The geometry of Sinkhorn divergences

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Workshop “Variational Analysis, Models and Methods in Measure Spaces”

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Joint work with

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UNIVERSITÄT GÖTTINGEN

Gilles Mordant

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Luca Tamanini

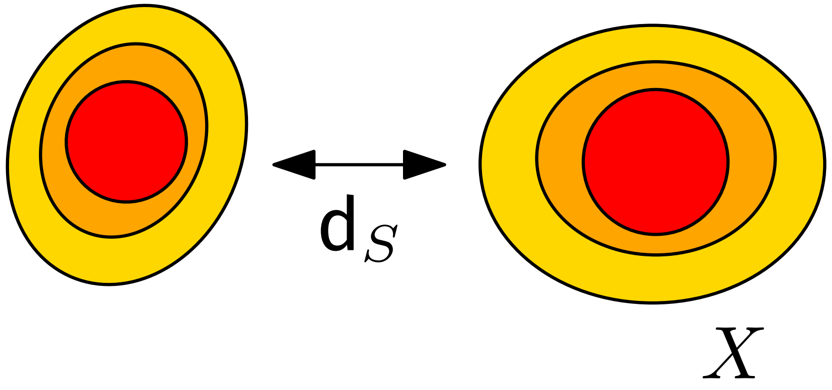
UNIVERSITAS CATHOLICA SACRI CORDIS IESU MEDIOLANI

Preprint on arxiv hopefully soon!

What I will present

$\mathcal{P}(X)$ probability distributions over (X, d) compact metric space.

We propose d_S a new distance over $\mathcal{P}(X)$:



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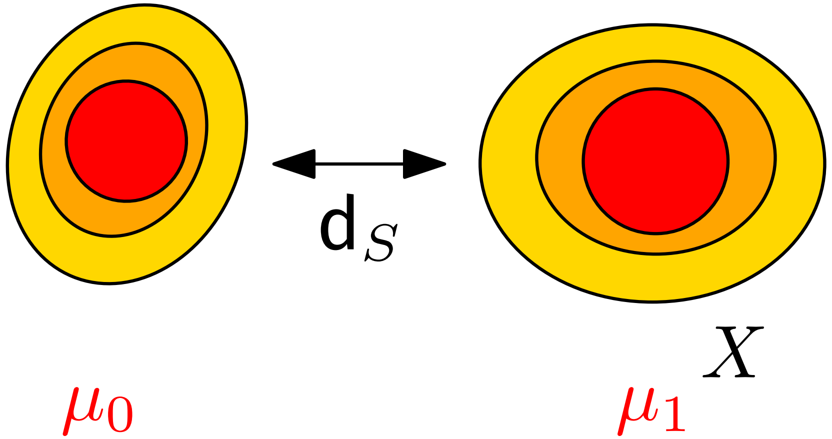
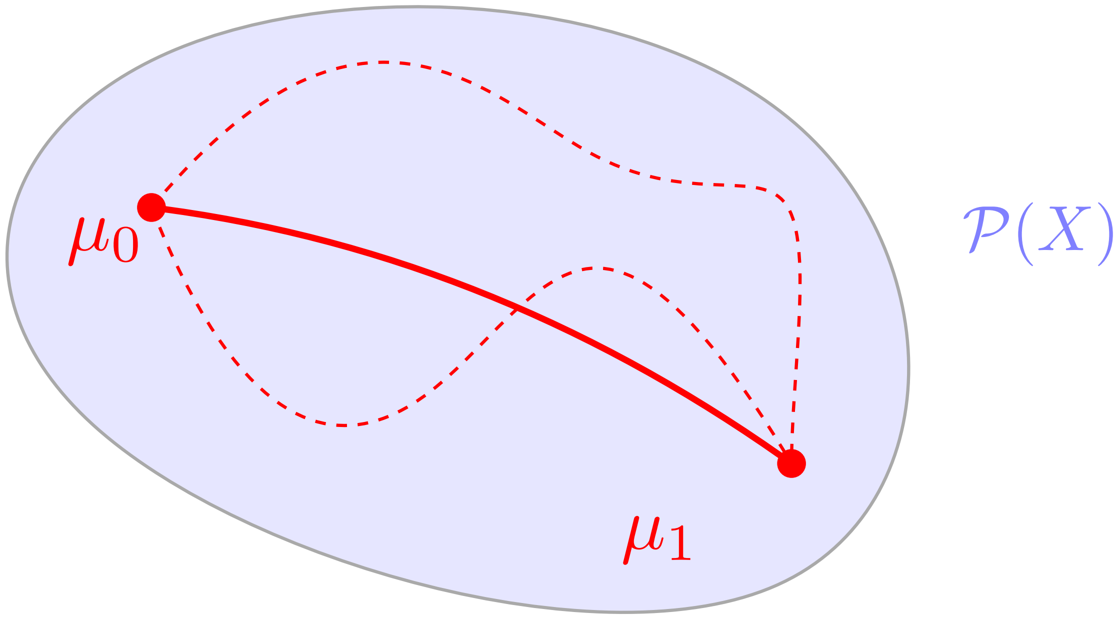


1. It is a "Riemannian" metric.



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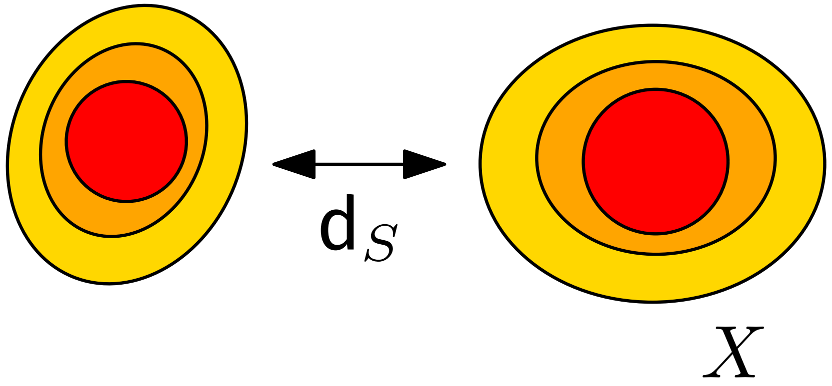

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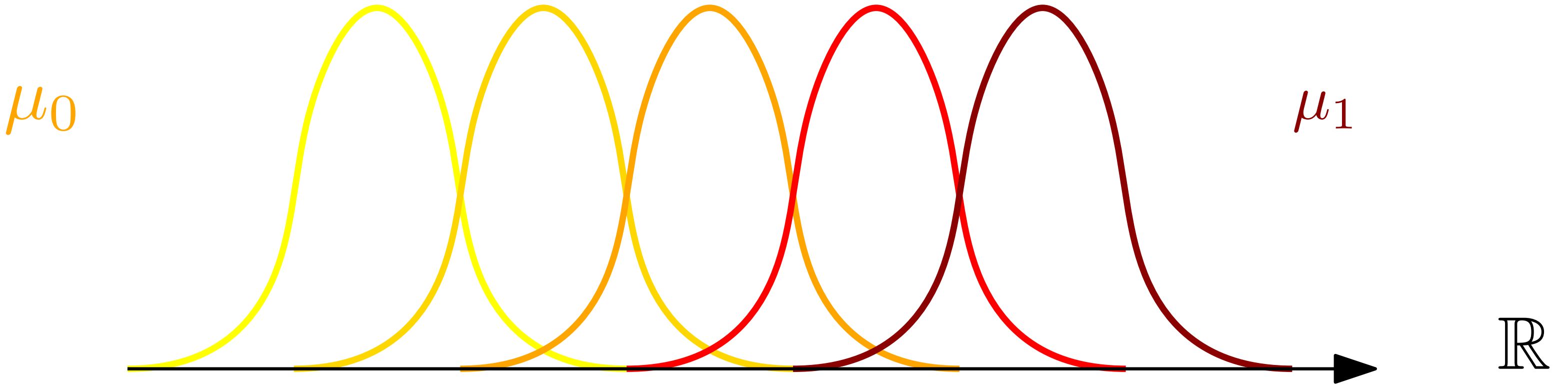

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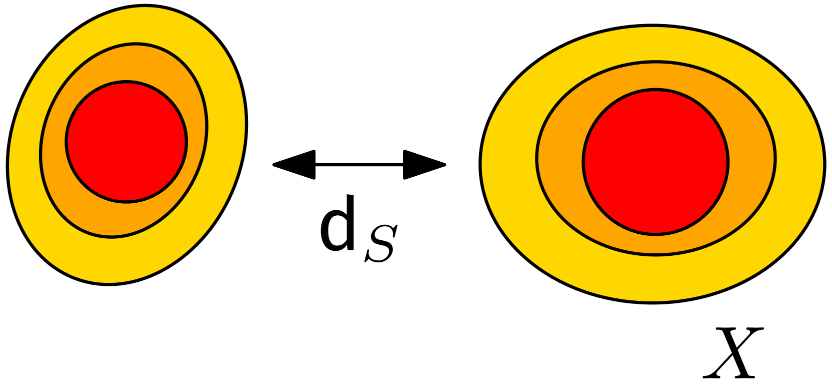

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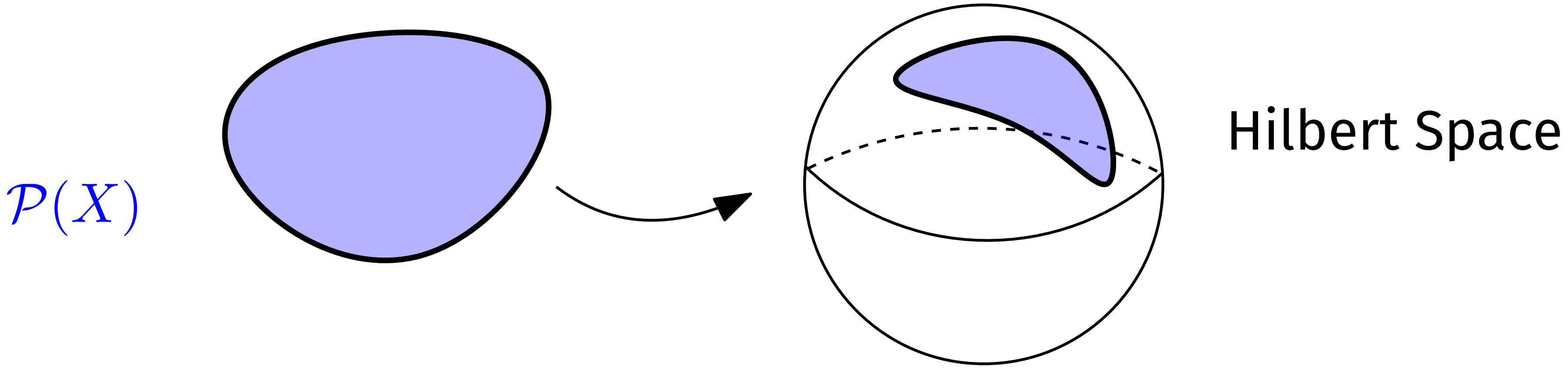

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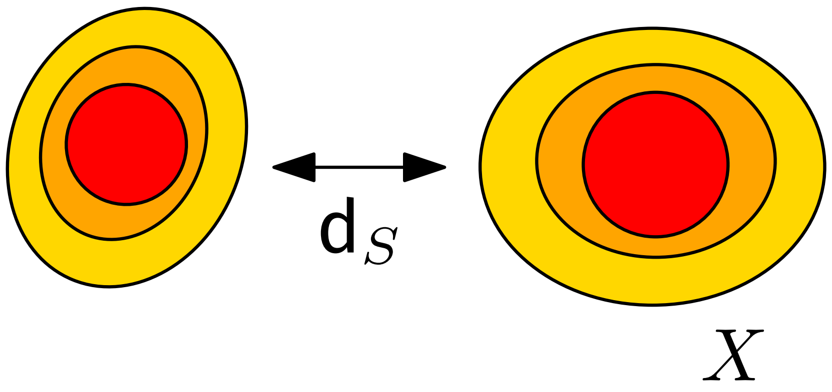

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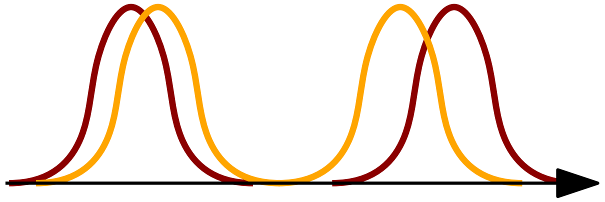
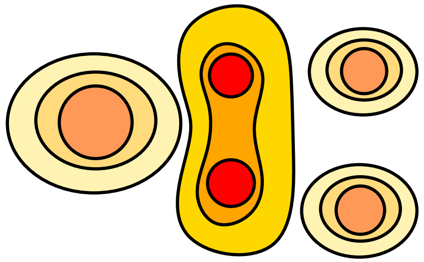
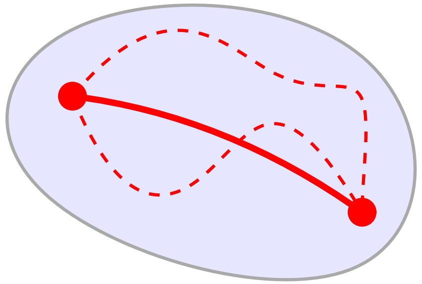
Idea: construct a Riemannian distance out of entropic optimal transport.



