Unbalanced optimal transport

Models, Numerical methods, Applications

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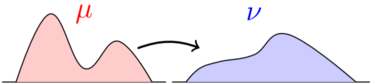
Aim

Monge's problem (1781)

How to move a pile of dirt from one configuration to another with least cost?



$\Rightarrow$ possible only if both piles have same mass

Aim

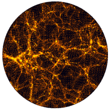
Extension to unbalanced piles

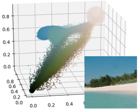
Why is it interesting?

Strong modelization power: nonnegative measure

- probability distribution, empirical distribution
- undistinguishable weighted particles
- density of a gaz, a crowd

Origins of universe (Brenier *et al.* '08)





Color transfer (Delon '10)

Crowd motions (Roudneff *et al.*, 12')

Point clouds

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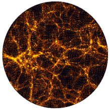

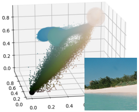

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Crowd motions (Roudneff *et al.*, 12')

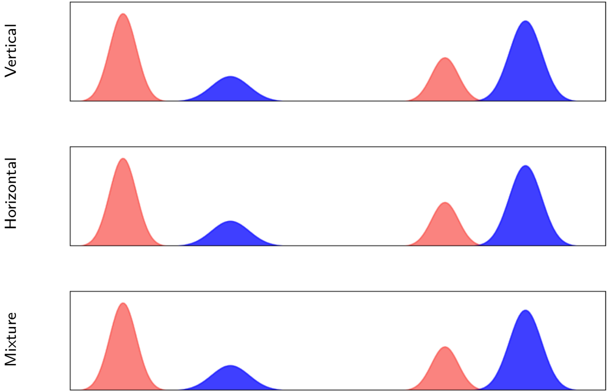
Point clouds

Provides with powerful tools

- geodesic distance faithful to the ground geometry
- transport plans, barycenters, gradient flows

Strategy

- preserve key properties of optimal transport
- combine two kind of geometries
  horizontal (transport) and *vertical* (linear)



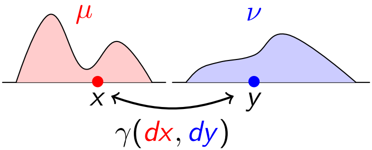
Content

Content

Classical theory

Ingredients

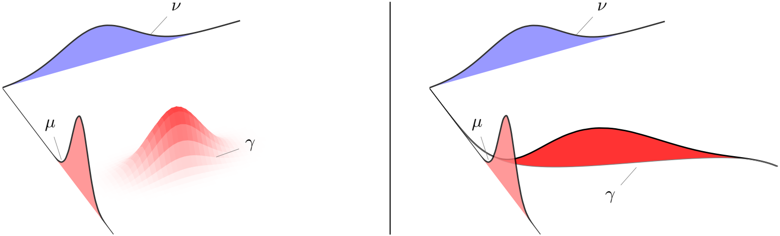
- Ambiant space $\mathcal{X}$ (compact metric in this talk)
- Cost function $c : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \cup \{\infty\}$
- Two probability measures μ, ν sur $\mathcal{X}$



Definition (Kantorovich formulation)

$$\min \left\{ \int_{\mathcal{X}\times\mathcal{X}} c(x,y)\gamma(dx,dy) \; ; \; \gamma \in \Pi(\mu,\nu) \right\}$$

Couplings



Definition (Couplings)

$$\Pi(\mu,\nu) := \left\{\gamma \in M_+(\mathcal{X}\times\mathcal{X}) : \pi^1_\#\gamma = \mu,\ \pi^2_\#\gamma = \nu\right\}$$

Generalizes: maps $\mathcal{X}\to\mathcal{X}$, permutations

Properties: convex, weakly compact

Properties

Theorem (Wasserstein distances)

