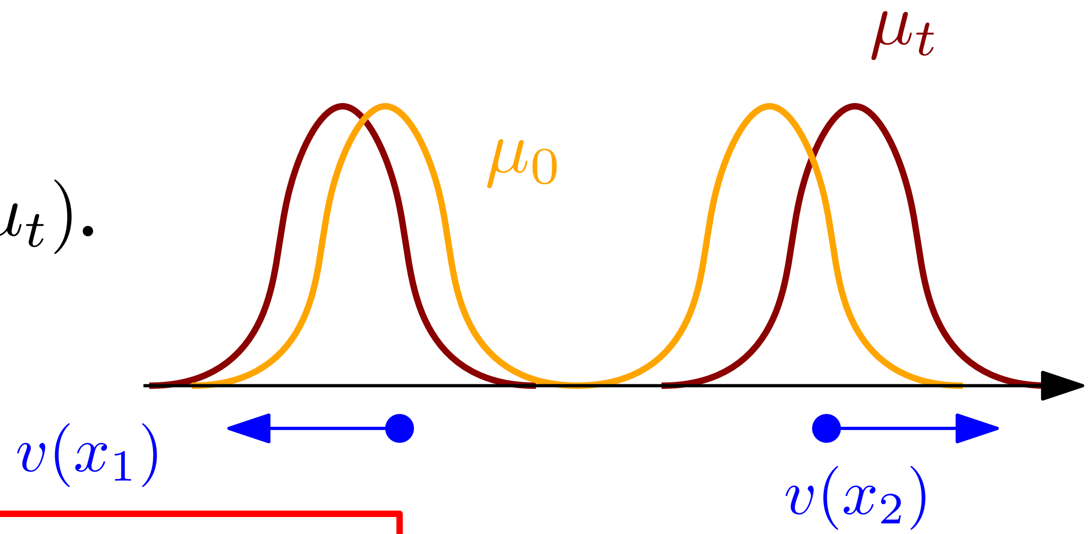


**Theorem.** $\mathrm{OT}(\mu_0, \mu_t) \sim t^2 \left( \min_v \int_{\mathbb{R}^d} |v(x)|^2 \, \mathrm{d}\mu_0(x) \right),$

where $v : \mathbb{R}^d \to \mathbb{R}^d$ such that $\left.\dfrac{\partial \mu}{\partial t}\right|_{t=0} = -\mathrm{div}(\mu_0 v)$.

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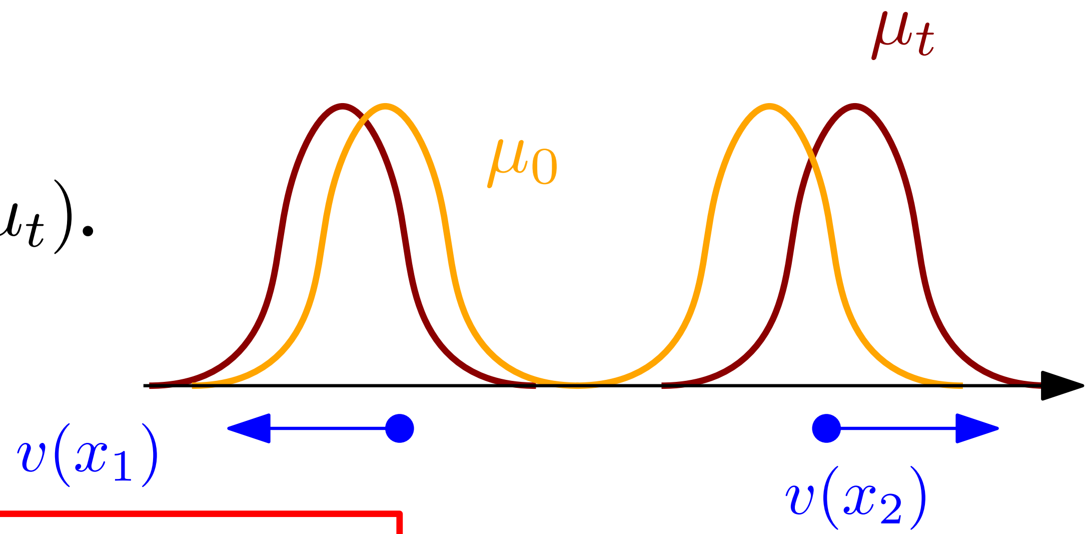


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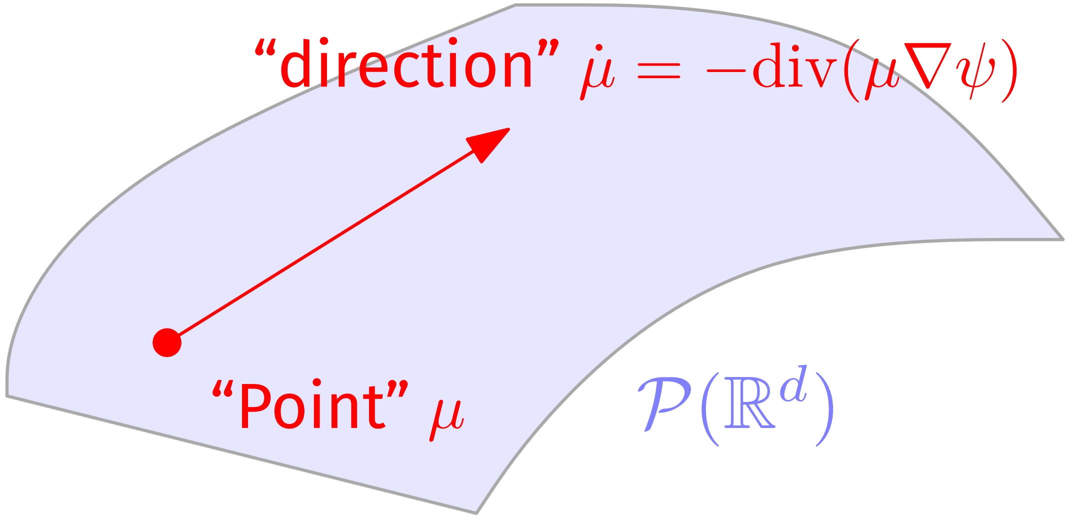
elliptic equation in $\psi$

Optimal $v$ is $\nabla\psi$, obtained by solving $-\mathrm{div}(\mu_0 \nabla \psi) = \dot{\mu}_0$.

Ambrosio, Gigli & Savaré (2008). Gradient flows: in metric spaces and in the space of probability measures.

# The metric tensor and the geometry of optimal transport




**Metric tensor:**

$$\mathbf{g}^{\mathrm{OT}}_{\mu}(\dot\mu,\dot\mu) = \int_X |\nabla\psi|^2 \,\mathrm{d}\mu.$$

Quadratic form in $\dot\mu$, depending on $\mu$.

Otto (2001). The geometry of dissipative evolution equations: the porous medium equation.

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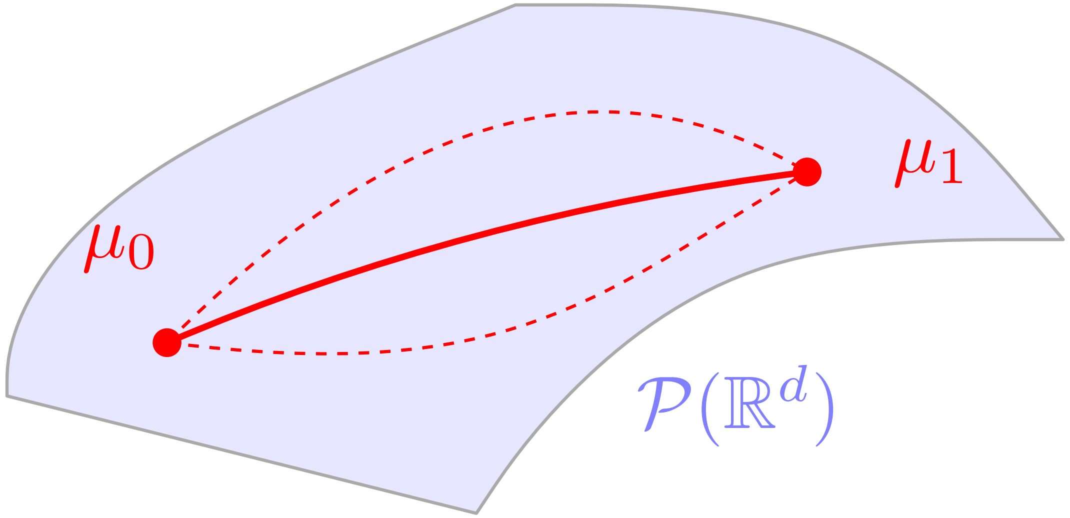


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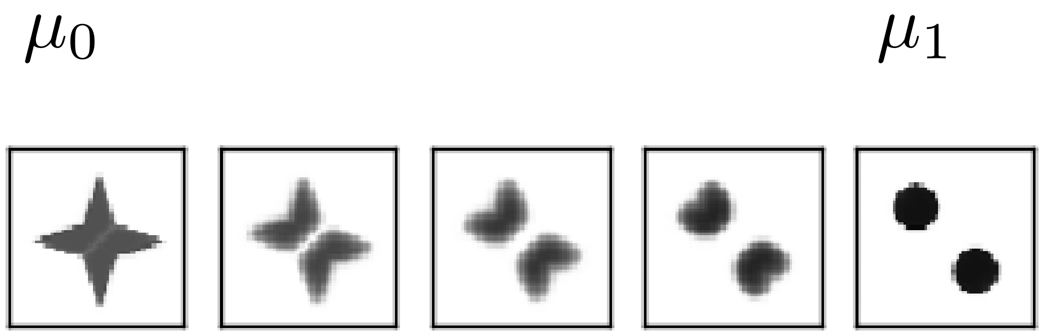
**Theorem** (Benamou and Brenier, 2000):

$$\mathrm{OT}(\mu_0, \mu_1) = \min_{(\mu_t)_t} \int_0^1 \mathbf{g}^{\mathrm{OT}}_{\mu_t}(\dot{\mu}_t, \dot{\mu}_t) \, \mathrm{d}t$$

with $\mu_0, \mu_1$ fixed.