1 - Optimal transport and its geometry

2 - Entropic optimal transport and Sinkhorn divergences





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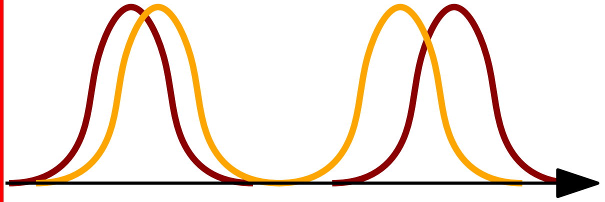

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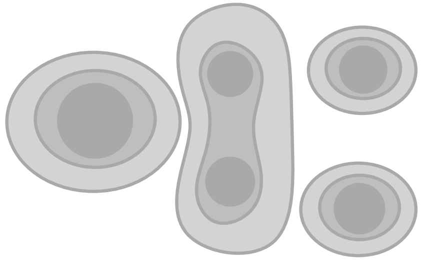
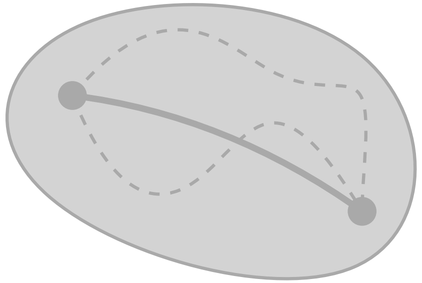




3 - Building a Riemannian geometry out of Sinkhorn divergences

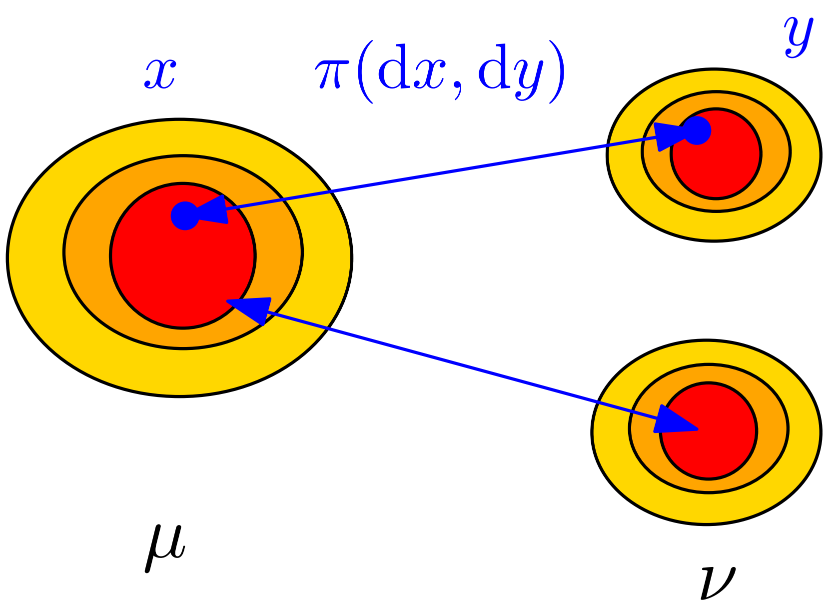
Quadratic optimal transport

(X, d) compact metric space.

Definition

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

Subset of $\mathcal{P}(X \times X)$, coupling between μ and ν



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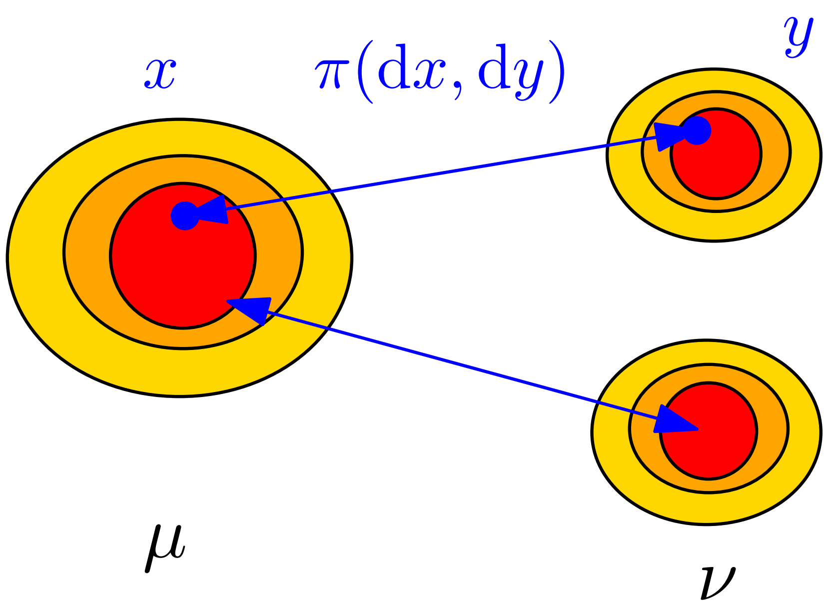
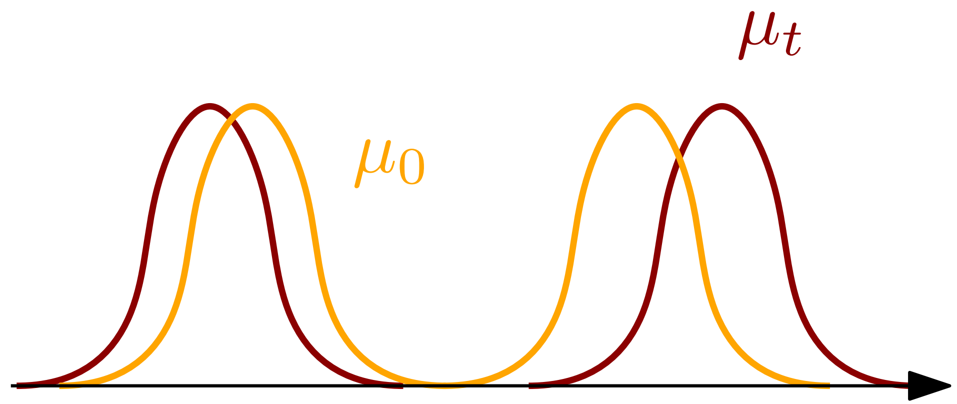


Theorem. OT is the square of a distance on $\mathcal{P}(X)$ metrizing the weak convergence.

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 $\mathrm{OT}(\mu_0, \mu_t)$.



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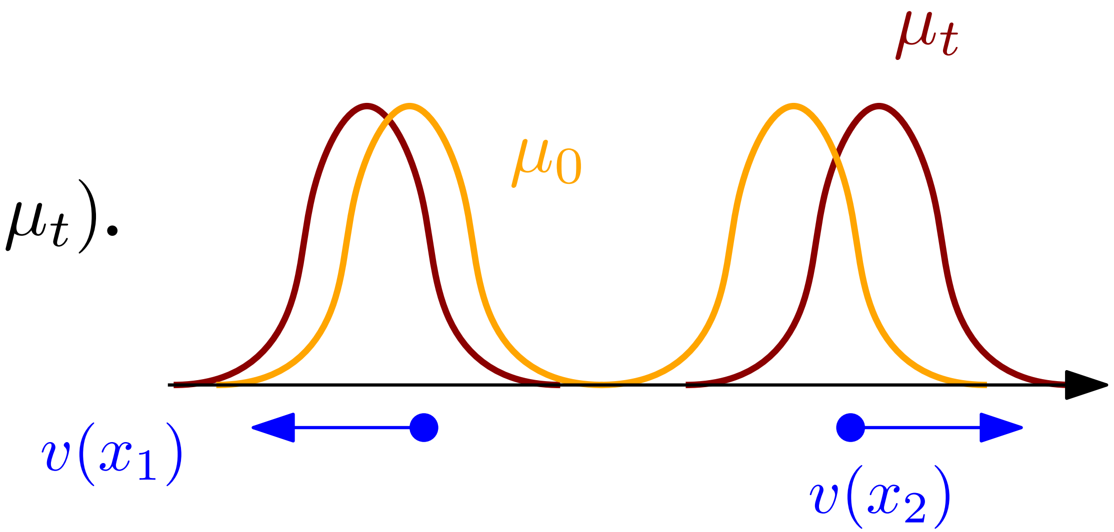

Theorem. $\mathrm{OT}(\mu_0,\mu_t) \sim t^2 \left(\min_v \int_{\mathbb{R}^d} |v(x)|^2 \, \mathrm{d}\mu_0(x) \right),$

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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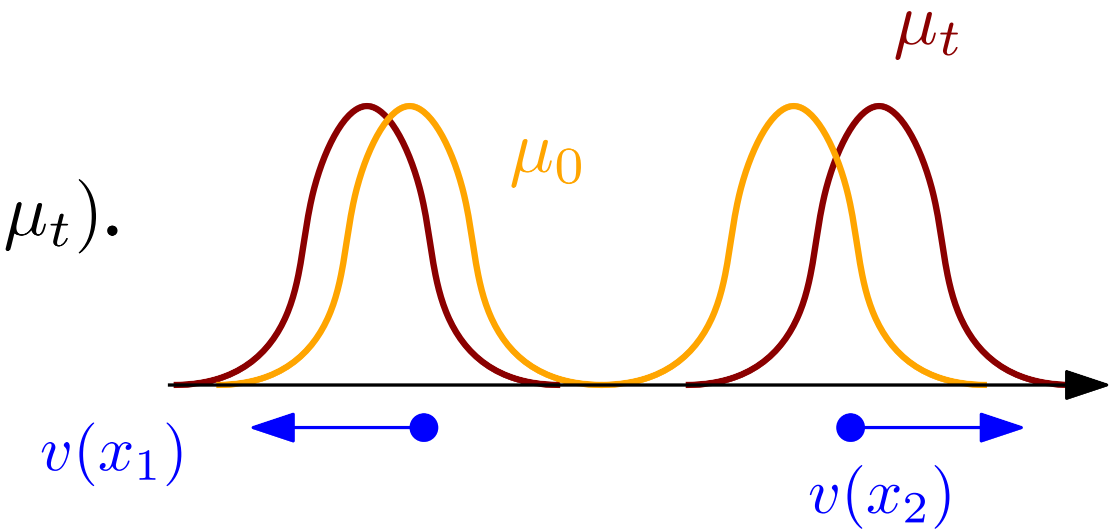

