An optimal transport problem with bulk/interface interactions

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Dynamics and Discretization: PDEs, Sampling, and Optimization
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UNIVERSITÉ DE LORRAINE

$\langle \phi | \mu \rangle$ *Grupo de Física Matemática da Universidade de Lisboa*

FCT Fundação para a Ciência e a Tecnologia
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Motivation

- [JKO '98, Otto '00] Fokker-Planck $=$ gradient-flow with respect to OT geometry
- [Maas '11, Mielke '11, Chow-Huang-Li-Zhou '12] discrete counterpart for irreducible reversible Markov processes

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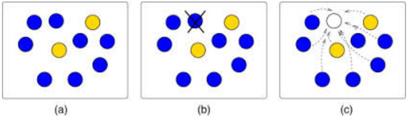

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$$\xrightarrow{N\to\infty}$$

$$\mathrm{d}X_t = \sqrt{X_t(1-X_t)}\mathrm{d}B_t$$

or

$$\partial_t \rho = \Delta\left(x(1-x)\rho\right)$$

Kimura eq. $x \in [0, 1]$

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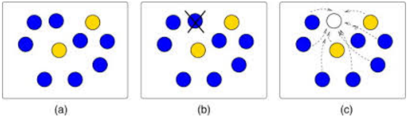

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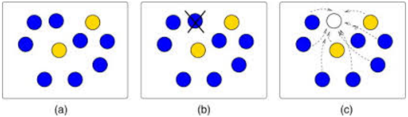

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Need for an adapted bulk/interface geometry!

(but failed in the end)

In this talk $\Omega \subset \mathbb{R}^d$ is compact and $\partial\Omega \subset \Omega$

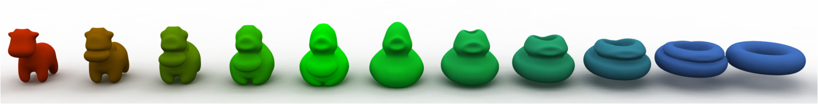
Dynamical OT

Theorem (Benamou-Brenier '00)

For $\rho_0, \rho_1 \in \mathcal{P}(\Omega)$ *the* **Wasserstein distance**

$$\mathcal{W}^2(\rho_0, \rho_1) = \min_{\rho, v} \left\{ \int_0^1 \int_\Omega \frac{1}{2} |v_t(x)|^2 \mathrm{d}\rho_t(x) \, \mathrm{d}t \quad s.t. \quad \partial_t \rho_t + \mathrm{div}(\rho_t v_t) = 0 \right\}$$

with $\rho|_{t=0,1} = \rho_{0,1}$ *and no-flux boundary conditions on* $\partial\Omega$



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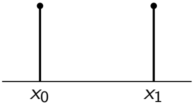
$\rho_t = \delta_{x_t}$



mass conservative, based on horizontal displacements

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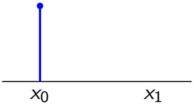

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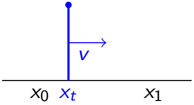

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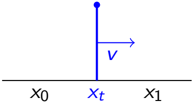

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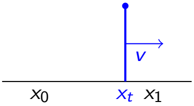

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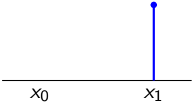

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Dynamical reaction

Definition (Fisher-Rao)

For $\rho_0, \rho_1 \in \mathcal{M}^+(\Omega)$ with possibly $|\rho_0| \neq |\rho_1|$

$$\mathcal{FR}^2(\rho_0, \rho_1) = \min_{\rho, r} \left\{ \int_0^1 \int_\Omega \frac{1}{2} |r_t(x)|^2 \mathrm{d}\rho_t(x)\, \mathrm{d}t \quad \text{s.t.} \quad \partial_t \rho_t = \rho_t r_t \right\}$$

popular in statistics and geometric information theory $\rightsquigarrow$ Fisher information metric

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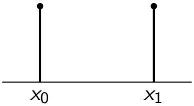

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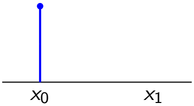