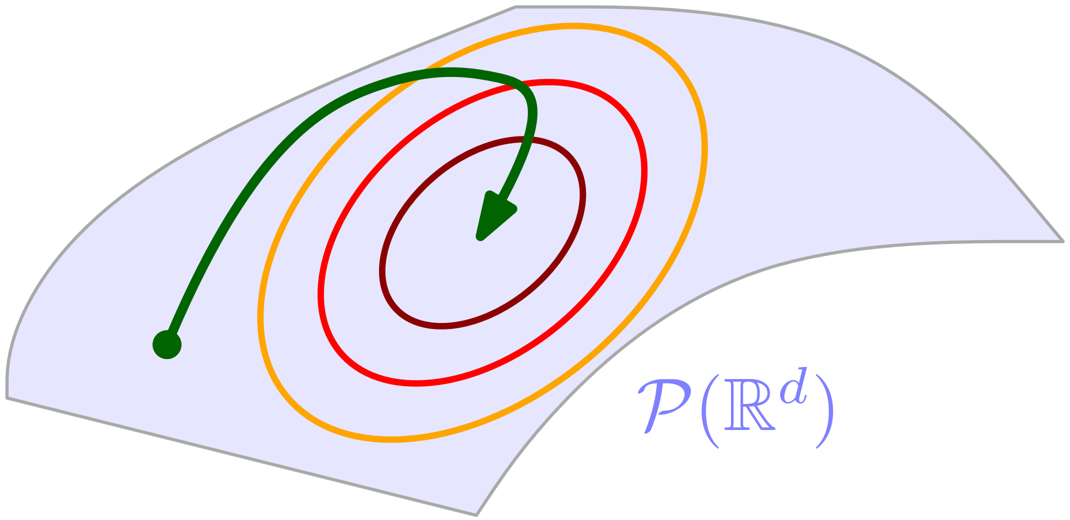
Minimizers are **geodesics**.




Example geodesic

Benamou and Brenier (2000). A computational fluid mechanics solution to the Monge-Kantorovich mass transfer problem.

# The metric tensor and the geometry of optimal transport

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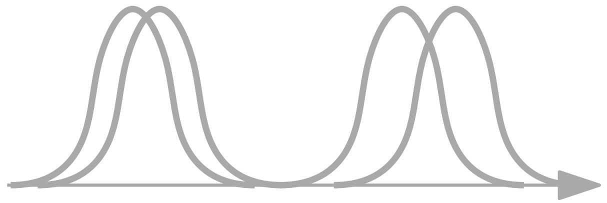
**Gradient flows:** JKO scheme

$$\mu^\tau_{k+1} \in \arg\min_{\mu} E(\mu) + \frac{\mathrm{OT}(\mu, \mu^\tau_k)}{2\tau},$$

becomes with $\tau \to 0$

$$\dot\mu_t \in \arg\min_{\sigma} DE(\mu_t)[\sigma] + \frac{\mathbf{g}^{\mathrm{OT}}_{\mu_t}(\sigma, \sigma)}{2}.$$



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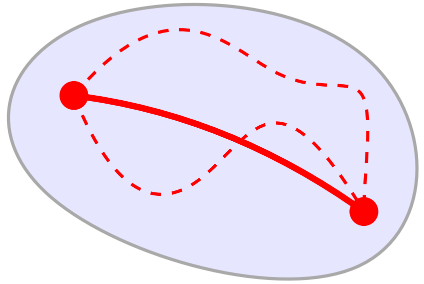
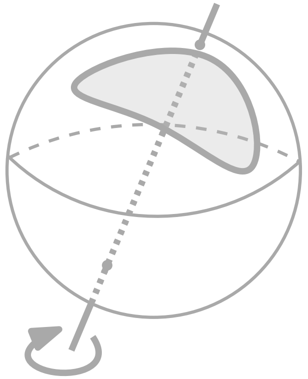


1. Define $\mathbf{g}_\mu(\dot\mu, \dot\mu)$ by $S_\varepsilon(\mu_0, \mu_t) \sim t^2 \mathbf{g}_{\mu_t}(\dot\mu_t, \dot\mu_t)$.
2. Define $\mathrm{d}_S(\mu_0, \mu_1)^2 = \inf \int_0^1 \mathbf{g}_{\mu_t}(\dot\mu_t, \dot\mu_t)\,\mathrm{d}t$.

See also Park & Slepčev (2023). Geometry and analytic properties of the sliced Wasserstein space.

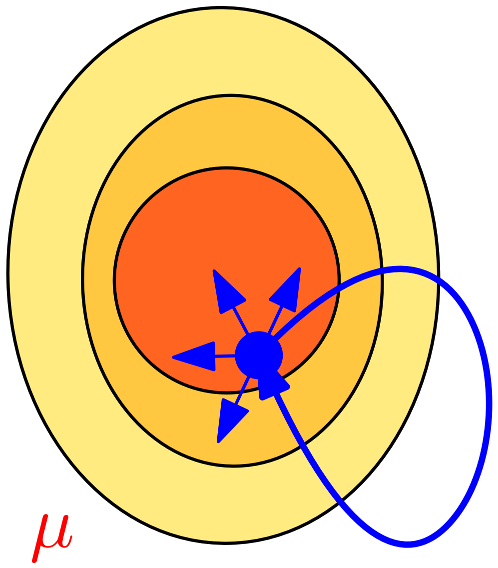


**3 - Gradient flows of potential energies for the Sinkhorn geometry**

# **Understanding** $\mathrm{OT}_\varepsilon(\mu,\mu)$

With $f_\mu : X \to \mathbb{R}$ Schrödinger potential, $\pi_\varepsilon$ entropic optimal plan between $\mu$ and $\mu$ is:

$$\mathrm{d}\pi_\varepsilon(x,y) = \exp\left(\frac{f_\mu(x) + f_\mu(y) - c(x,y)}{\varepsilon}\right)\mathrm{d}\mu(x)\mathrm{d}\mu(y).$$



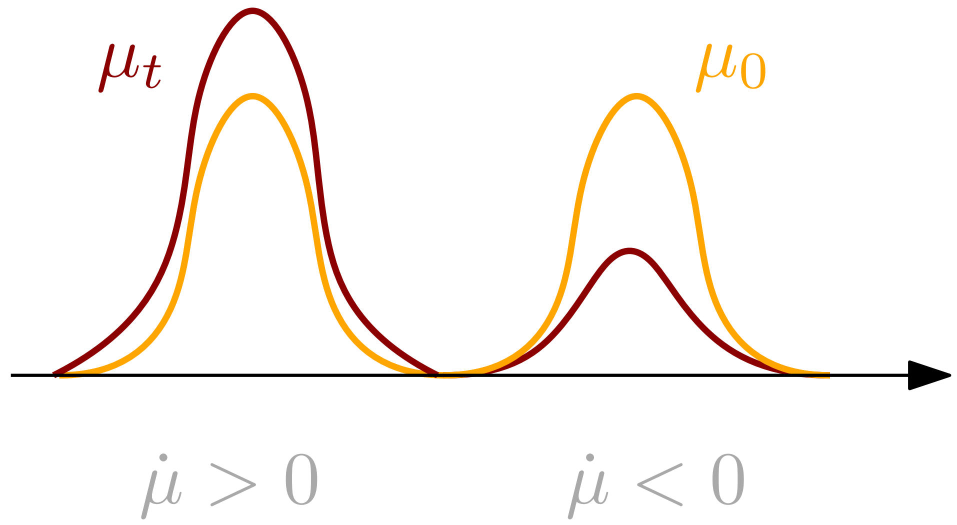

(Defines a reversible Markov chain with equilibirum measure $\mu$.)

**Definition:**

$$k_\mu(x,y) = \exp\left(\frac{f_\mu(x) + f_\mu(y) - c(x,y)}{\varepsilon}\right).$$

# The Hessian of the Sinkhorn divergence

$\mu_t = \mu + t\dot{\mu}$, with $\dot{\mu}$ signed measure with zero mass.