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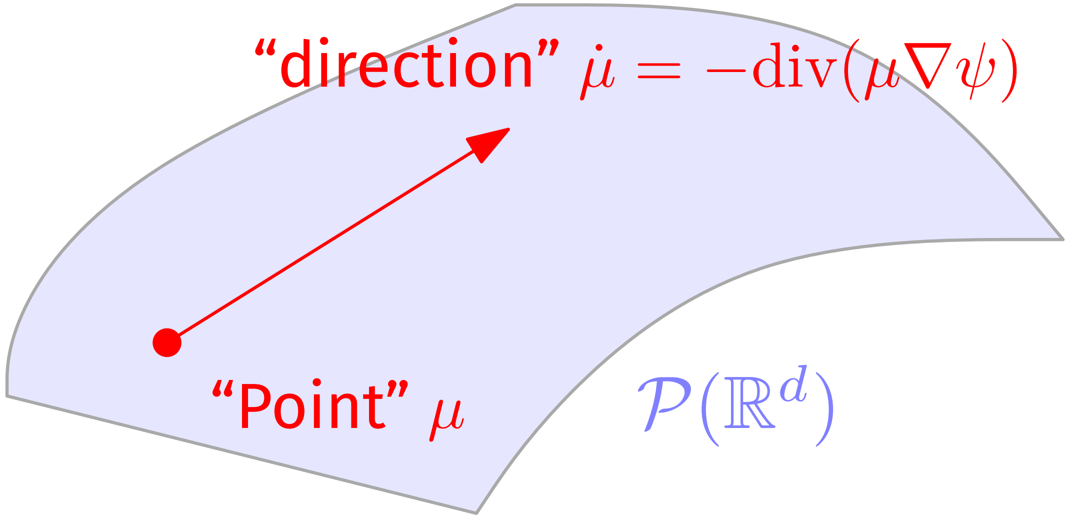
elliptic equation in ψ

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:

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

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

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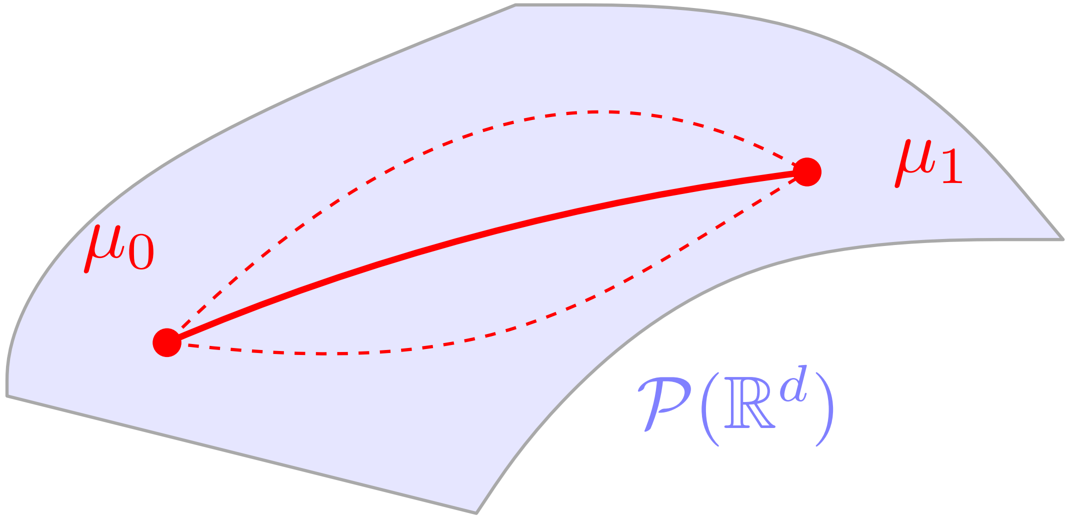

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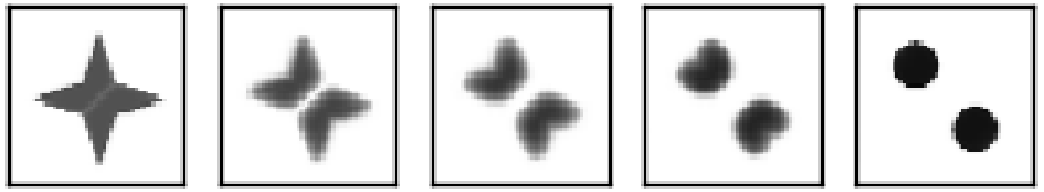
$$\mathrm{OT}(\mu_0, \mu_1) = \min_{(\mu_t)_t} \int_0^1 \mathbf{g}^{\mathrm{OT}}_{\mu_t}(\dot{\mu}_t, \dot{\mu}_t)\,\mathrm{d}t$$

with μ_0, μ_1 fixed.

Minimizers are **geodesics**.

μ_0 μ_0



Example geodesic

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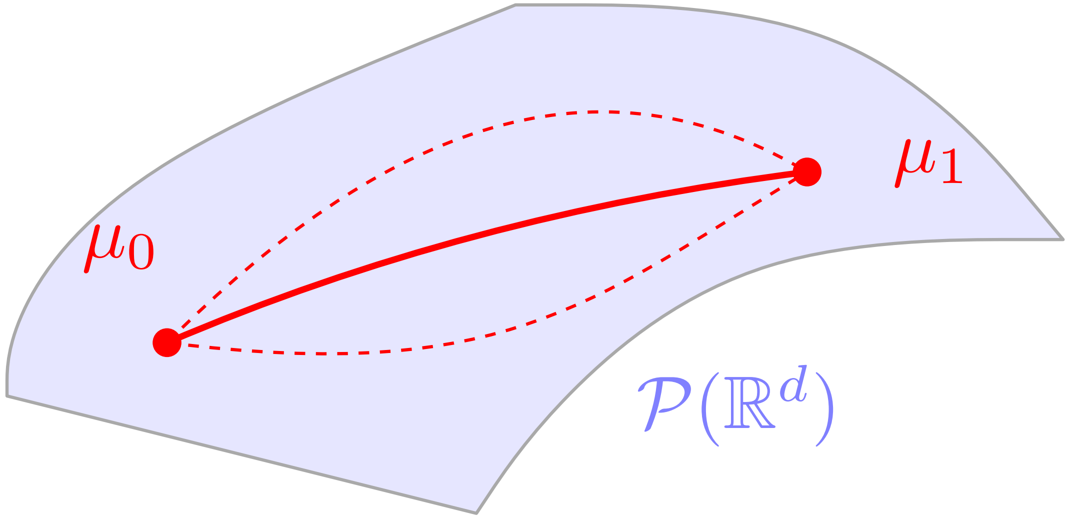

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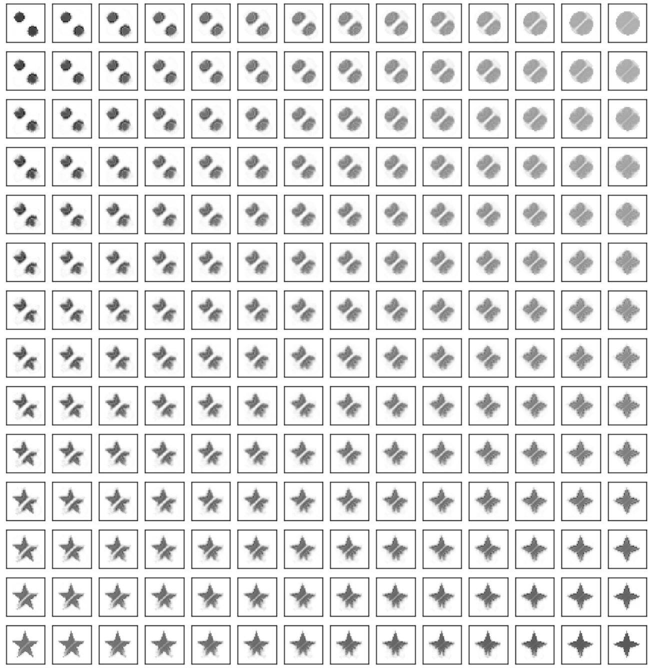

Example harmonic map

Lavenant (2019). Harmonic mappings valued in the Wasserstein space.

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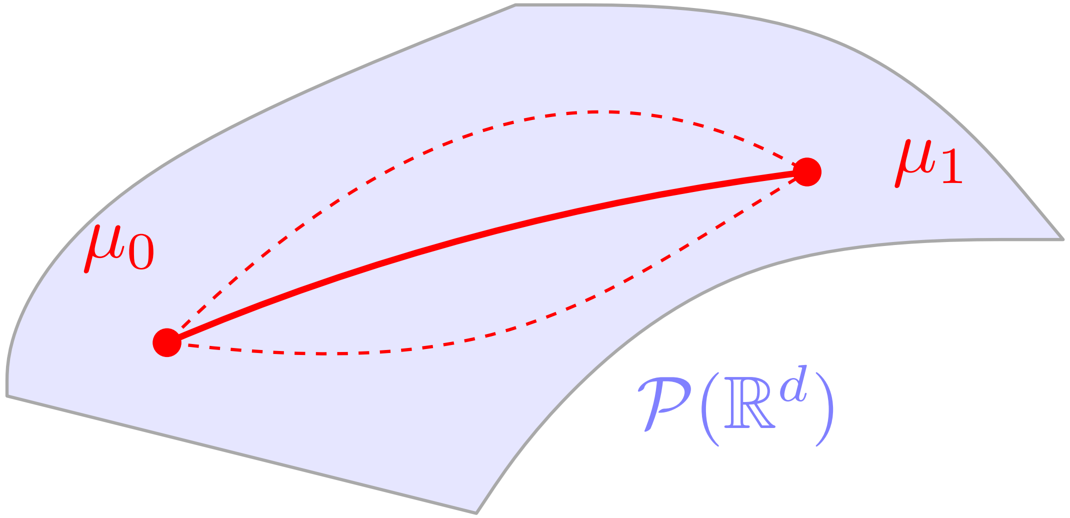

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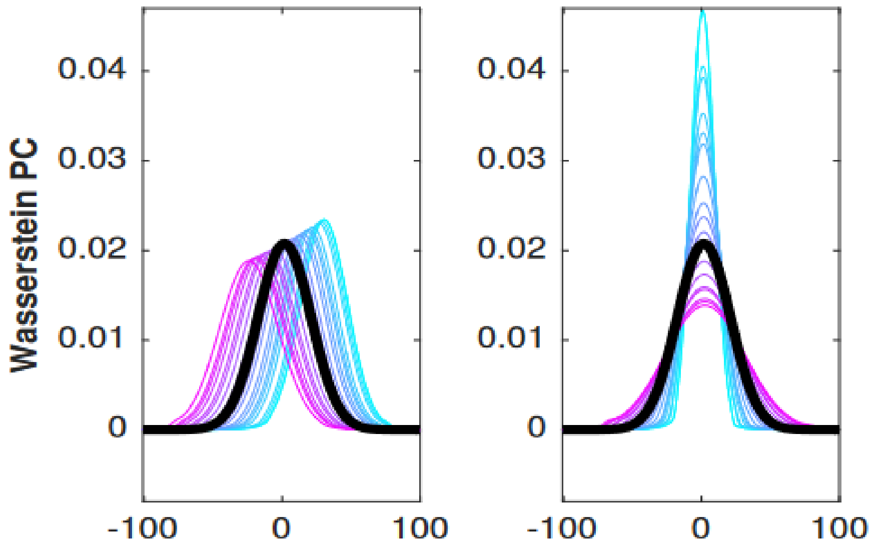
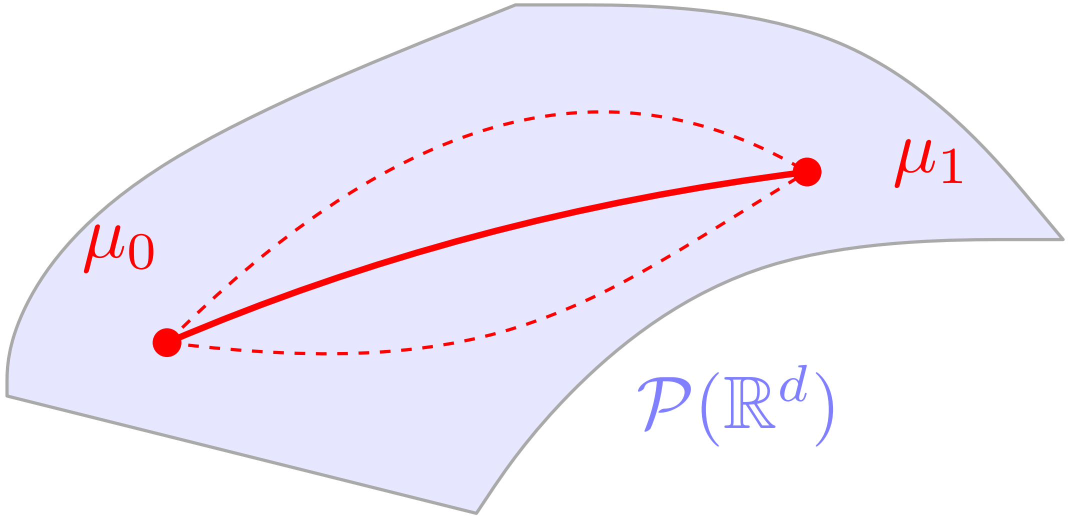


Example: Wasserstein PCA

Cazelles, Seguy, Bigot, Cuturi & Papadakis (2017). Log-PCA versus Geodesic PCA of histograms in the Wasserstein space.