If $(\mathcal{X}, \mathrm{dist})$ *is a geodesic space,* $p \geq 1$*, then the function*

$$W_p(\mu,\nu)^p := \min \left\{ \int_{\mathcal{X}\times\mathcal{X}} \mathrm{dist}(x,y)^p \gamma(dx,dy) : \gamma \in \Pi(\mu,\nu) \right\}$$

defines a geodesic metric on $P(\mathcal{X})$ *which metrizes weak convergence.*

Properties

Theorem (Wasserstein distances)

If $(\mathcal{X}, \mathrm{dist})$ is a geodesic space, $p \geq 1$, then the function

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defines a geodesic metric on $P(\mathcal{X})$ which metrizes weak convergence.

Dynamic formulation (Benamou-Brenier)

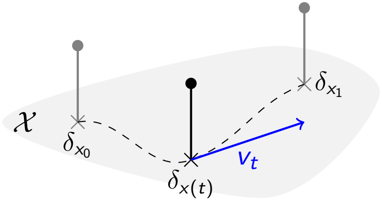
For μ, ν probability measures on $\Omega \subset \mathbb{R}^d$, it holds

$$W_p(\mu,\nu)^p = \min_{(\rho_t, v_t)_{t\in[0,1]}} \left(\int_0^1 \int_{\mathbb{R}^d} \|v(t,x)\|^p d\rho_t(x) dt \right)$$

subject to $\partial_t \rho_t = -\mathrm{div}(\rho_t v_t)$ and $(\rho_0, \rho_1) = (\mu, \nu)$.

More generally: convex Lagrangian $L(v(t,x))$.

From dynamic to coupling



Minimal-path cost

Given a convex Lagrangian $L : \mathbb{R}^d \to \mathbb{R}$, let

$$c_L(x_0, x_1) := \inf \int_0^1 L(v(t))dt$$

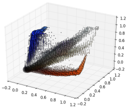
where $\delta_{x(t)}$ continuously interpolates between δ_{x_0} et δ_{x_1} and $v_t = x'(t)$.

Equivalence (Benamou-Brenier, Jimenez, Villani):

dynamic with $L \quad \Leftrightarrow \quad$ coupling with c_L

Content

Color transfer



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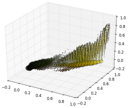
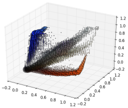


(Delon *et al.*)
(Rabin, Papadakis)

Color transfer



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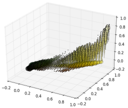

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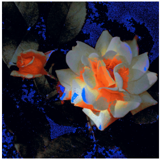
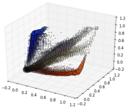


classical

Color transfer



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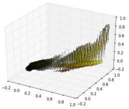

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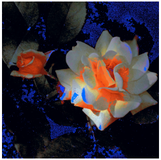
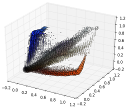
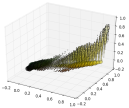


classical

partial

Color transfer





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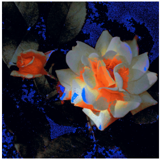


classical

partial

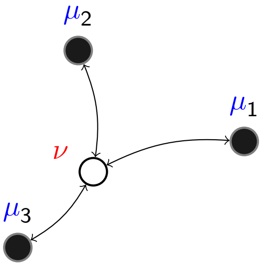
unbalanced ($\widehat{W}_2$)

Barycenters / Fréchet means

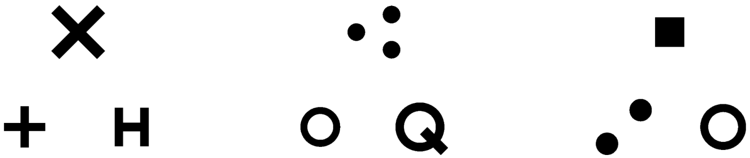
Wasserstein barycenters (Agueh et Carlier)