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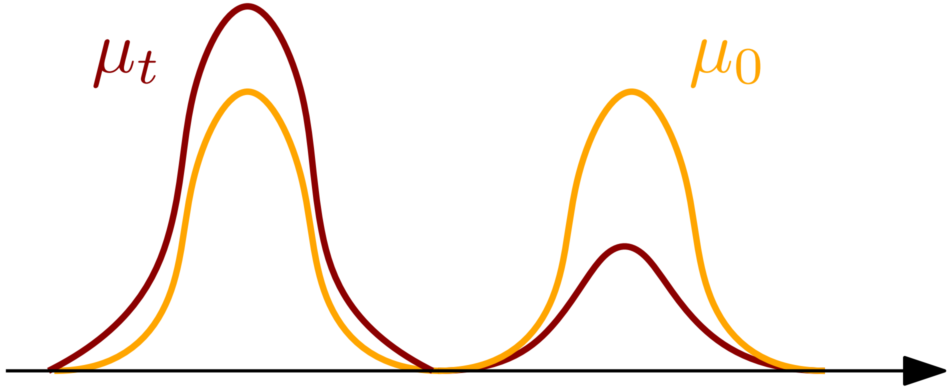
**Theorem.**

$$S_\varepsilon(\mu_0, \mu_t) \sim t^2 \frac{\varepsilon}{2} \langle \dot{\mu}, (\mathrm{Id} - K_\mu^2)^{-1} H_\mu[\dot{\mu}] \rangle.$$




Where $k_\mu(x, y) = \exp((f_\mu(x) + f_\mu(y) - c(x, y))/\varepsilon)$ and:

$$K_\mu(\phi)(x) = \int_X k_\mu(x, y)\phi(y)\,\mathrm{d}\mu(y),$$

$$H_\mu[\sigma](x) = \int_X k_\mu(x, y)\,\mathrm{d}\sigma(y).$$

$(\mathrm{Id} - K_\mu^2)/\varepsilon \sim$ Laplacian

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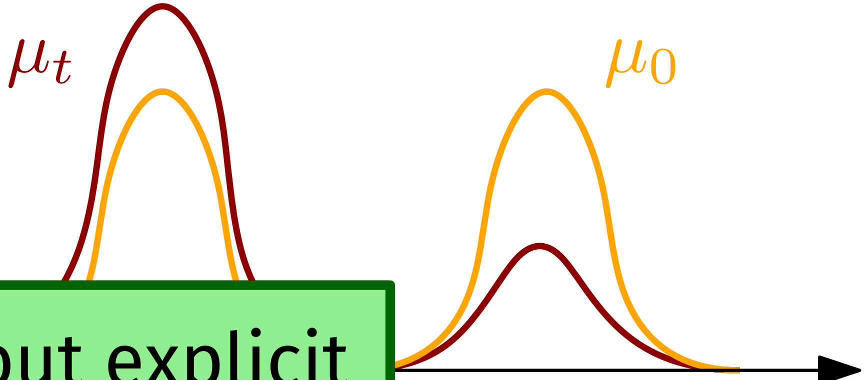


Main message: heavy but explicit and interpretable formula!

Where $k_\mu(x, y) = \exp((f_\mu(x$

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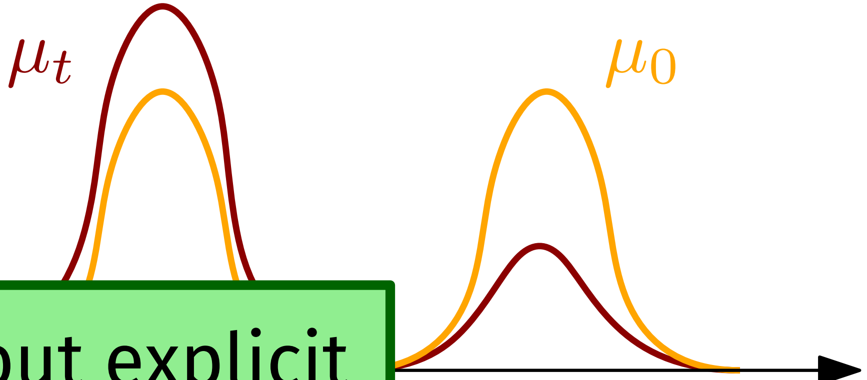
$$S_\varepsilon(\mu_0, \mu_t) \sim t^2 \frac{\varepsilon}{2} \langle \dot{\mu}, (\mathrm{Id} - K_\mu^2)^{-1} H_\mu[\dot{\mu}] \rangle.$$




Main message: heavy but explicit and interpretable formula!

Where $k_\mu(x, y) = \exp((f_\mu(x$

$$K_\mu(\phi)(x) = \int_X k_\mu(x, y)\phi(y)\,\mathrm{d}\mu(y),$$

$$H_\mu[\sigma](x) = \int_X k_\mu(x, y)\,\mathrm{d}\sigma(y).$$

$(\mathrm{Id} - K_\mu^2)/\varepsilon \sim$ Laplacian

Same formula

**Definition.** $\mathbf{g}_\mu(\dot{\mu}, \dot{\mu}) = \frac{\varepsilon}{2} \langle \dot{\mu}, (\mathrm{Id} - K_\mu^2)^{-1} H_\mu[\dot{\mu}] \rangle.$

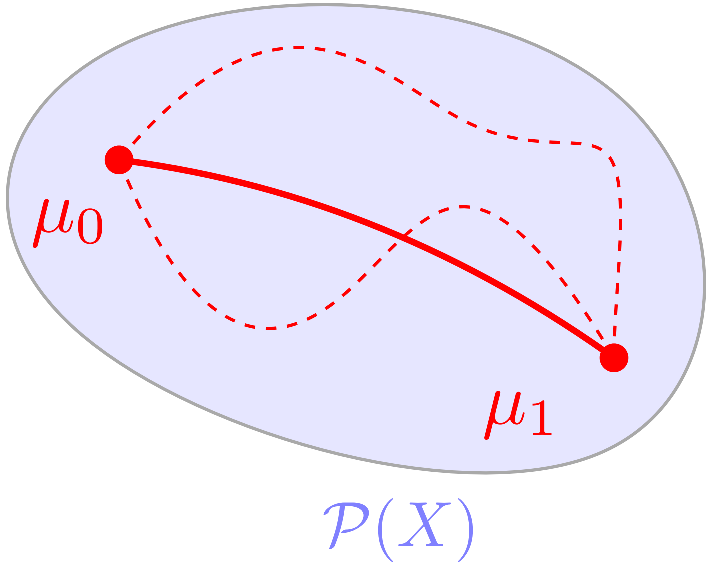
# Definition of the Riemannian distance and main results

Recall $X$ compact, $\mathbf{g}_\mu(\dot\mu, \dot\mu) = \frac{\varepsilon}{2}\langle \dot\mu, (\mathrm{Id} - K_\mu^2)^{-1} H_\mu[\dot\mu]\rangle$.

**Definition.** Given $\mu_0, \mu_1$:

$$\mathrm{d}_S(\mu_0, \mu_1)^2 = \inf \int_0^1 \mathbf{g}_{\mu_t}(\dot\mu_t, \dot\mu_t)\,\mathrm{d}t$$

where infimum over $(\mu_t)$ on a class of path to be specified in the next slides.

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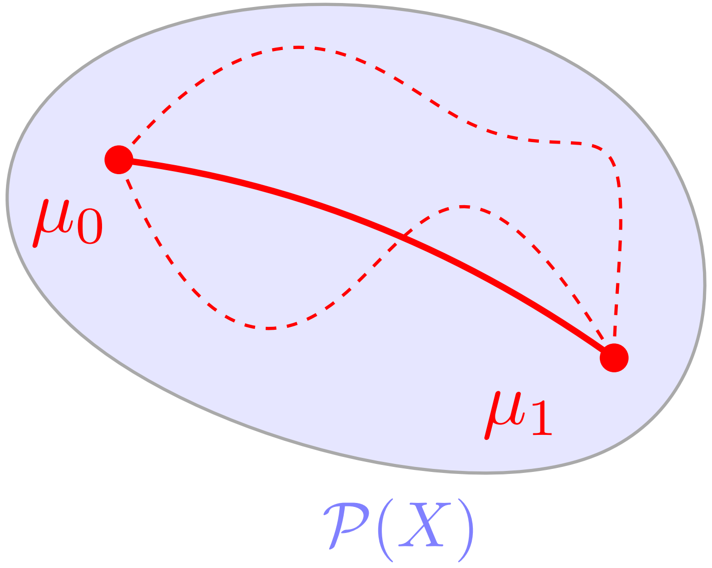


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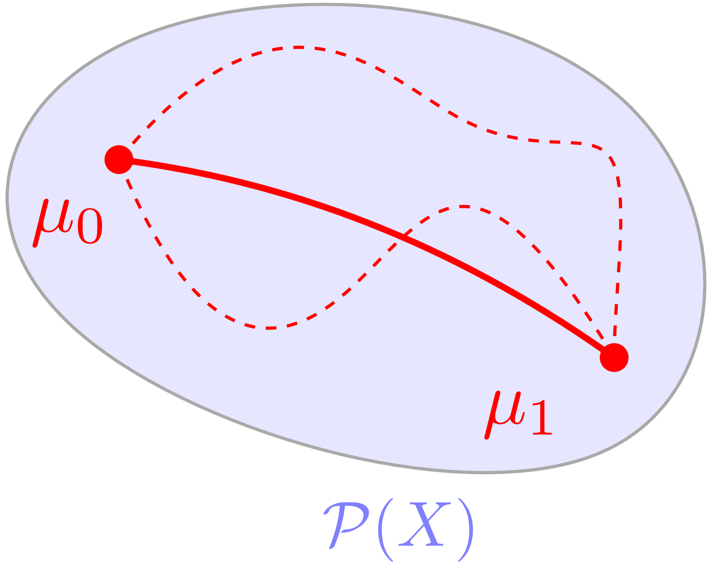


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**Elements of the proof**: next slides.