The metric tensor and the geometry of optimal transport



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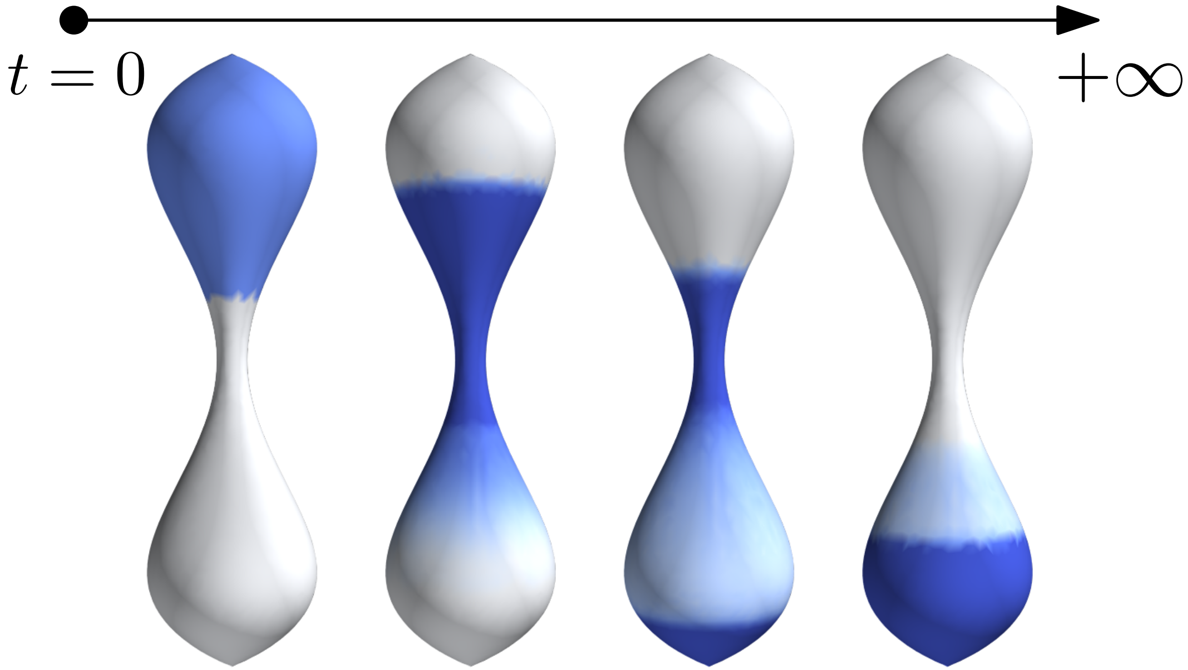
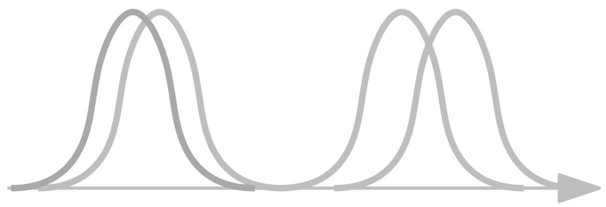


Example gradient flow

Jordan, Kinderlehrer & Otto (1998). The variational formulation of the Fokker–Planck equation.
Ambrosio, Gigli & Savaré (2008). Gradient flows: in metric spaces and in the space of probability measures.



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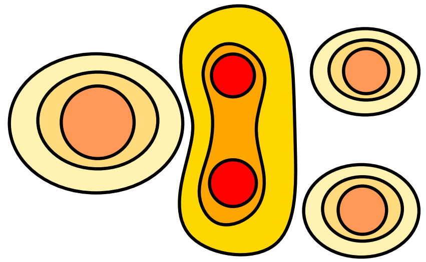
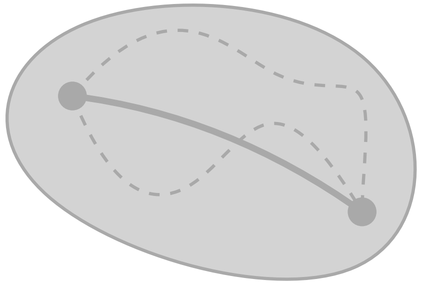




3 - Building a Riemannian geometry out of Sinkhorn divergences

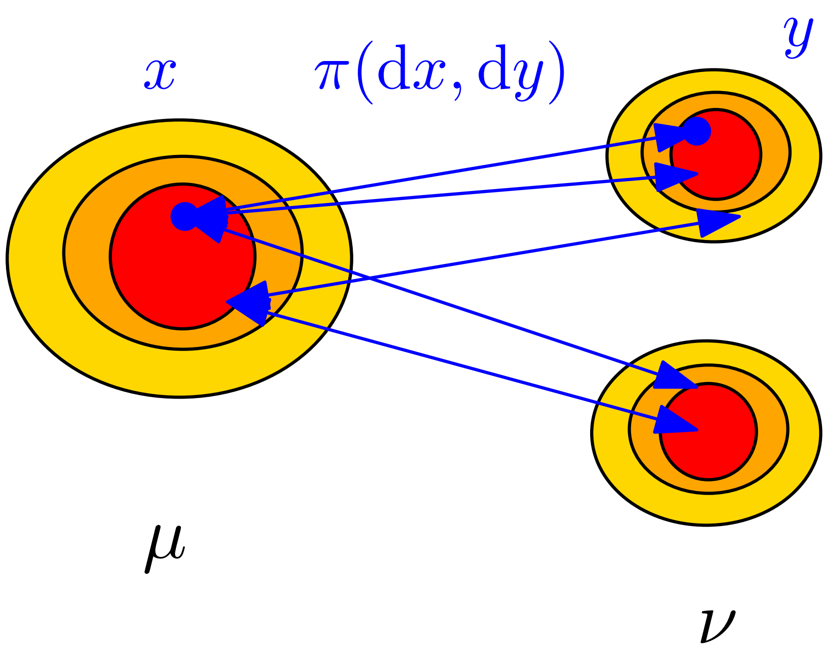
Entropic optimal transport

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

Definition

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

$$\mathrm{KL}(\alpha|\beta) = \int \log(\mathrm{d}\alpha/\mathrm{d}\beta)\mathrm{d}\alpha.$$



Peyré & Cuturi (2019). Computational optimal transport.

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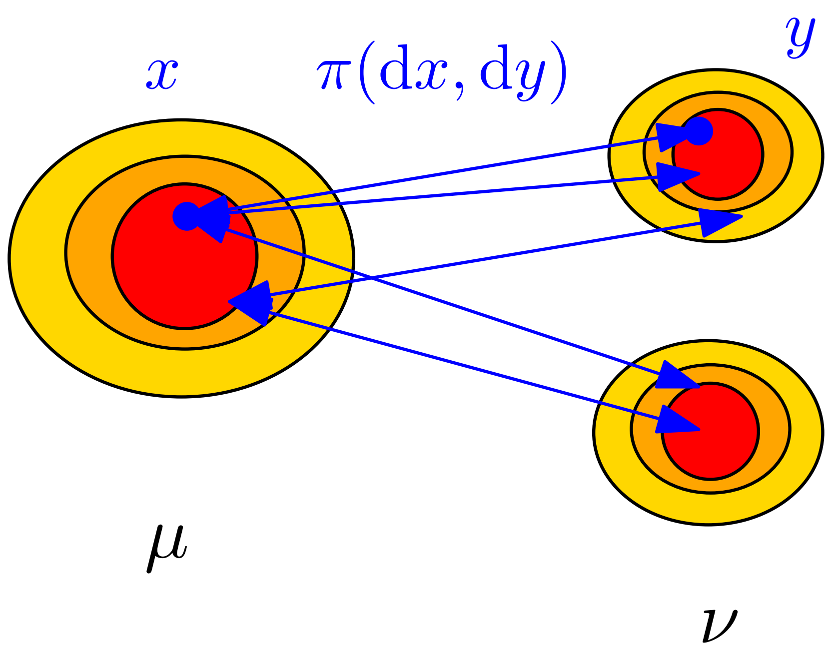


Why?

1. easier to compute (**Sinkhorn algorithm**),
2. better statistical complexity,
3. smoother dependence in (μ,ν).

Peyré & Cuturi (2019). Computational optimal transport.

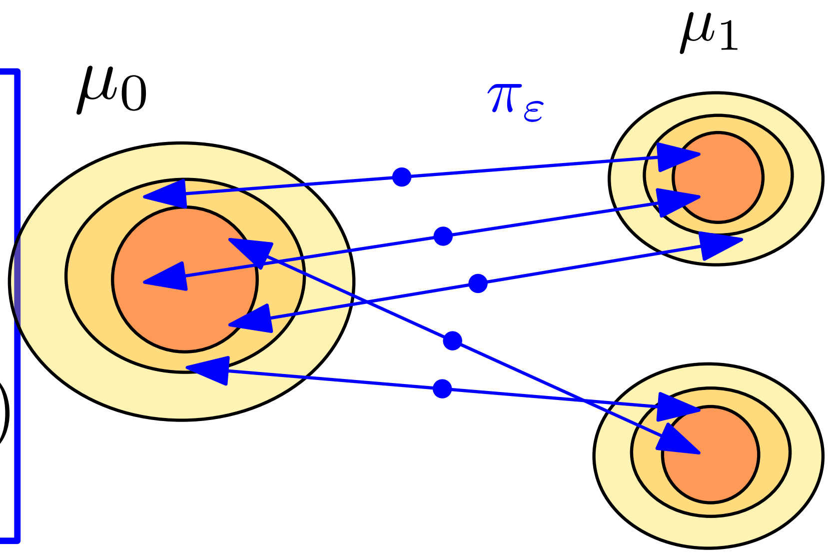
Schrödinger bridges as generalizations of geodesics?

Take c the quadratic cost on $\mathbb{R}^d$.

Select the entropic optimal coupling π_ε and define $(\mu_t)_t$ **Schrödinger bridge** between μ_0 and μ_1:

$$\mu_t = \iint_{\mathbb{R}^d \times \mathbb{R}^d} \mathcal{N}\left((1-t)x + ty, \frac{t(1-t)\varepsilon}{2} \right) \, \mathrm{d}\pi_\varepsilon(x,y)$$

Gaussian distribution



Léonard (2013). A survey of the Schrödinger problem and some of its connections with optimal transport.