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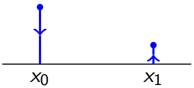

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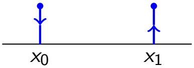

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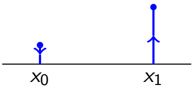

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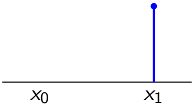

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Unbalanced OT

Definition/theorem (Wasserstein-Fisher-Rao)

For $\rho_0, \rho_1 \in \mathcal{M}^+(\Omega)$ and $\kappa > 0$

$$\mathcal{WFR}_\kappa^2(\rho_0, \rho_1) := \min_{\rho, v, r} \left\{ \int_0^1 \int_\Omega \frac{1}{2} \left(|v_t(x)|^2 + \kappa^2 |r_t(x)|^2 \right) \mathrm{d}\rho_t(x)\, \mathrm{d}t \quad \text{s.t.} \quad \partial_t \rho_t + \mathrm{div}(\rho_t v_t) = \rho_t r_t \right\}$$

is a distance on $\mathcal{M}^+(\Omega)$ with nice properties [KMV '16, LMS '18, CPSV '18]

Infimal convolution between horizontal Wasserstein and vertical Fisher-Rao

Some convex analysis

$$\partial_t \rho_t + \mathrm{div}(\rho_t v_t) = \rho_t r_t \qquad \int_0^1 \int_\Omega \frac{1}{2} \left(|v_t(x)|^2 + \kappa^2 |r_t(x)|^2 \right) \mathrm{d}\rho_t(x) \, \mathrm{d}t$$

- mass/momentum variables, convex 1-homogeneous action

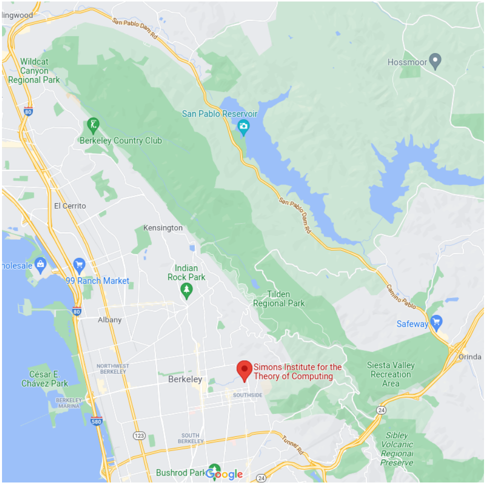
$$(\rho, G, f) = (\rho, \rho v, \rho r) \qquad \text{and} \qquad (|v|^2 + \kappa^2 r^2)\rho = \frac{|G|^2 + \kappa^2 |f|^2}{\rho}$$

- convex constraint/functional over measures $(\rho, G, f) \in \mathcal{M}^+ \times \mathcal{M}^d \times \mathcal{M}$

$$\partial_t \rho_t + \mathrm{div}\, G_t = f_t \qquad \frac{1}{2} \int_0^1 \int_\Omega \frac{|G_t|^2 + \kappa^2 |f_t|^2}{\rho_t} \mathrm{d}t$$

The bulk/interface setup

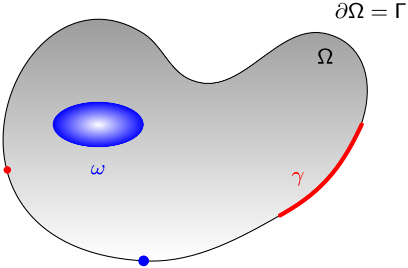
(AKA the ring-road)



Key ingredients:

- ✓ transport in the city
- ✓ transport on the road
- ✓ a toll cost $\kappa > 0$

Ω = downtown, $\Gamma = \partial\Omega$ = ring-road



Think ω = cars in the city Ω, and γ = cars on the road Γ

$$\mathcal{P}^{\oplus}(\Omega) := \left\{ \rho = (\omega, \gamma) \in \mathcal{M}^+(\Omega) \times \mathcal{M}^+(\Gamma) \quad \text{s.t.} \quad |\omega| + |\gamma| = 1 \right\}$$