# Reminder on Reproducing Kernel Hilbert Spaces (RKHS)

Fix $k : X \times X \to \mathbb{R}$ positive definite.

**Definition.** $\mathcal{H}_k$ Hilbert space of functions $X \to \mathbb{R}$: start with

$$\operatorname{span}\{k(\cdot, x) \ : \ x \in X\}$$

with $\langle k(\cdot, x), k(\cdot, y)\rangle_{\mathcal{H}_k} = k(x, y)$. Then take completion.

$k$ positive definite if this defines dot product

($k$ universal $\Leftrightarrow$ $\mathcal{H}_k$ dense in $C(X)$ )

Paulsen & Raghupathi (2016). An Introduction to the Theory of Reproducing Kernel Hilbert Spaces.

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In our case:

- $k = \exp(-c/\varepsilon)$, space $\mathcal{H}_c$.
- $k = k_\mu = \exp((f_\mu \oplus f_\mu - c)/\varepsilon)$, space $\mathcal{H}_\mu$.

Typically smooth functions!

Paulsen & Raghupathi (2016). An Introduction to the Theory of Reproducing Kernel Hilbert Spaces.

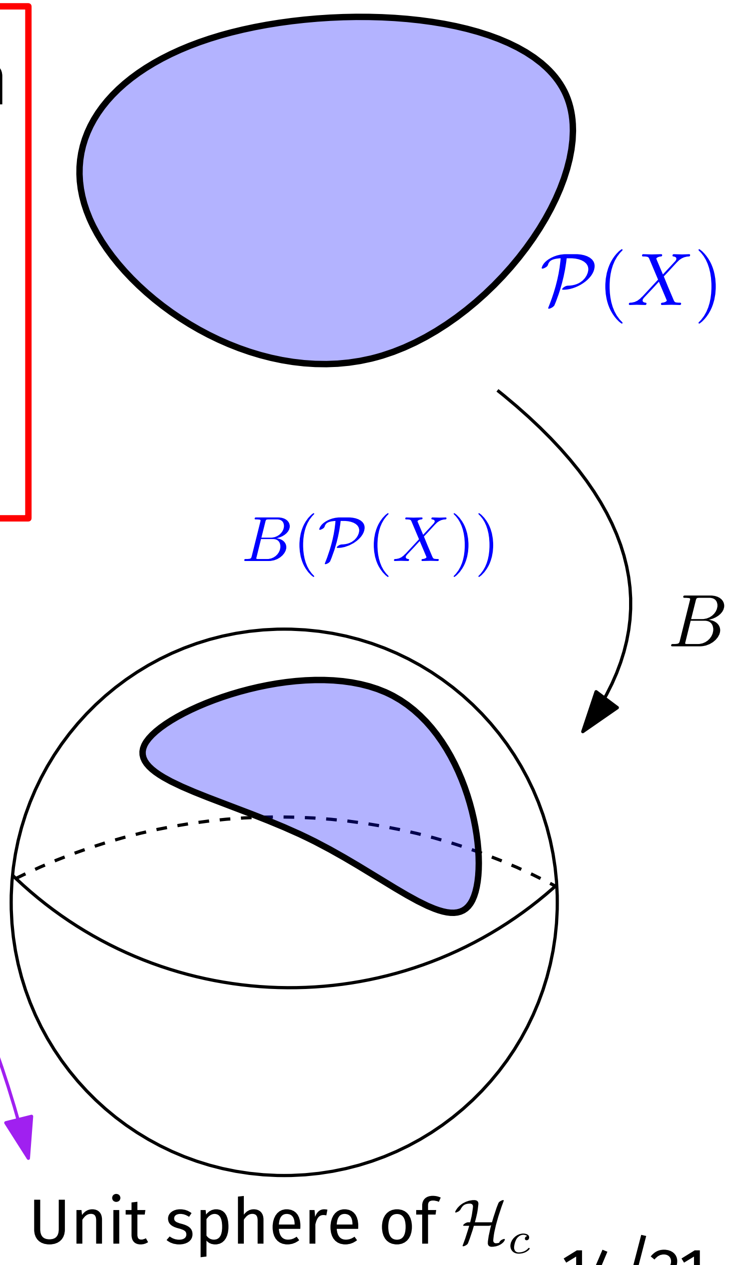
# A useful change of variable

**Define:**

$$b = B(\mu) = \exp\left(-\frac{f_\mu}{\varepsilon}\right)$$

where $f_\mu : X \to \mathbb{R}$ self Schrödinger potential.

**Theorem.** The map $B$ is an homeomorphism between $\mathcal{P}(X)$ and the intersection of a convex cone and the unit sphere of $\mathcal{H}_c$.




$\mathcal{H}_c$: Reproducing Kernel Hilbert Space built on $\exp(-c/\varepsilon)$.

(Change of variable suggested by Feydy et al, Séjourné et al)


Feydy, Séjourné, Vialard, Amari, Trouvé & Peyré (2019). Interpolating between optimal transport and MMD using Sinkhorn divergences.
Séjourné, Feydy, Vialard, Trouvé & Peyré (2019). Sinkhorn divergences for unbalanced optimal transport.

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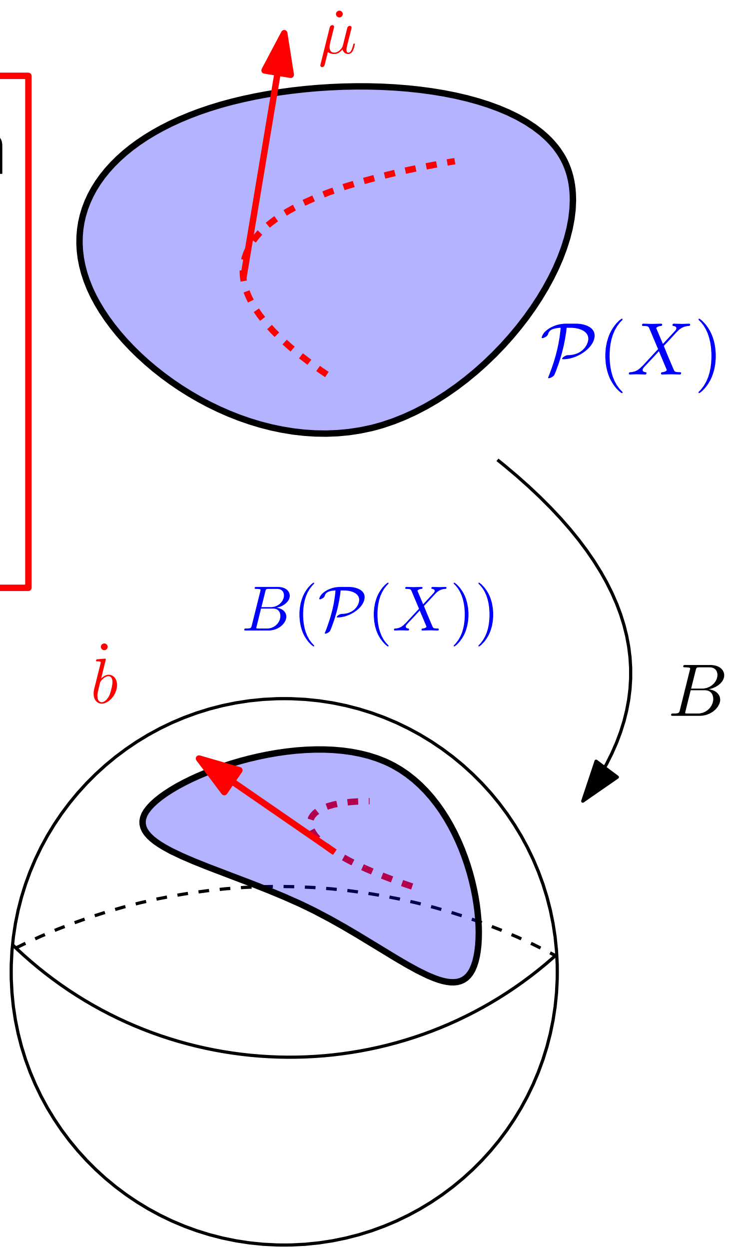