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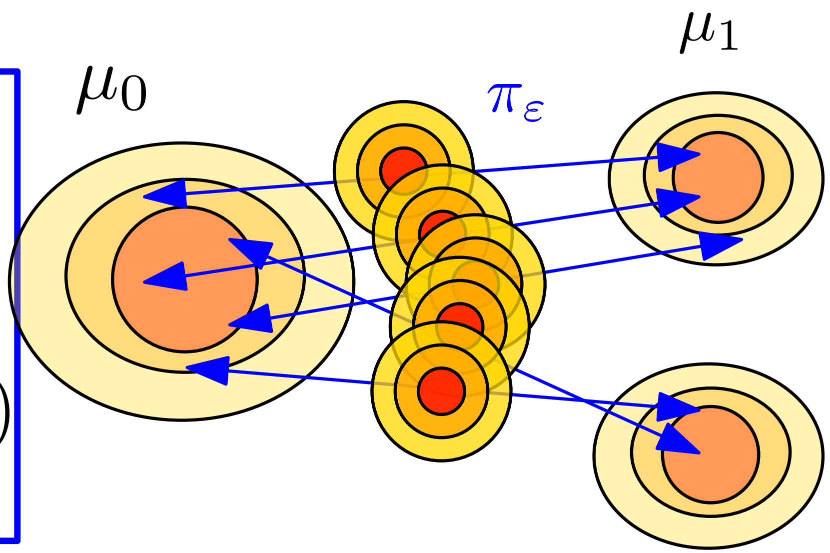

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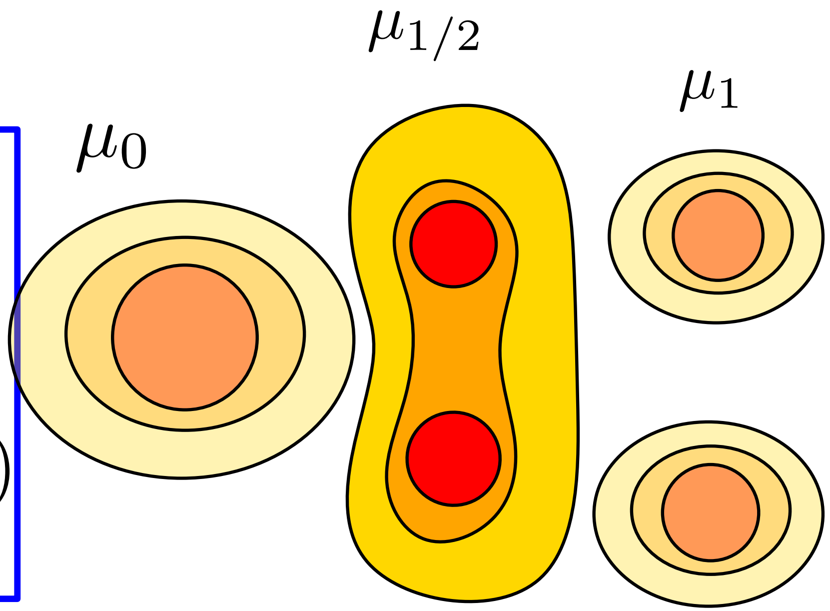

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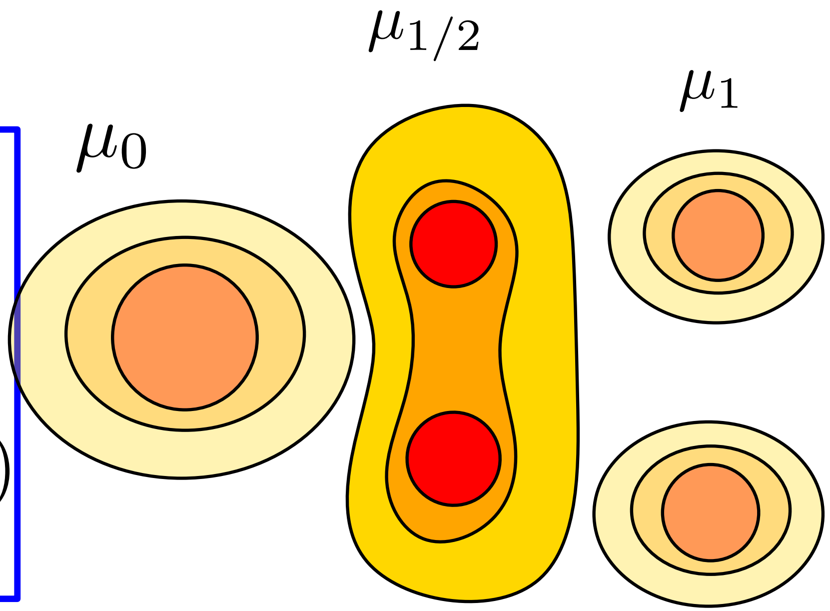

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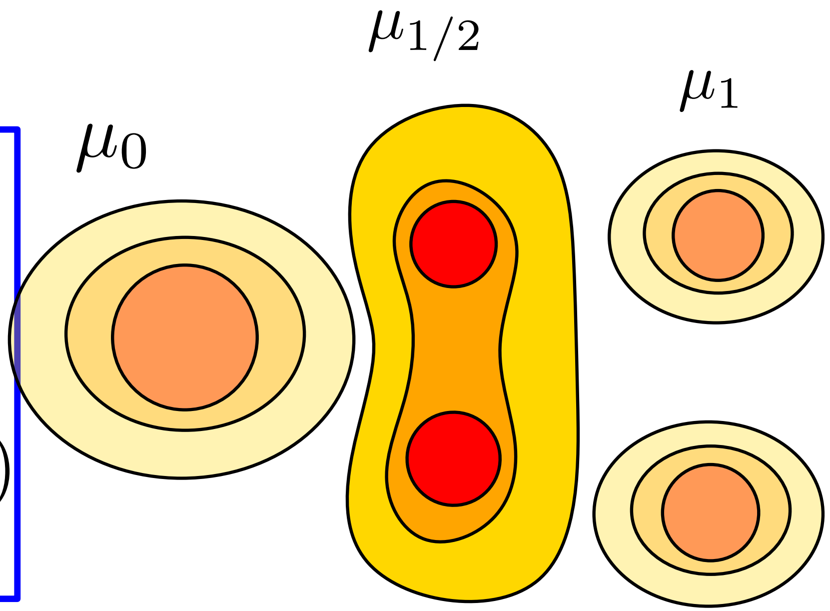

- Interpolates between μ_0 and μ_1, converges to OT geodesic as $\varepsilon \to 0$.
- **But** the bridge between μ and itself is **not** $\mu_t = \mu$ for all t.
- **But** the temporal rescaling of a ε-bridge by τ is a $\tau\varepsilon$-bridge.

Léonard (2013). A survey of the Schrödinger problem and some of its connections with optimal transport.

Sinkhorn divergence as a distance?

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

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

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

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Theorem (Feydy et al., 2019). Assume $\exp(-c/\varepsilon)$ positive definite universal kernel.

1. $S_\varepsilon(\mu,\nu) \geq 0$ with equality iff $\mu = \nu$.
2. $S_\varepsilon(\mu_n,\mu) \to 0$ iff $\mu_n \to \mu$ weakly.
3. S_ε convex in each of its inputs.

Assumption until the end of the talk

Genevay, Peyré, & Cuturi (2018). Learning generative models with Sinkhorn divergences.
Feydy, Séjourné, Vialard, Amari, Trouvé & Peyré (2019). Interpolating between optimal transport and MMD using Sinkhorn divergences.

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But $\sqrt{S_\varepsilon}$ does not satisfy the triangle inequality.

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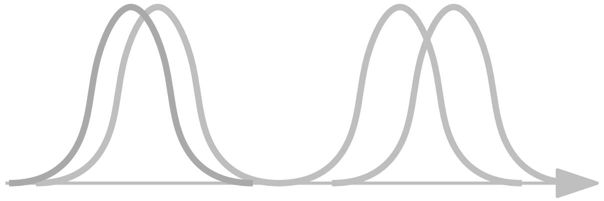
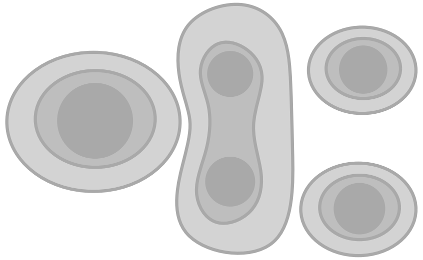
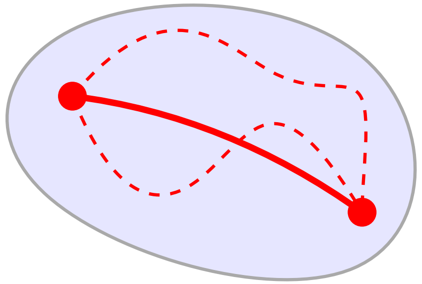


1 - Optimal transport and its geometry

2 - Entropic optimal transport and Sinkhorn divergences





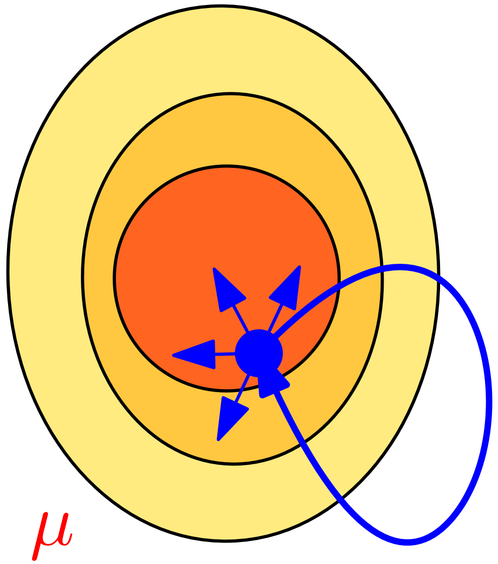
3 - Building a Riemannian geometry out of Sinkhorn divergences

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

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

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

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



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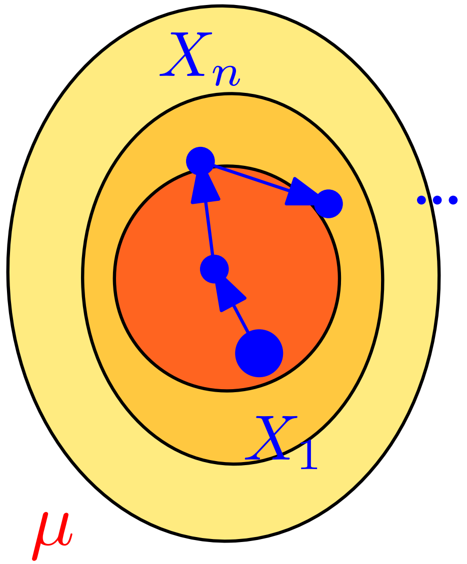

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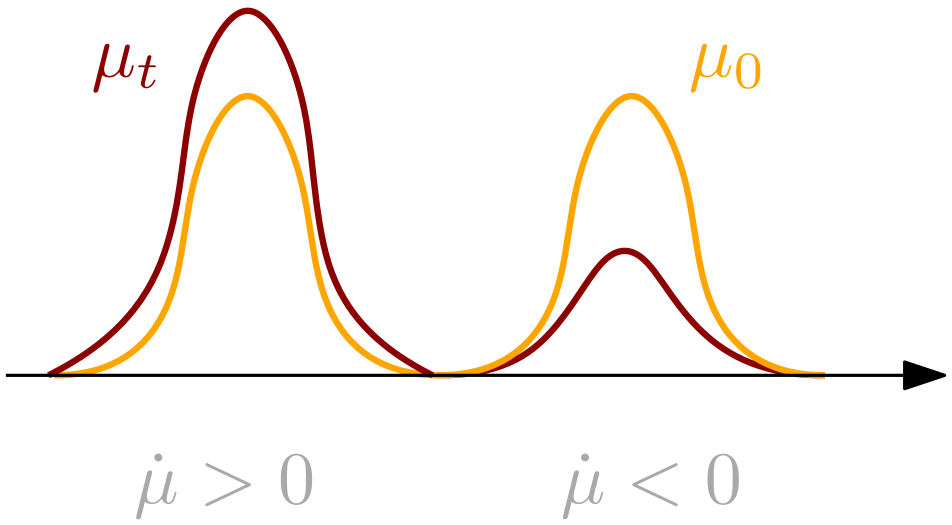
Interpretation. Take $X_1, \ldots, X_n, \ldots$ Markov chain with $(X_n, X_{n+1}) \sim \pi_\varepsilon$. Then:

1. Invariant distribution μ,
2. Reversible Markov chain,
3. Transition probability close to $\exp(-c(x, y)/\varepsilon)$.