The ring-road distance

Definition/theorem [M '20]

For $\rho_0, \rho_1 \in \mathcal{P}^{\oplus}(\Omega)$

$$\mathcal{W}_\kappa^2(\rho_0,\rho_1) = \min \left\{ \int_0^1 \int_\Omega \frac{|F_t|^2}{2\omega_t} \mathrm{d}t + \int_0^1 \int_\Gamma \frac{|G_t|^2 + \kappa^2 |f_t|^2}{2\gamma_t} \mathrm{d}t \right.$$

$$\left. \text{s.t.} \quad \begin{array}{ll} \partial_t \omega_t + \mathrm{div}(F_t) = 0 & \text{in } \Omega \\ F_t \cdot n = f_t & \text{on } \partial\Omega \end{array} \quad \text{and} \quad \partial_t \gamma_t + \mathrm{div}(G_t) = f_t \text{ in } \Gamma \right\}$$

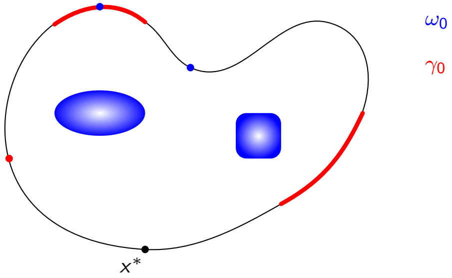
is a distance on $\mathcal{P}^{\oplus}(\Omega)$, and minimizing geodesics $t \mapsto \rho_t$ always exist with

$$\varrho_t = \omega_t + \gamma_t \in \mathcal{P}(\Omega).$$

- only coupled through the flux condition
- weak formulation allows $f \neq 0$ even if $F = 0$
- local stoichiometry $\omega \rightleftharpoons \gamma$ with rate $\partial_t \gamma = f = -\partial_t \omega$

A typical proof: $\mathcal{W}_\kappa(\rho_0, \rho_1) < +\infty$

$$\begin{cases} \partial_t \omega + \operatorname{div} F = 0 & \text{in } \Omega \\ F \cdot n = f & \text{on } \partial\Omega \end{cases} \qquad \text{and} \qquad \partial_t \gamma + \operatorname{div} G = f \quad \text{in } \Gamma$$



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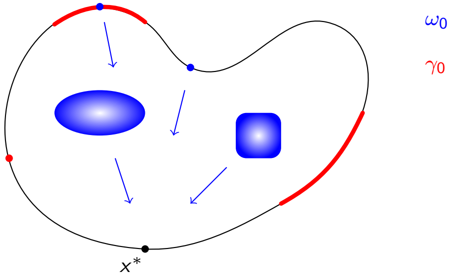

Step 1: pure Wasserstein transport inside Ω with $f = 0$, $G = 0$

finite cost $\quad \mathcal{W}^2_\Omega < \infty$

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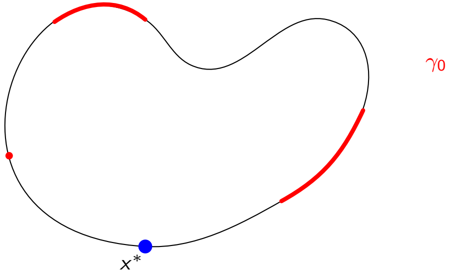

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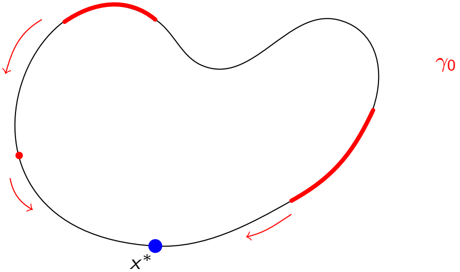