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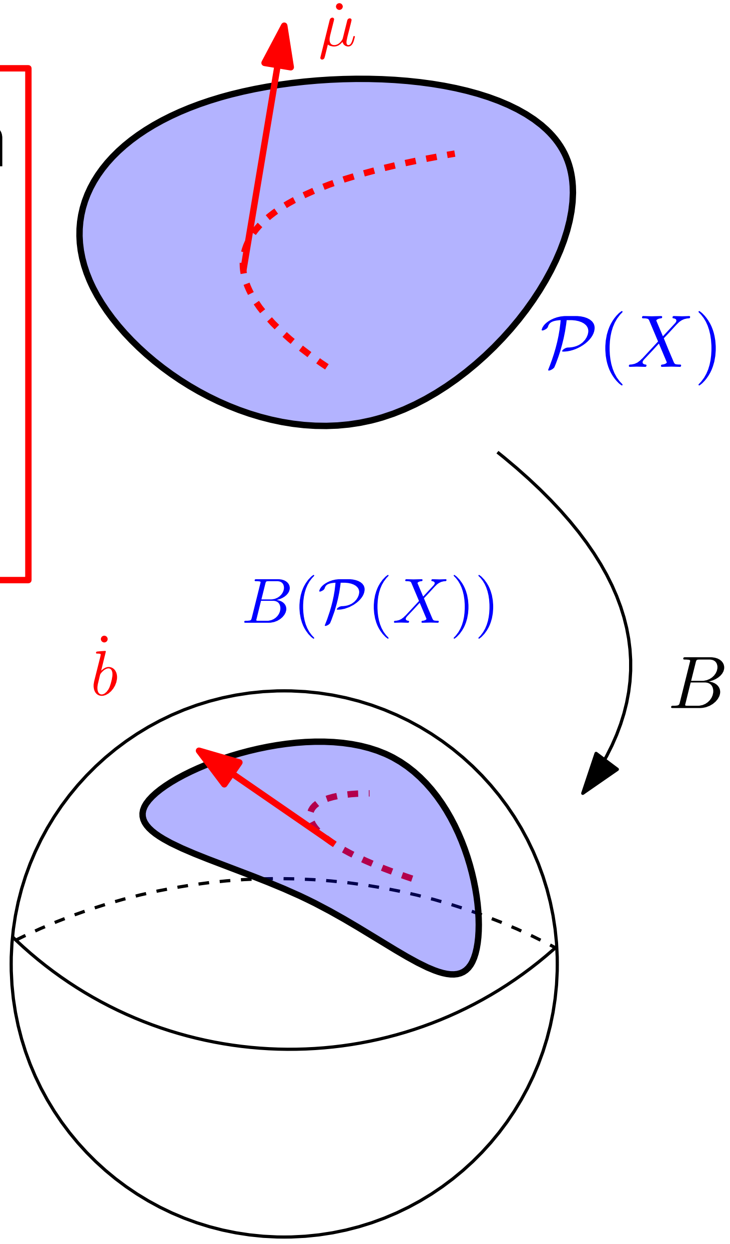
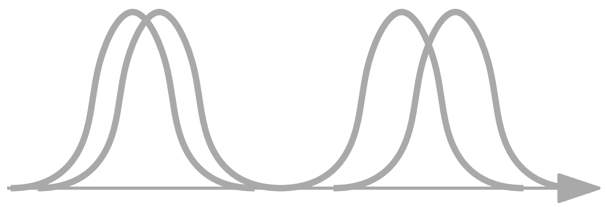
**Consequence.** Admissible paths: $(b_t)$ $H^1$ valued in $\mathcal{H}_c$,

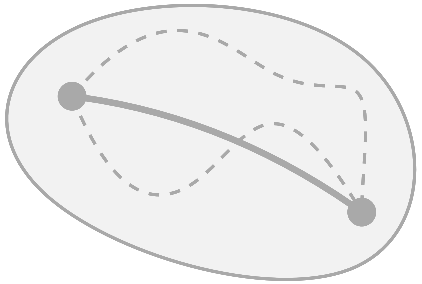
$$\mathsf{d}_S(\mu_0, \mu_1) \asymp \|b_1 - b_0\|_{\mathcal{H}_c}.$$

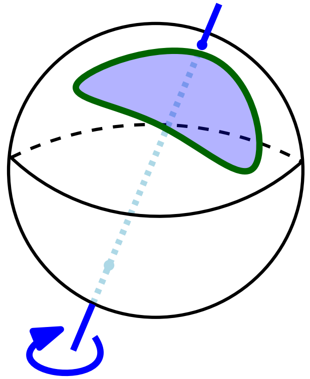




**1 - Optimal transport: metric tensor, geometry, gradient flows**

**2 - Building a Riemannian geometry out of Sinkhorn divergences**





**3 - Gradient flows of potential energies for the Sinkhorn geometry**

## Notations, object of study

$X$ compact metric, $\exp(-c/\varepsilon)$ p. d. and universal, and $V : X \to \mathbb{R}$ continuous.

**Sinkhorn JKO:**

$$\mu_{k+1}^\tau \in \arg\min_\mu \; E(\mu) + \frac{S_\varepsilon(\mu, \mu_k^\tau)}{2\tau}.$$

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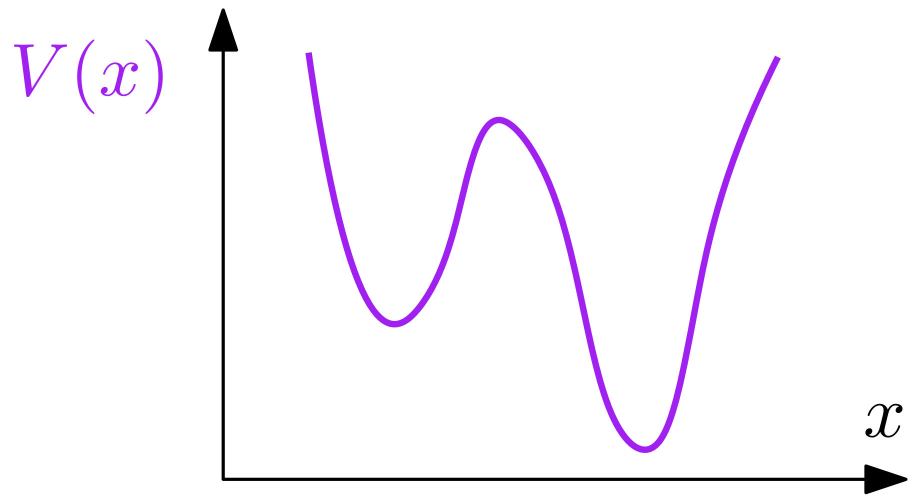

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**Formal** limit when $\tau \to 0$:

Evolution equation, **Sinkhorn flow**

$$\frac{\varepsilon}{2}(\mathrm{Id} - K^2_{\mu_t})^{-1} H_{\mu_t}[\dot{\mu}_t] + V + p_t = \text{Cst.}$$

$p_t$ pressure: $p_t \leq 0$, and $p_t = 0$ on $\mathrm{supp}(\mu_t)$

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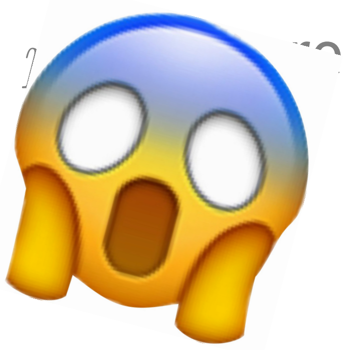

So $\dot{\mu}_t = H_{\mu_t}^{-1}[\ldots]$ with $H_{\mu_t}$ "convolution".
**Non local** equation **of infinite order**.

# Sinkhorn flow in the Hilbert space $\mathcal{H}_c$

Recall $b_t = \exp(-f_{\mu_t}/\varepsilon) \in \mathcal{H}_c$ and $V : X \to \mathbb{R}$.