Gaussian kernel if c quadratic

The Hessian of the Sinkhorn divergence

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



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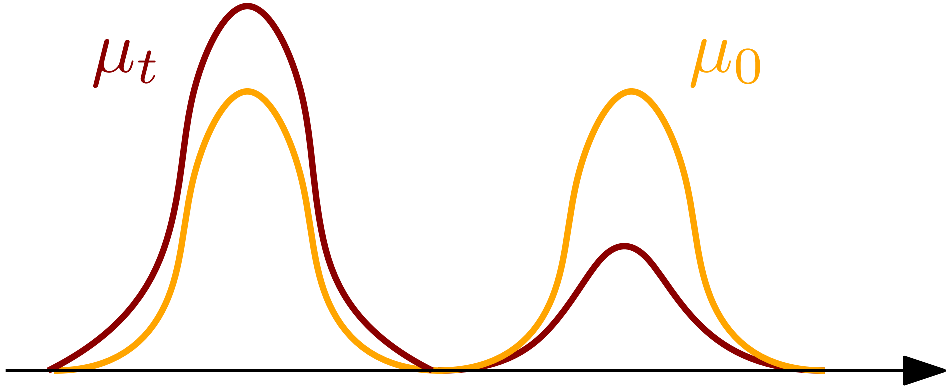
Theorem.

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



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

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

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

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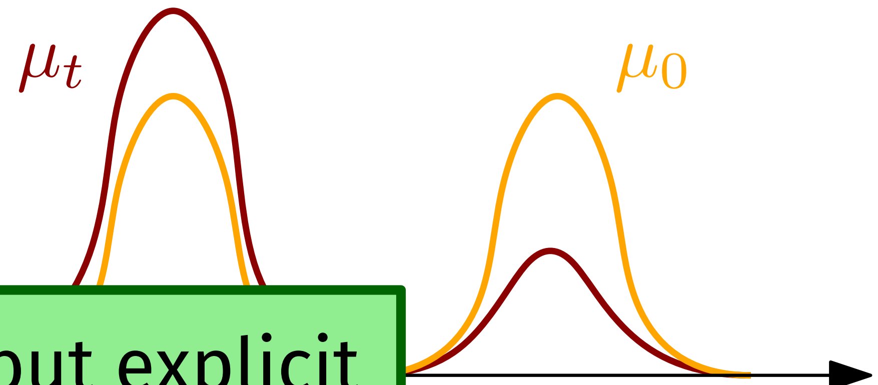

Main message: heavy but explicit and interpretable formula!

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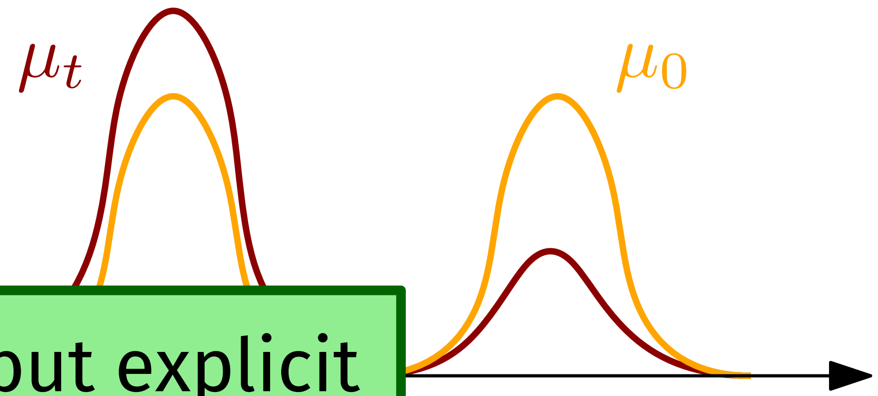

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Same formula

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

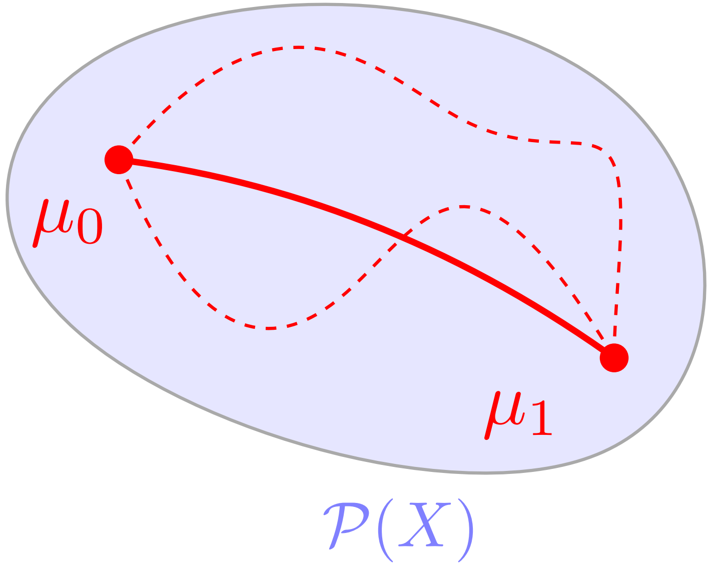
Definition of the distance and main results

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

Definition. Given μ_0, μ_1:

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

where infimum over (μ_t) on a class of path to be specified later.



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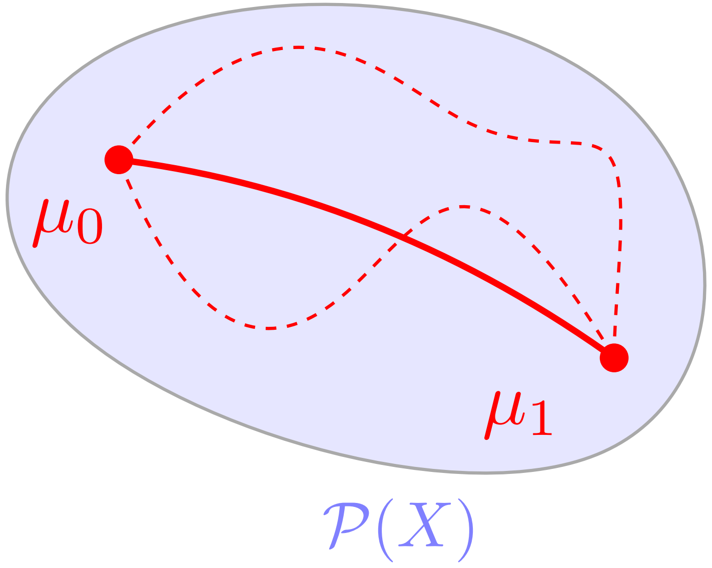

Theorem. d_S is a distance over $\mathcal{P}(X)$ **metrizing weak convergence of measures,** and the infimum in the definition is reached (**geodesics exist**).

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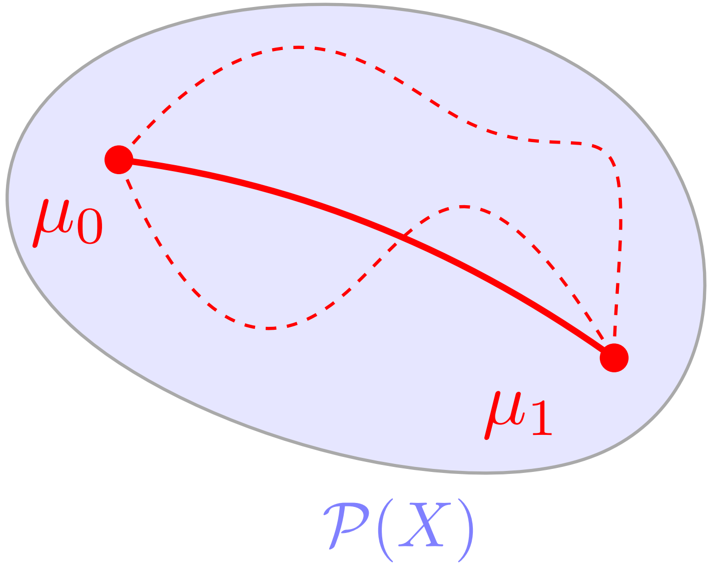

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Next slides: elements of the proof (and of functional analysis!).

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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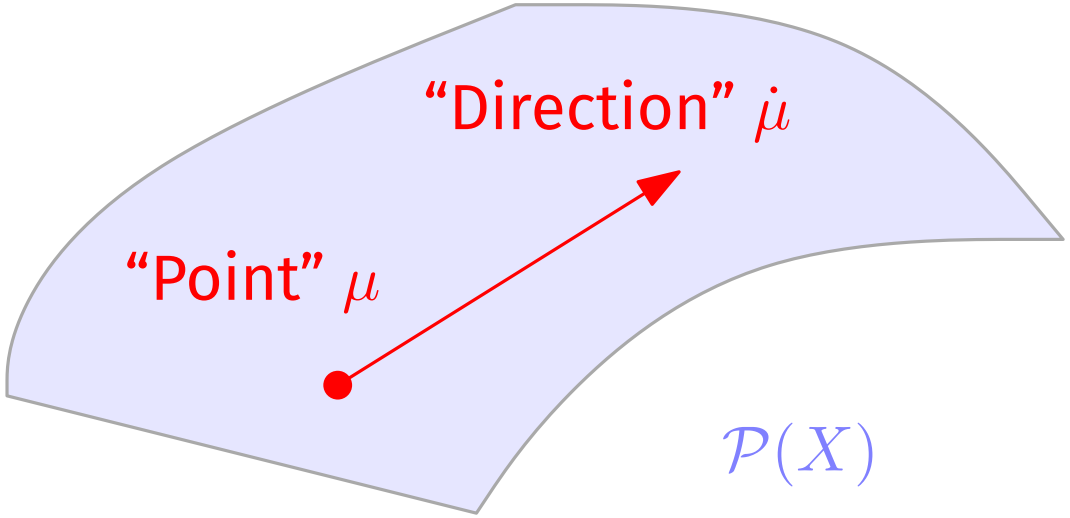
In our case:

Typically smooth functions!

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

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

The tangent space



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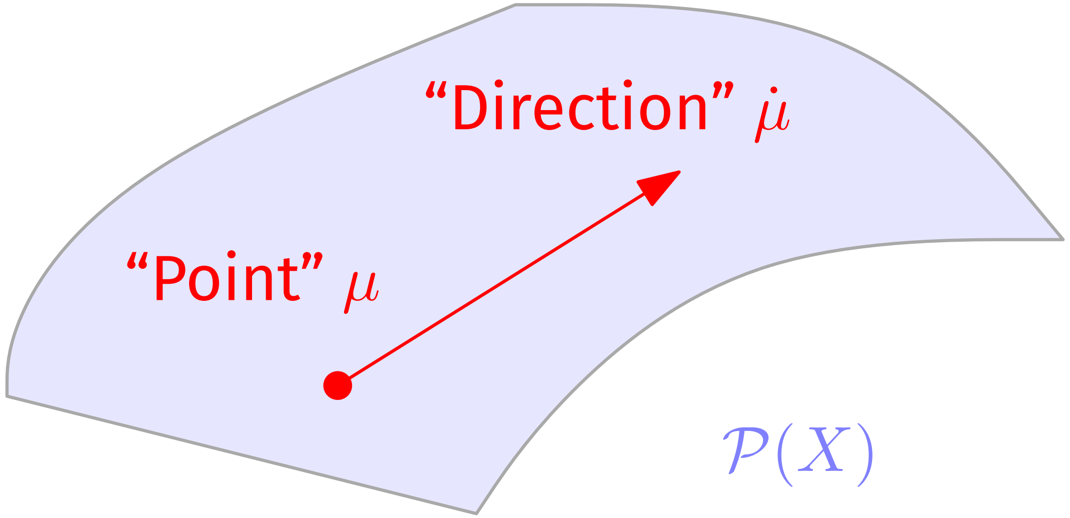
- $\mathbf{g}_\mu(\dot{\mu}, \dot{\mu}) = \frac{\varepsilon}{2} \langle \dot{\mu}, (\mathrm{Id} - K_\mu^2)^{-1} H_\mu[\dot{\mu}] \rangle$
  quadratic form in $\dot{\mu}$
- $\mathcal{H}_\mu$ RKHS with kernel k_μ.