Step 2: pure Wasserstein transport along Γ with $F = 0, f = 0$

finite cost $\quad \mathcal{W}_\Gamma^2 < \infty$

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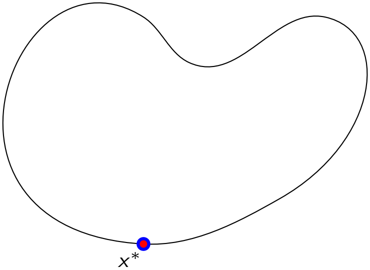

Step 2: pure Wasserstein transport along Γ with $F = 0, f = 0$

finite cost $\quad \mathcal{W}_\Gamma^2 < \infty$

A typical proof: $\mathcal{W}_\kappa(\rho_0, \rho_1) < +\infty$

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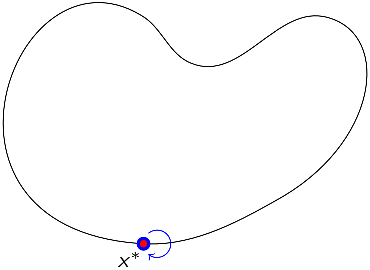

Step 3: pure Fisher-Rao reaction $\omega \rightleftharpoons \gamma$ with $F = 0, G = 0$ and $f > 0$

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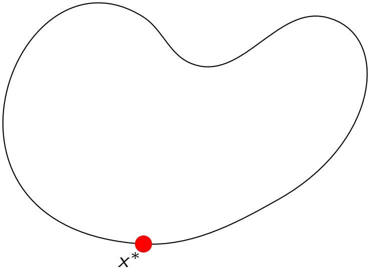

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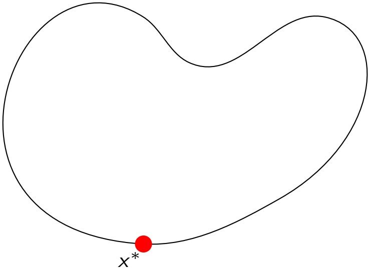

Conclusion: we just connected any arbitrary ρ_0 to $\rho^* = (0, \delta_{x^*})$ with finite cost. □

Duality

Existence by Fenchel-Rockafellar (von Neumann min-max)

$$\inf_{(\omega,\gamma)\in L} \mathcal{A}$$

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$$\mathcal{W}_\kappa^2(\rho_0,\rho_1) = \sup_{\phi,\psi} \left\{ \int_\Omega \phi_1\omega_1 - \phi_0\omega_0 + \int_\Gamma \psi_1\gamma_1 - \psi_0\gamma_0 \quad \text{s.t. } \phi,\psi \in C^1 \text{ and} \right.$$
$$\left. \begin{cases} \partial_t\phi + \frac{1}{2}|\nabla\phi|^2 \leq 0 & \text{in } (0,1)\times\Omega \\ \partial_t\psi + \frac{1}{2}|\nabla\psi|^2 + \frac{1}{2\kappa^2}|\psi-\phi|^2 \leq 0 & \text{in } (0,1)\times\Gamma \end{cases} \right\}$$

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Corollary

For fixed ρ_0, ρ_1 the map $\kappa \mapsto \mathcal{W}_\kappa(\rho_0,\rho_1)$ is monotone $\uparrow$

Proof: $S_{\kappa'} \subset S_\kappa$ for $\kappa' < \kappa$.

□

Optimality and geodesics

$$\mathcal{W}_\kappa^2(\rho_0,\rho_1) = \sup\left\{ \int_\Omega \phi_1\omega_1 - \phi_0\omega_0 + \int_\Gamma \psi_1\gamma_1 - \psi_0\gamma_0 \quad \text{s.t. } (\phi,\psi) \text{ subsolutions} \right\}$$

Hopf-Lax monotonicity suggests saturating HJ inequalities

Theorem (certification)

If $\begin{cases} \partial_t\omega + \mathrm{div}(\omega\nabla\phi) = 0 \\ \partial_t\gamma + \mathrm{div}(\gamma\nabla\psi) = \gamma\frac{\psi-\phi}{\kappa^2} \end{cases}$ with $\begin{cases} \partial_t\phi + \frac{1}{2}|\nabla\phi|^2 = 0 & \omega - \text{a.e.} \\ \partial_t\psi + \frac{1}{2}|\nabla\psi|^2 + \frac{1}{2\kappa^2}|\psi-\phi|^2 = 0 & \gamma - \text{a.e.} \end{cases}$

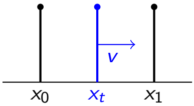
then $t \mapsto \rho_t = (\omega_t,\gamma_t) \in \mathcal{P}^\oplus$ is a minimizing geodesic between ρ_0,ρ_1.