**Sinkhorn flow** in the $b$-variable.

$$\dot{b}_t + \frac{2}{\varepsilon}(V - V^*)\, b_t + p_t = 0.$$

$p_t \leq 0$, and $p_t = 0$ on $\operatorname{supp}(\mu_t)$

multiplication by $V$ in $\mathcal{H}_c$

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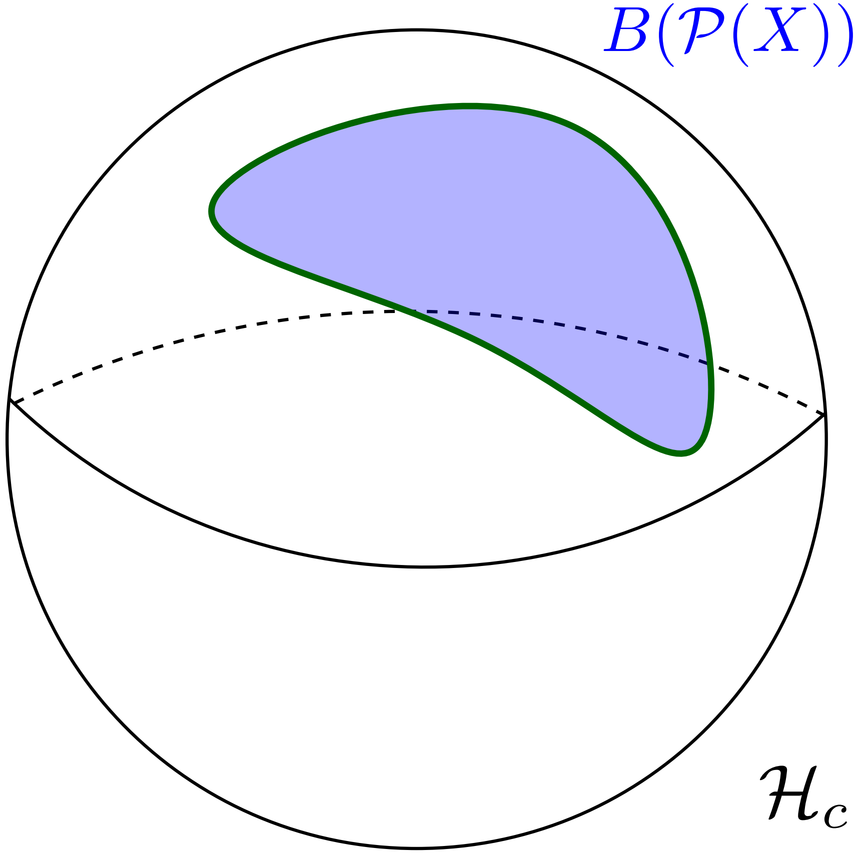

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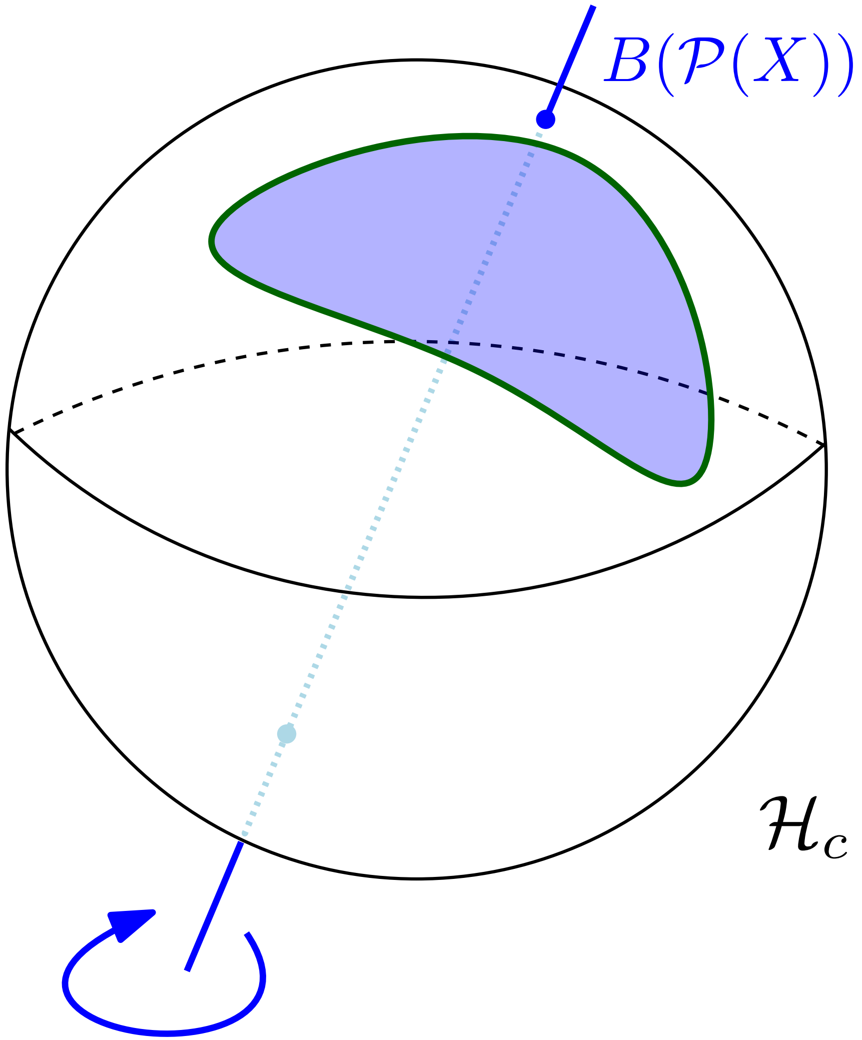
$\frac{2}{\varepsilon}(V - V^*)$ skew-symmetric: generates group of unitary operators, but unbounded.

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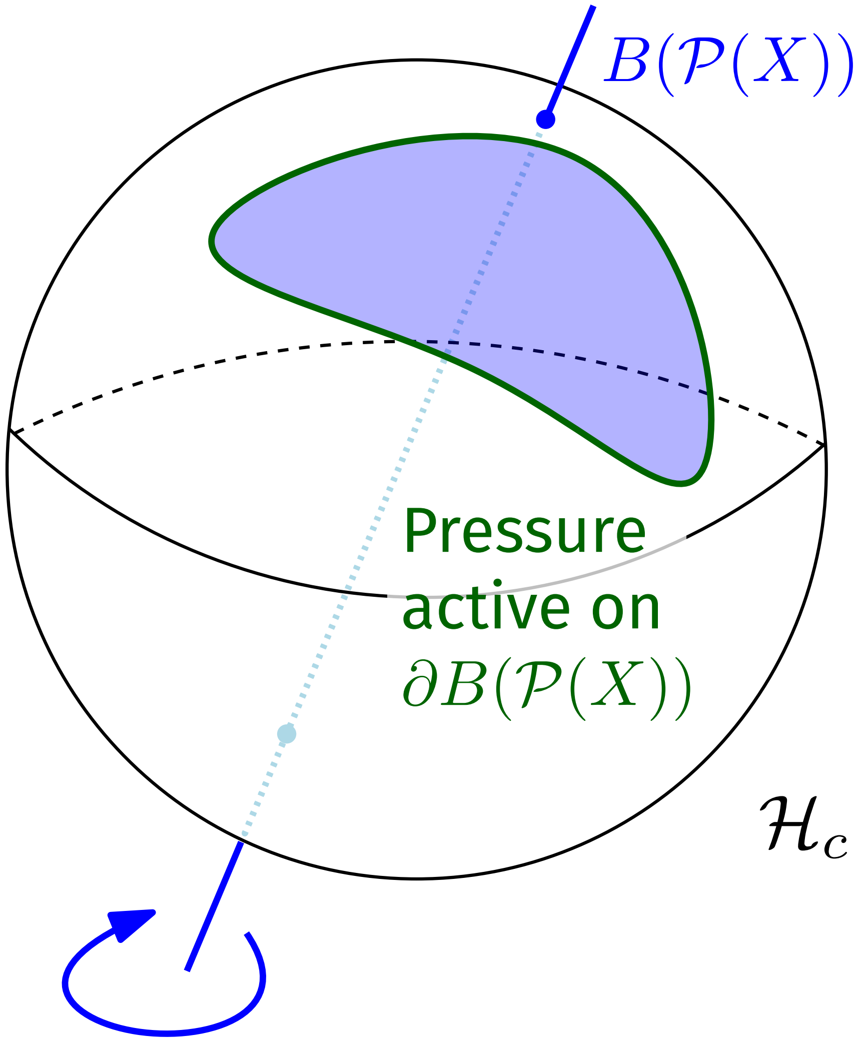