The tangent space



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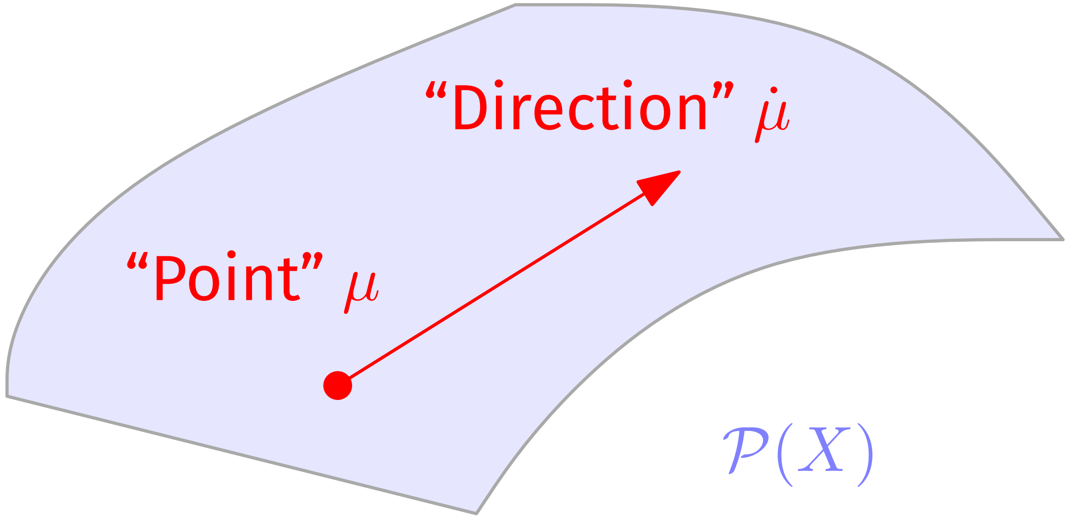
Theorem. The completion of signed measures with zero mass with respect to $\mathbf{g}_\mu$ is $\mathcal{H}^*_{\mu,0}$ the space of linear forms σ on $\mathcal{H}_\mu$ with $\langle \sigma, 1\rangle = 0$.

That is, we want $\left| \frac{\mathrm{d}}{\mathrm{d}t} \int \phi \, \mathrm{d}\mu_t \right| \leq C \|\phi\|_{\mathcal{H}_\mu}$ for any $\phi \in \mathcal{H}_\mu$.

The tangent space



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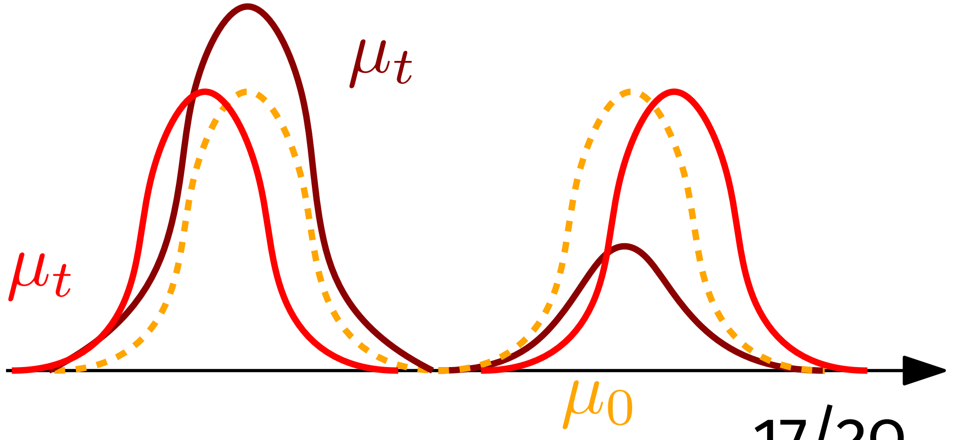
If c quadratic cost, both $\dot\mu$ signed measure (“**vertical**”) and $\dot\mu = -\mathrm{div}(\mu v)$ (“**horizontal**”) are in the tangent space $\mathcal{H}^*_{\mu,0}$.



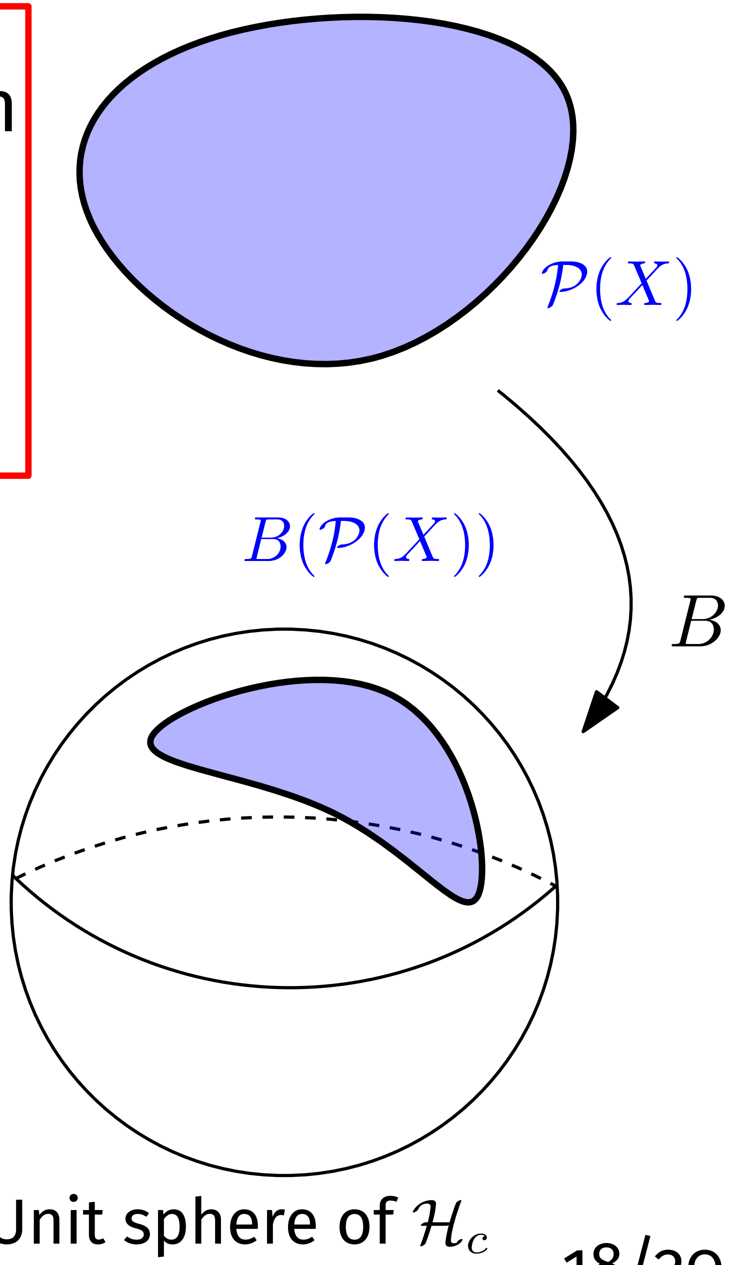
A useful change of variable

Define:

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

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

Theorem. The map B is an homeomorphism onto its image, included in unit sphere of $\mathcal{H}_c$.



(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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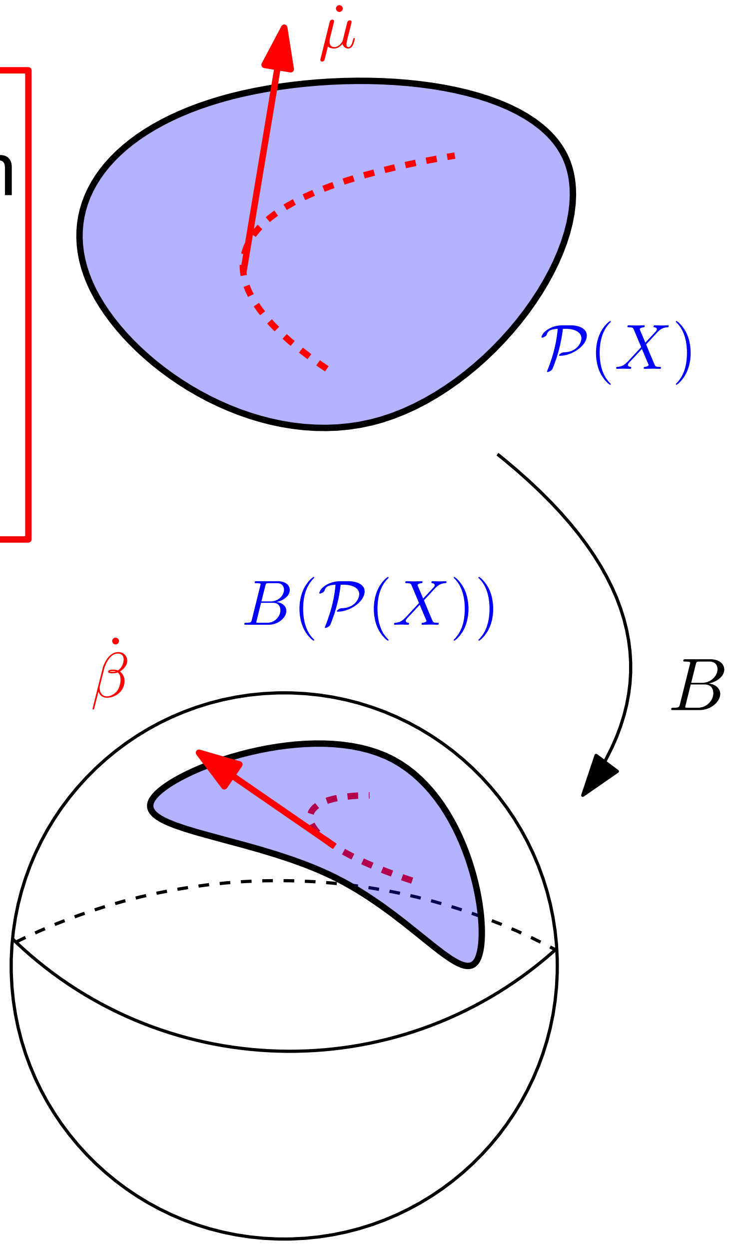
- $\tilde{\mathbf{g}}_\mu(\dot\beta, \dot\beta) \asymp \|\dot\beta\|^2_{\mathcal{H}_c}$ uniformly in μ (but not in ε).