- $\mu_1, \dots, \mu_n$ probability measures
- $w_1, \dots, w_n$ positive weights
- Definition of the barycenter ν^* :

$$\nu^* \in \arg \min_{\nu \in P(\mathcal{X})} \sum_{k=1}^{n} w_k \, W_2^2(\mu_k, \nu)$$

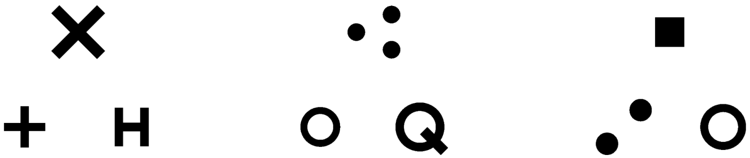


Barycenters of mesures



μ_1 μ_2 μ_3

Barycenters of mesures



μ_1 μ_2 μ_3

Iso-barycenter ν^* for W_2

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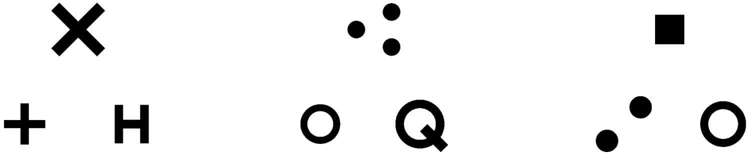

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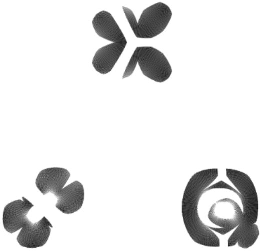
Iso-barycenter ν^* for W_2



Iso-barycenter ν^* for $\widehat{W_2}$

Gradient flows

Gradient flows (formal)

Let E a metric space, $F : E \to \bar{\mathbb{R}}$ et $\mu_0 \in E$,

$$\partial_t \mu_t = -\operatorname{grad}_E F(\mu_t) \qquad t > 0$$

metric	$\operatorname{grad}_E F(\mu)$
L^2	$F'(\mu)$
Hellinger	$\mu F'(\mu)$
W_2	$-\mathrm{div}(\mu \nabla F'(\mu))$

Example: the Laplacian operator $-\Delta$ is the gradient of...

- the Dirichlet energy for L^2 : $F(\mu) = \int |\nabla \mu|_2^2$
- the entropy for W_2 : $F(\mu) = \int \mu(\log \mu - 1)$

Wasserstein gradient flows

Interest

- characterize certain evolution PDEs

$$\partial_t \mu_t + \mathrm{div}(\mu_t v_t) = 0$$

- theoretical : existence, uniqueness, asymptotics
- numerical : intrisic mass conservation and nonnegativity

Crowd motion
(Roudneff-Chupin, Maury and Santambrogio)

Metric structure for equations with mass variations?

References and history

Before 2015

- re-normalization
- optimal partial transport (Kantorovich), (Mc Cann, Cafarelli), (Figalli), (Piccoli, Rossi)
- various specific models (Benamou), (Lombardi, Maître), (Rumpf *et al.*)

References and history

Before 2015

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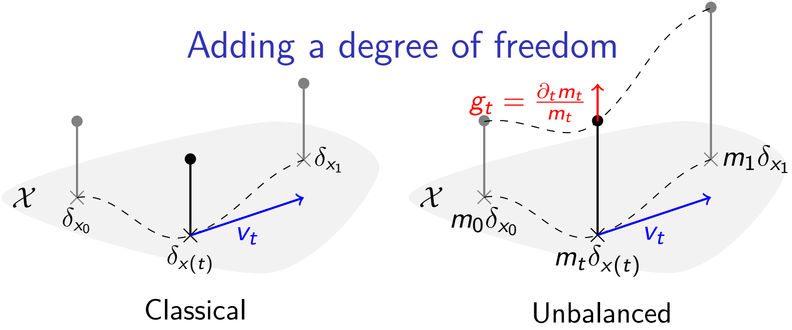
Since 2015