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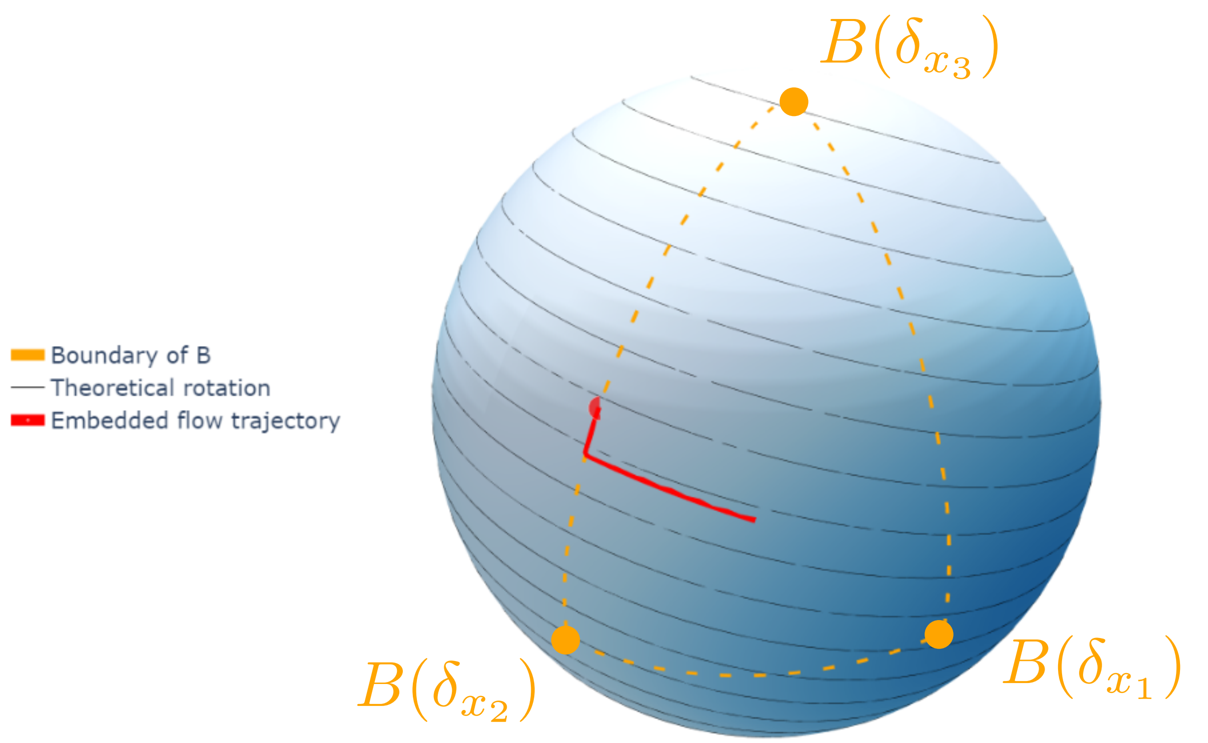
$X = \{x_1, x_2, x_3\}$

$V(x_3) \leq V(x_2) \leq V(x_1)$



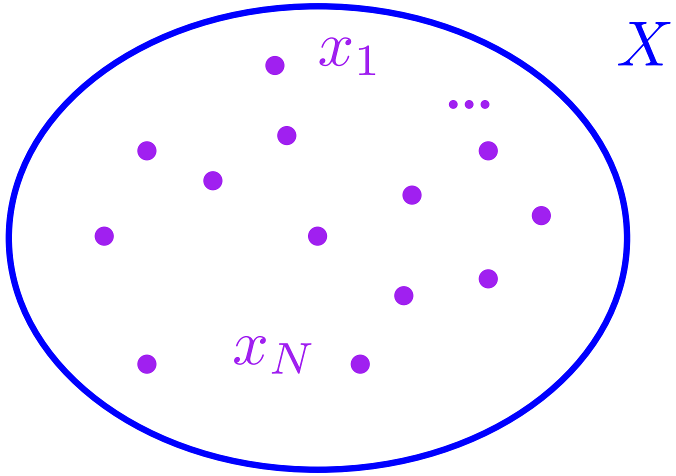

Obtained by solving the **SJKO** scheme.

# Main theoretical results

**Theorem** (on the Sinkhorn flow).

1. **Existence**: for any $b_0 = B(\mu_0)$, there exists a solution, with $(b_t) \in H^1([0,+\infty), \mathcal{H}_c)$.

**Proof idea**: approximate $X$ by a finite space $X_N = \{x_1, \dots, x_N\}$. For measures supported on $X_N$, the Sinkhorn flow is a maximal monotone evolution.



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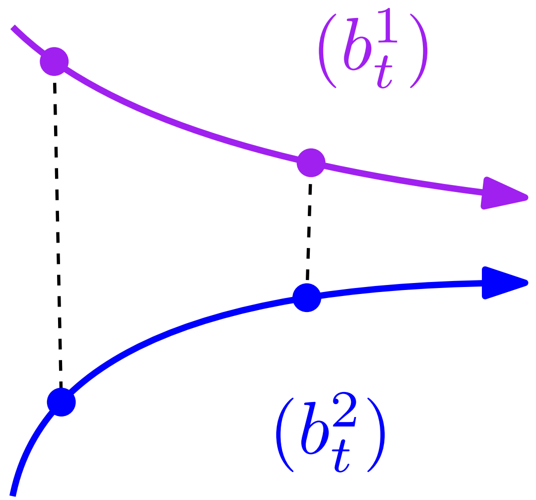
**Proof idea**: Maximal monotone operators are non-expansive.



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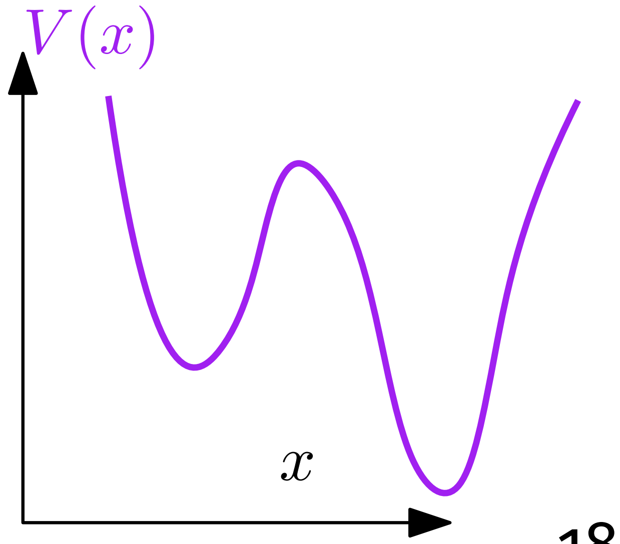
3. Convergence to **global minimum**: $E(\mu_t) \to \min E$ as $t \to +\infty$.

**Recall**. The flow of the Wasserstein GF $\partial \mu_t = \mathrm{div}(\mu_t \nabla V)$ gets trapped in local minima.



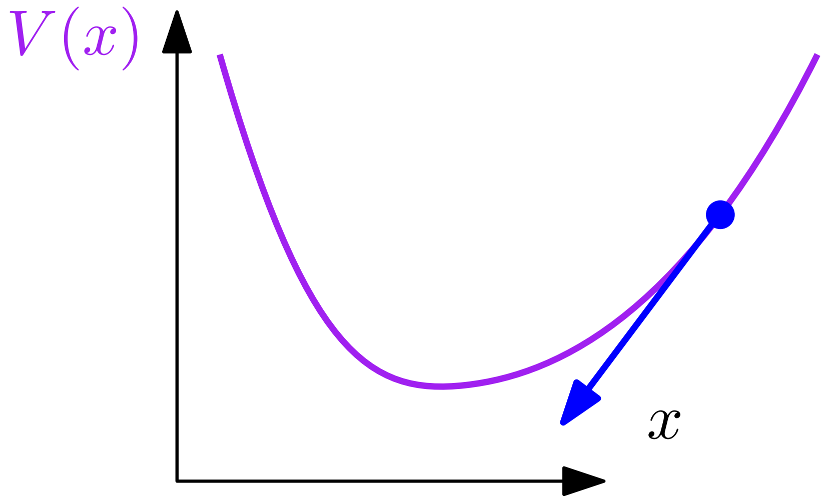

**Proof idea**. The only critical points of $E$ are global minima because vertical perturbations (teleportation) is allowed in the Sinkhorn geometry (no convexity of $V$ needed).

## Examples

**Proposition.** If $X = \mathbb{R}^d$, $V$ convex, $c$ quadratic cost and $\mu_0 = \delta_{x_0}$ then $\mu_t = \delta_{x_t}$ with

$$\dot{x}_t \in -\partial V(x_t).$$

(Same as Wasserstein GF).