Unit sphere of $\mathcal{H}_c$

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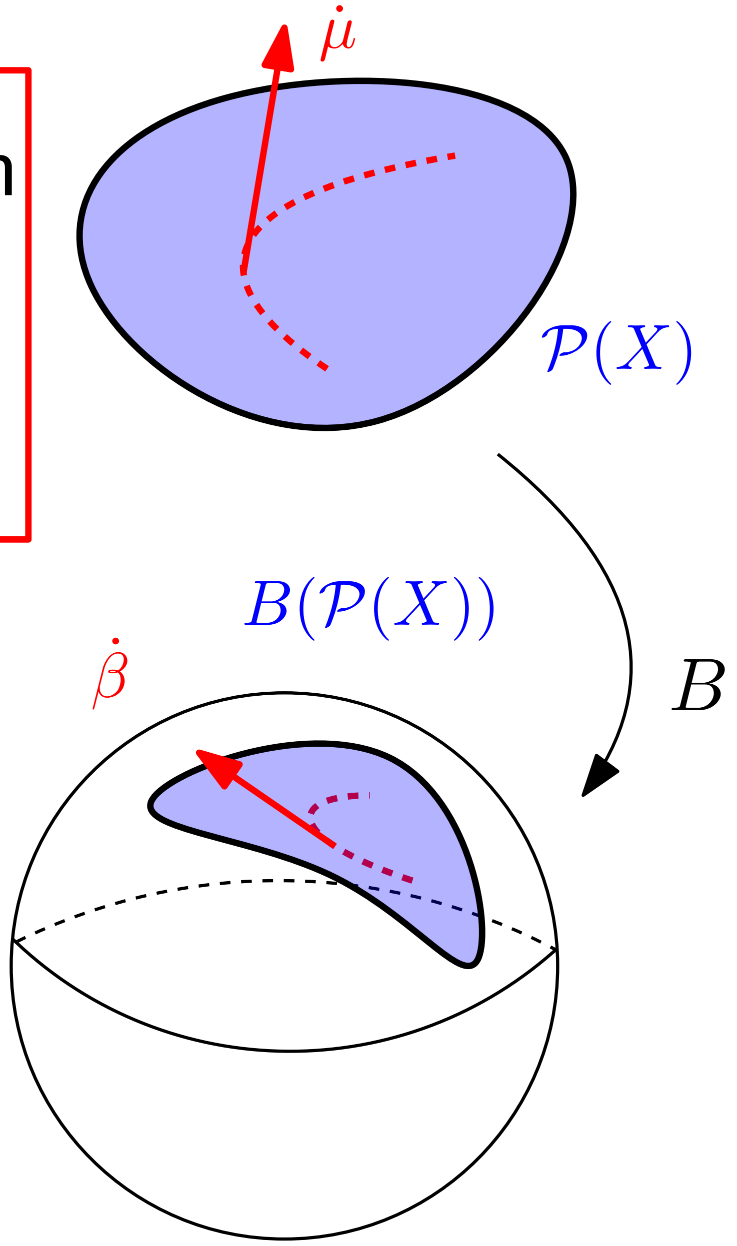

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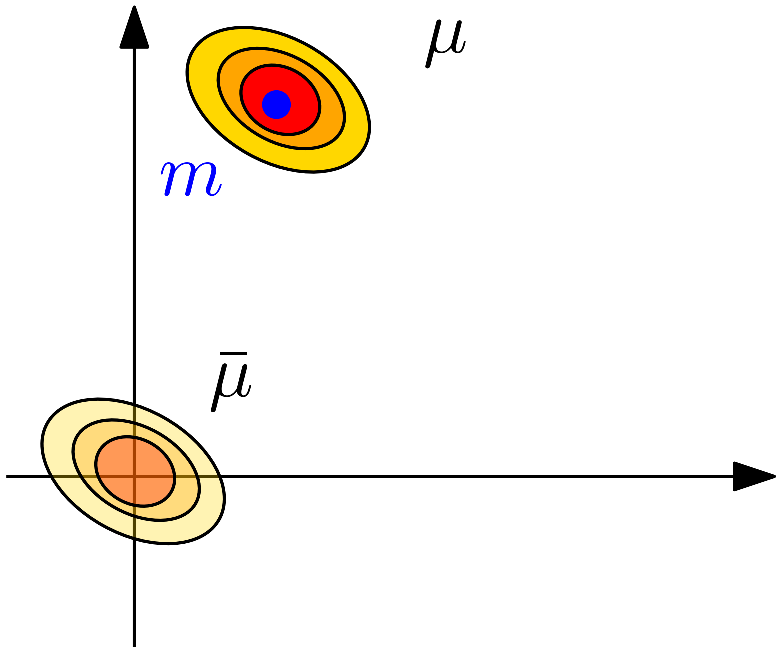
Consequence. Admissible paths: $(\beta_t)_t$ H^1 valued in $\mathcal{H}_c$,

$$c_\varepsilon \|\beta_1 - \beta_0\|_{\mathcal{H}_c} \leq \mathbf{d}_S(\mu_0, \mu_1) \leq C_\varepsilon \|\beta_1 - \beta_0\|_{\mathcal{H}_c}.$$

The quadratic case

Previous results hold for **any** compact space X if $\exp(-c/\varepsilon)$ positive definite universal kernel.



Now $X \subset \mathbb{R}^d$ and $c(x, y) = |x - y|^2$.

If $\mu \in \mathcal{P}(X)$, m barycenter and $\bar{\mu}$ centered part.

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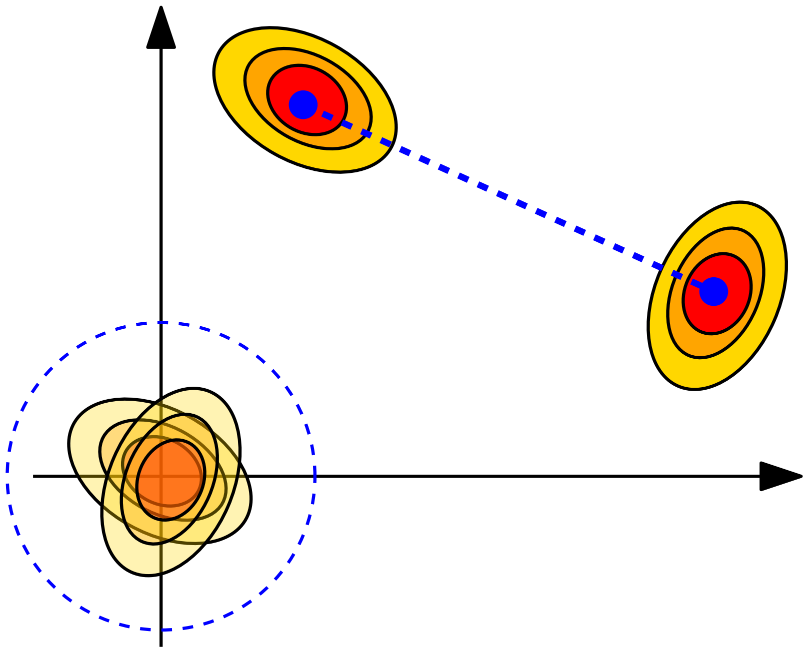

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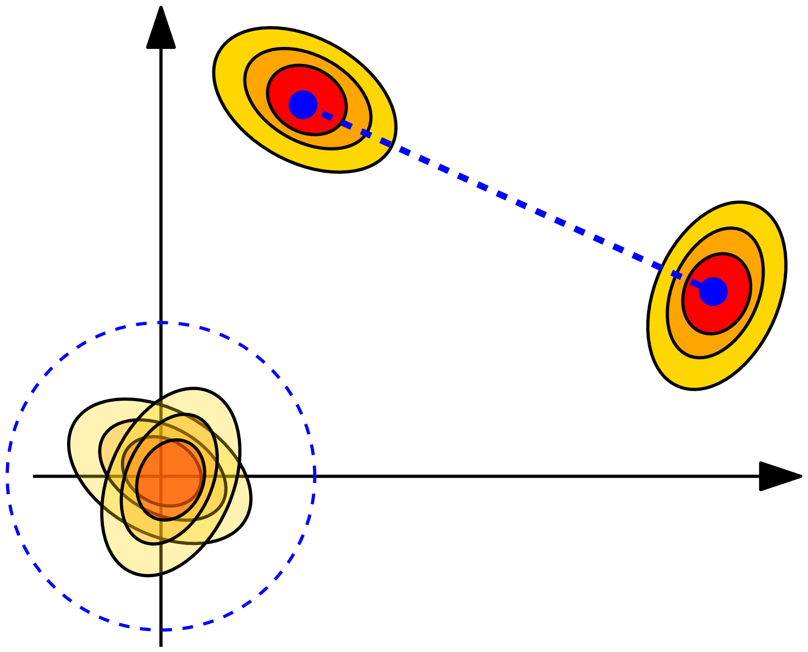

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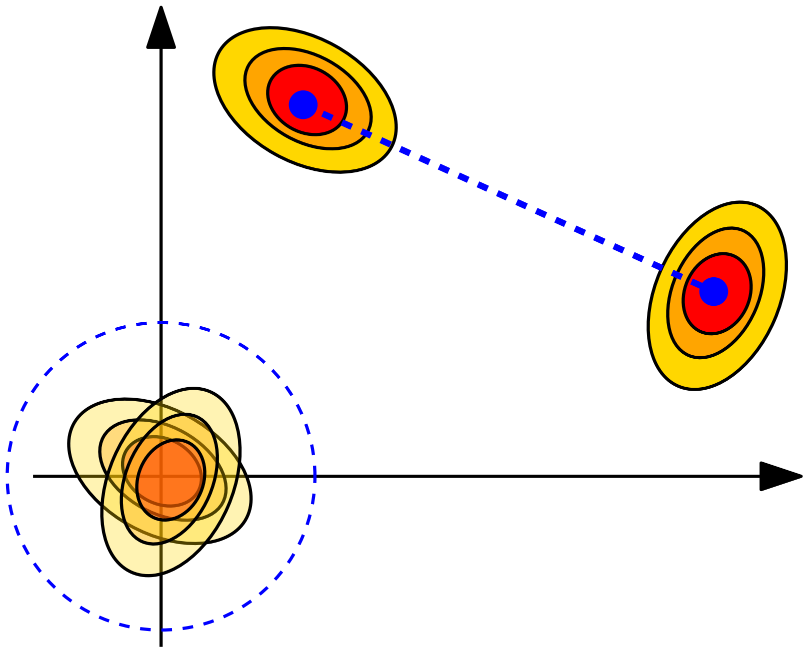

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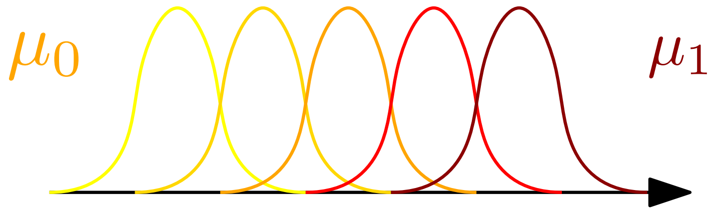

Consequence: constant-speed translations are geodesics.

Conclusion and open questions

What I have not presented

- Explicit formula for Gaussians and the “two points” space.
- Example showing the Sinkhorn divergence is **not** jointly convex.

Open questions and future directions

- Limit $\varepsilon \to 0$ towards optimal transport.
- Numerical approximation of the distance?
- Gradient flows with respect to d_S (ongoing work with Mathis Hardion).

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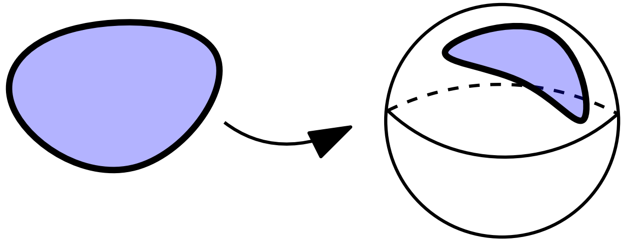

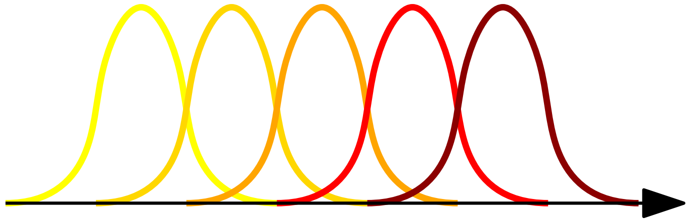

Thank you for your attention