- Quadratic model (Liero *et al.*), (Kondratiev *et al.*), (Chayes, Lei), (C. *et al.*)
- General theory (Liero *et al.*), (C. *et al.*)
- Emerging applications : imaging (Feydy *et al.*), statistical learning (Schiebinger *et al.*), (Frogner *et al.*)

Content

Adding a degree of freedom



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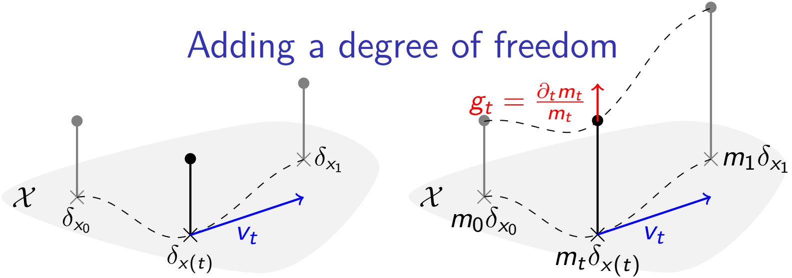


Classical

Unbalanced

Dynamic formulation (C. *et al.*)

For μ, $\nu \in M_+(\Omega)$ measures with *potentially* different masses, let

$$C_L(\mu,\nu) := \min_{(\rho_t, v_t, g_t)_{t\in[0,1]}} \int_0^1 \int_{\mathbb{R}^d} L(v_t(x), g_t(x)) d\rho_t(x) dt$$

subject to $\partial_t \rho_t = -\mathrm{div}(\rho_t v_t) + \rho_t g_t$ and $(\rho_0, \rho_1) = (\mu, \nu)$.

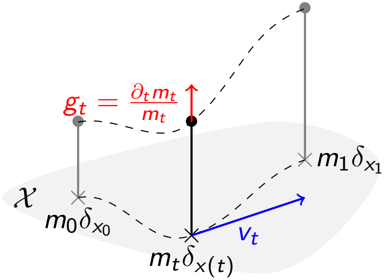
- L convex Lagrangian, continuous, minimal at $L(0,0) = 0$.

Properties

Proposition (C. *et al.*)

- *$C_L(\mu, \nu)$ is finite, minimizers exist*
- *C_L continuous under weak convergence*
- *if L is even and p-homogeneous then $C_L^{1/p}$ defines a metric on $M_+(\Omega)$*

From dynamic to coupling (I)



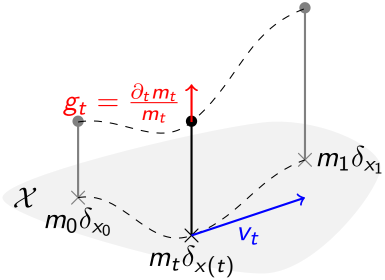
Minimal path cost (unbalanced case)

Given a convex Lagrangian L,

$$c_L((x_0, m_0), (x_1, m_1)) = \inf \int_0^1 L(v(t), g(t))m(t)dt$$

where $m(t)\delta_{x(t)}$ interpolates between $m_0\delta_{x_0}$ and $m_1\delta_{x_1}$.

From dynamic to coupling (I)



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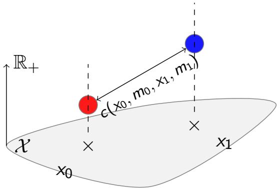
- What is the corresponding *coupling* formulation?

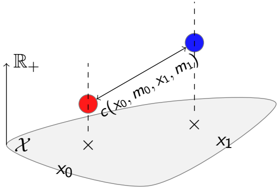
Semi-couplings



Semi-couplings

Measures $\gamma_0, \gamma_1 \in M_+(\mathcal{X}^2)$ such that $\pi^1_\# \gamma_0 = \mu$ and $\pi^2_\# \gamma_1 = \nu$.