- allows to check optimality of possible ansatz
- determines the built-in Riemannian structure *à la Otto*

One-point geodesics

In classical OT, Eulerian/Lagrangian duality $d^2(x_0, x_1) = \mathcal{W}^2(\delta_{x_0}, \delta_{x_1})$

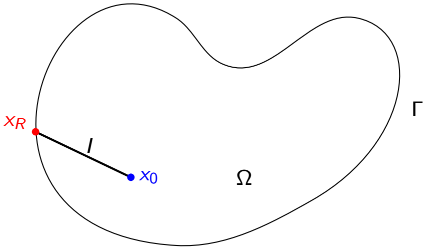
$$\rho_t = \delta_{x_t}$$



$\Longleftrightarrow$

minimizing $\mathcal{W}$-geodesics constant-speed particles

One-point geodesics



Question

Compute the $\mathcal{W}_\kappa$ distance and geodesic between $\rho_0 = (\delta_{x_0}, 0)$ and $\rho_1 = (0, \delta_{x_R})$?

- clearly a 1D problem along I, coordinate $r \in [0, R]$ with $R = |x_R - x_0|$
- cannot simply be a traveling Dirac (∞ cost)

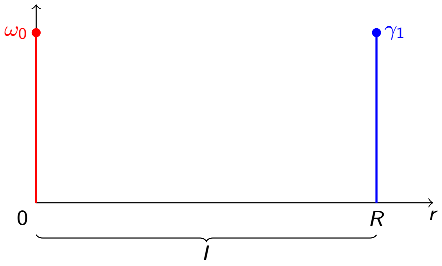
Theorem (one-point geodesics)

For $\rho_0 = (\delta_0, 0)$ and $\rho_1 = (0, \delta_R)$ we have

$$\boxed{\mathcal{W}_\kappa^2(\rho_0, \rho_1) = \frac{1}{2}\frac{\alpha}{\alpha - 1}(R^2 + \alpha\kappa^2)} \qquad \alpha = 1 + \sqrt{1 + \frac{R^2}{\kappa^2}} > 2$$

and the geodesic is

$$\omega_t = \alpha \left(\frac{Rt}{r}\right)^\alpha \frac{1}{r}\chi_{[Rt,R]}(r)\mathrm{d}r \qquad \text{and} \qquad \gamma_t = t^\alpha$$



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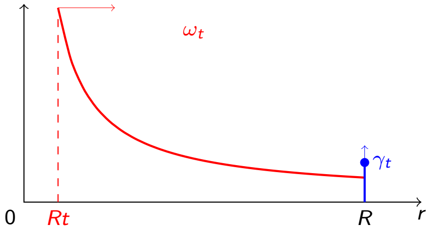

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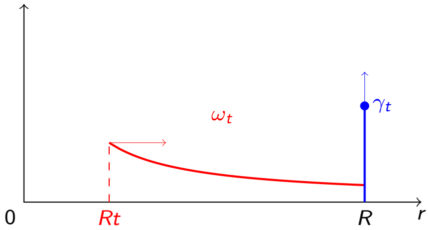

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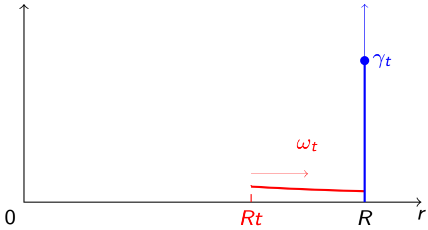