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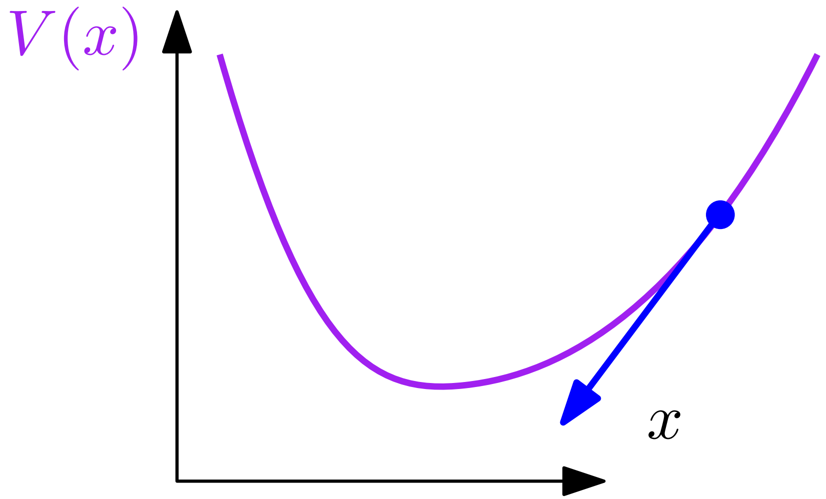
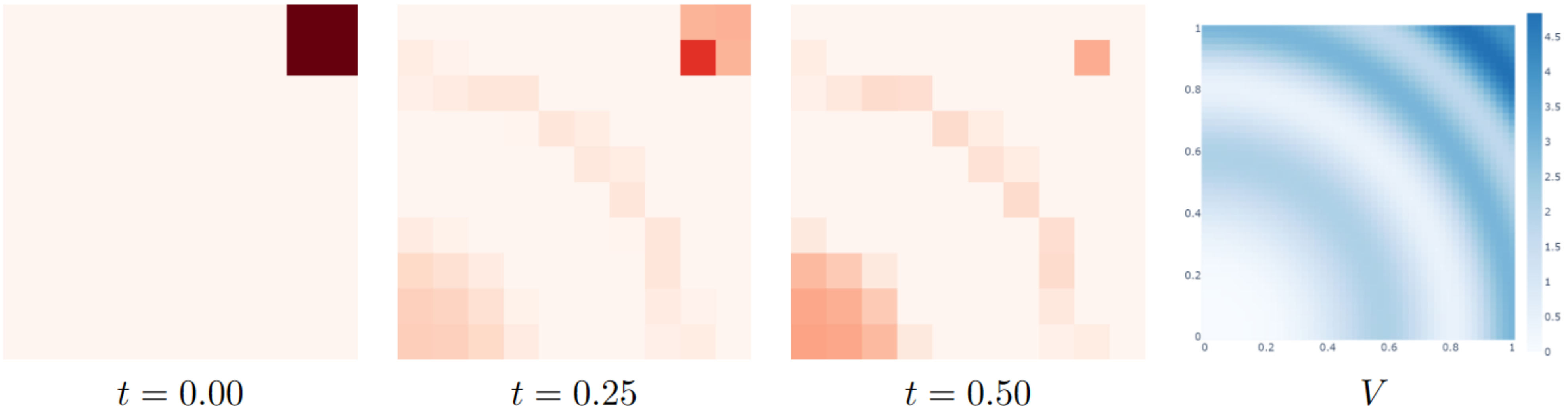



But if $V$ not convex there can be **teleportation**!

Here a **Lagrangian** discretization won't work.



# Link with the Sinkhorn JKO scheme

**Sinkhorn JKO:**

$$\mu_{k+1}^\tau \in \arg\min_\mu \; E(\mu) + \frac{S_\varepsilon(\mu, \mu_k^\tau)}{2\tau}.$$

with $S_\varepsilon$ Sinkhorn divergence and $E(\mu) = \int V \, \mathrm{d}\mu$ **potential energy**.

**Sinkhorn flow** in the $b$-variable:

$$\dot{b}_t + \frac{2}{\varepsilon}(V - V^*)\, b_t + p_t = 0.$$

with $b_t = \exp(-f_{\mu_t}/\varepsilon)$.

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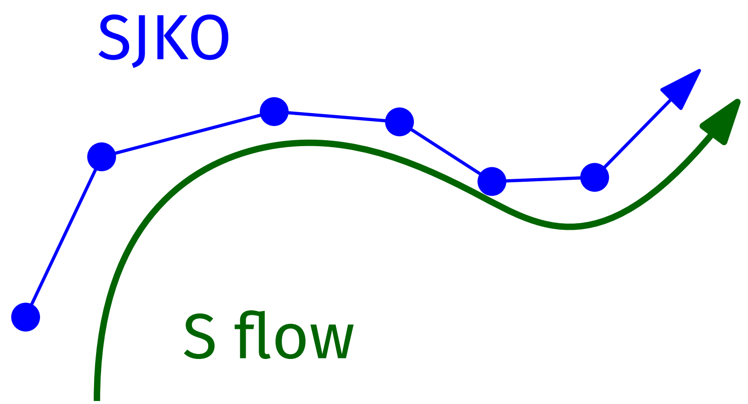
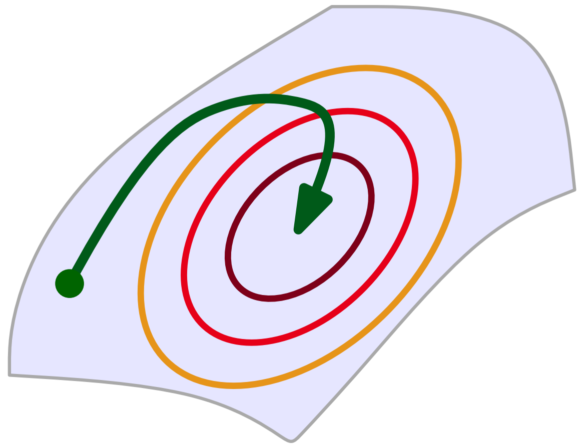


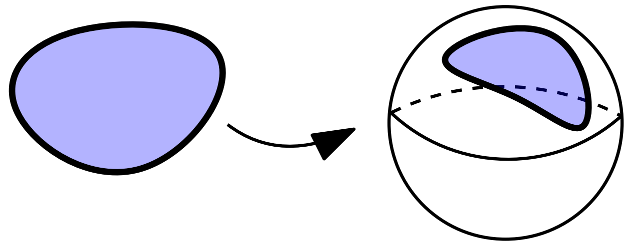

**Proposition.** If $X$ is a **finite set**, the solutions of the Sinkhorn JKO scheme, properly interpolated in time, converge to the Sinkhorn flow as $\tau \to 0$ in $C([0,T], \mathcal{P}(X))$.

# Future works

**What I have not presented:**

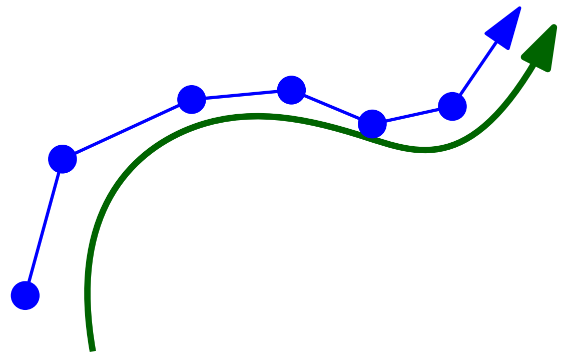
- Explicit computations for Gaussians, two points space,
- Proof that Sinkhorn divergence is not jointly convex,
- Proof that Sinkhorn divergence is not a metric.





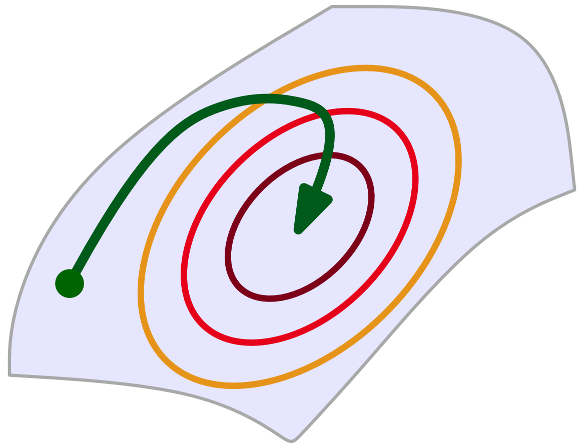
**Some topics we are working on:**

- Extend the convergence SJKO $\to$ Sinkhorn flow,
- Numerical approximation of geodesics,
- Limit $\varepsilon \to 0$ towards optimal transport,
- Homogeneization when space is refined.

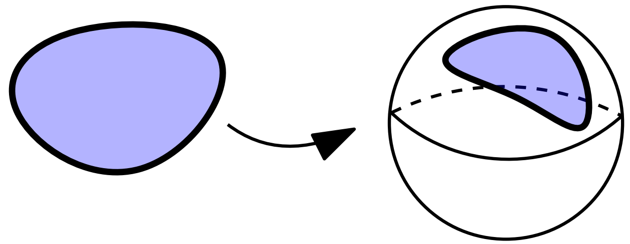


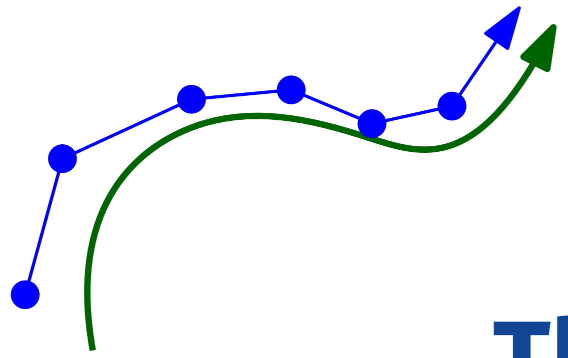
# Future works

## What I have not presented:



- Explicit computations for Gaussians, two points space,
- Proof that Sinkhorn divergence is not jointly convex,
- Proof that Sinkhorn divergence is not a metric.





## Some topics we are working on:

- Extend the convergence SJKO $\to$ Sinkhorn flow,
- Numerical approximation of geodesics,
- Limit $\varepsilon \to 0$ towards optimal transport,
- Homogeneization when space is refined.

# Thank you for your attention