Semi-couplings



Semi-couplings

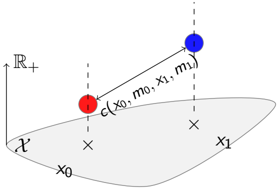
Measures $\gamma_0, \gamma_1 \in M_+(\mathcal{X}^2)$ such that $\pi^1_\# \gamma_0 = \mu$ and $\pi^2_\# \gamma_1 = \nu$.

Definition (Semi-coupling formulation (C. *et al.*))

Let $c((x_0, m_0), (x_1, m_1))$ a cost function, *sublinear* in (m_0, m_1). We define, minimizing over the space of semi-couplings (γ_0, γ_1),

$$C_c(\mu, \nu) := \inf \int_{\mathcal{X}^2} c((x_0, \frac{d\gamma_0}{d\lambda}), (x_1, \frac{d\gamma_1}{d\lambda}))d\lambda \quad \gamma_0, \gamma_1 \ll \lambda.$$

Properties



Theorem (Metric property, $p \geq 1$)

If $c^{1/p}$ is a metric on $Cone(\mathcal{X}) := (\mathcal{X} \times \mathbb{R}_+)/\sim$ then $C_c^{1/p}$ is a metric on $M_+(\mathcal{X})$.

- equivalence with the transport problem *lifted* on $\mathcal{X} \times \mathbb{R}_+$ of (Liero *et al.*)
- dual formulation, weak continuity

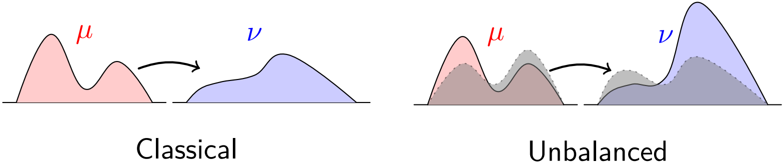
From dynamic to coupling (II)

Theorem (C. *et al.*)

Let $\Omega \subset \mathbb{R}^d$ a regular compact domain, L a Lagrangian and c_L the convex regularization of the associated cost. Then, for all nonnegative measures $\mu, \nu \in M_+(\Omega)$,

$$C_L(\mu,\nu) = C_c(\mu,\nu).$$

Third approach



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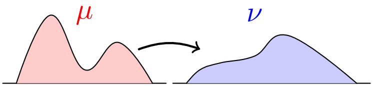
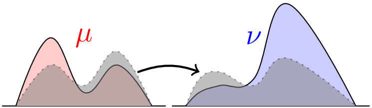




Optimal entropy-transport problems (Liero *et al.*)

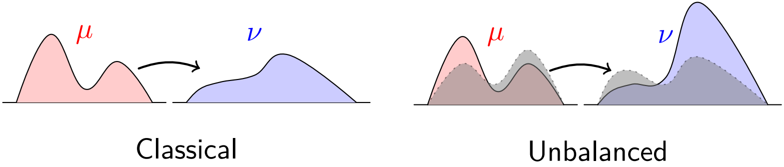
$$C_{c,f}(\mu,\nu) := \min_{\gamma\in M_+(\mathcal{X}^2)} D_f(\pi^1_\#\gamma|\mu) + D_f(\pi^2_\#\gamma|\nu) + \int_{\mathcal{X}^2} c\, d\gamma$$

f-divergence (Csiszár)

$$D_f(\mu|\nu) := \int_{\mathcal{X}} f(\frac{d\mu}{d\nu})d\nu + \mu^\perp(\mathcal{X})\, f'(\infty) \qquad \mu,\nu \in M_+(\mathcal{X})$$

with $f : \mathbb{R}_+ \to \mathbb{R}$ convex, minimal at $f(1) = 0$.