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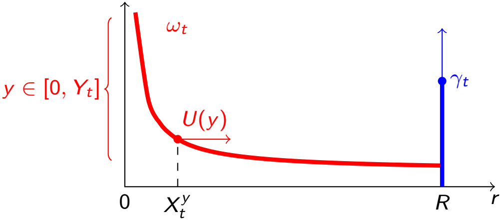
- Mass splitting and unbounded speeds $\neq$ classical OT
- $\mathcal{W}^2_\kappa(\rho_0, \rho_1) \xrightarrow{\kappa\to\infty} +\infty$ and $\mathcal{W}^2_\kappa(\rho_0, \rho_1) \xrightarrow{\kappa\to 0} \frac{1}{2}R^2$

Idea of proof

(clever ansatz + certification)



1. superposition of Lagrangian particles $(X_t^y)_{y \in [0,1]}$ with mass $\mathrm{d}y$
2. constant speeds, only keep $y \in [0, Y_t]$

$$\omega_t(\bullet) = \int_0^{Y_t} \delta_{X_t^y}(\bullet)\,\mathrm{d}y \qquad \text{and} \qquad \frac{d}{dt} X_t^y = U(y)$$

3. optimize with respect to $U(\cdot)$

$$\text{cost} = \int_0^1 \int_0^{\tau(y)} \frac{1}{2} \mathrm{d}y |U(y)|^2 \mathrm{d}t + \text{“reaction”}$$

□

Geometrical/topological properties

Theorem

Writing $\varrho_i = \omega_i + \gamma_i \in \mathcal{P}(\Omega)$, *there holds*

$$\boxed{\mathcal{W}^2_\Omega(\varrho_0,\varrho_1) \le \underbrace{\mathcal{W}^2_\kappa(\rho_0,\rho_1)}_{\uparrow \text{ in } \kappa} \le \mathcal{W}^2_\Omega(\omega_0,\omega_1) + \mathcal{W}^2_\Gamma(\gamma_0,\gamma_1)} \tag{1}$$

Moreover

$$\mathcal{W}_\kappa(\rho_n,\rho) \to 0 \quad \text{iff} \quad \omega_n \overset{*}{\rightharpoonup} \omega \text{ and } \gamma_n \overset{*}{\rightharpoonup} \gamma$$

and $(\mathcal{P}^\oplus, \mathcal{W}_\kappa)$ *is complete.*

Remarks:

- Completeness needed for the "Italian voodoo" [AGS '08]
- For fixed κ all inequalities are sharp but can be strict
- In (1) the r.h.s. can be $+\infty$ if $|\omega_0| \neq |\omega_1|$ or $|\gamma_0| \neq |\gamma_1|$

The small- and large-toll limits

Theorem

There holds

$$\lim_{\kappa\to 0} \mathcal{W}_\kappa^2(\rho_0,\rho_1) = \mathcal{W}_\Omega^2(\varrho_0,\varrho_1) \qquad \textit{with} \qquad \varrho = \omega + \gamma$$

and

$$\lim_{\kappa\to +\infty} \mathcal{W}_\kappa^2(\rho_0,\rho_1) = \mathcal{W}_\Omega^2(\omega_0,\omega_1) + \mathcal{W}_\Gamma^2(\gamma_0,\gamma_1) \qquad \in [0,+\infty]$$

and geodesics converge as well (Gamma-limit).

Interpretation:

- As $\kappa \to 0$ the (ω, γ) cars need not be distinguished and superpose into $\varrho = \omega + \gamma$
- As $\kappa \to +\infty$ transfer of mass becomes infinitely expensive, hence independent OT problems in Ω, Γ

Perspectives

- static formulation ??
- gradient-flows and PDEs
- dynamical evolution of interfaces [Cancès-Merlet?]
- complex structures, different flux costs

$$\kappa^2 \frac{|f|^2}{\theta(\omega,\gamma)} \qquad \text{e.g. } \theta(\omega,\gamma) = [\omega-\gamma]^+$$

- numerics, with T. Gallouët and M. Laborde (ALG2-JKO)

Thank you for listening