Third approach



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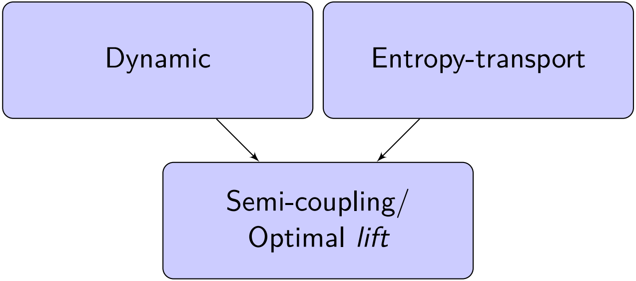
Theorem (Liero *et al.*)

$C_{c,f}$ is equivalent to the semi-coupling problem with the cost

$$\tilde{c}((x_0,m_0),(x_1,m_1)) := C_{c,f}(m_0\delta_{x_0}, m_1\delta_{x_1})$$

Summary



Content

Analog of W_p

We define, for $p \geq 1$ and the scale parameter $\alpha > 0$,

$$L(v, g) = (|v|/\alpha)^p + (|g|/p)^p.$$

Definition ($\widehat{W}_{p,\alpha}$ distance)

For $\mu, \nu \in M_+(\Omega)$, we define

$$\widehat{W}_{p,\alpha}(\mu,\nu)^p := \min_{(\rho_t, v_t, g_t)_{t\in[0,1]}} \int_0^1 \int_{\mathbb{R}^d} L(v_t(x), g_t(x)) d\rho_t(x) dt$$

subject to $\partial_t \rho_t = -\mathrm{div}(\rho_t v_t) + \rho_t g_t$ and ρ_0, ρ_1 fixed.

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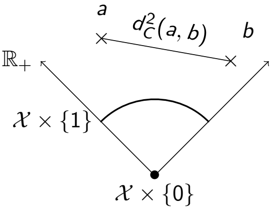
subject to $\partial_t \rho_t = -\mathrm{div}(\rho_t v_t) + \rho_t g_t$ and ρ_0, ρ_1 fixed.

Properties (C. *et al.*)

- $\widehat{W}_{p,\alpha}$ is a geodesic metric, weak convergence
- limit models (Γ-convergence):
  - $\alpha \to \infty$: optimal transport W_p (generalized)
  - $\alpha \to 0$: family of "vertical" metrics (Hellinger, TV)

Quadratic case (i)

$$L(v, g) = |v|^2 + \frac{1}{4}|g|^2$$



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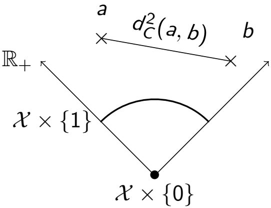


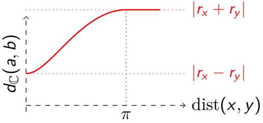
Proposition (Minimal path cost)

The minimal path cost is given by the cone metric

$$c_L((x_0,m_0),(x_1,m_1)) = d_C((x_0,\sqrt{m_0}),(x_1,\sqrt{m_1}))^2$$

where

$d_C((x_0,r_0),(x_1,r_1))^2 = r_0^2 + r_1^2 - 2r_0 r_1 \cos(\min\{\mathrm{dist}(x_0,x_1),\pi\})$.



Quadratic case (ii)

Theorem (Liero *et al.*, C. *et al.*)

There is an explicit semi-coupling formulation, and the entropy-transport formulation

$$\widehat{W}_2(\mu,\nu)^2 = \min_{\gamma \in M_+(\mathcal{X}^2)} \mathcal{H}(\pi^1_{\#}\gamma|\mu) + \mathcal{H}(\pi^2_{\#}\gamma|\nu) + \int_{\mathcal{X}^2} c_\ell d\gamma.$$

- $c_\ell(x,y) := -\log\cos^2(\min\{\mathrm{dist}(x,y), \pi/2\})$.
- $\mathcal{H}$ is the relative entropy (or Kullback-Leibler divergence):

$$\mathcal{H}(\mu|\nu) := \int_{\mathcal{X}} \log(d\mu/d\nu)d\mu - \mu(\mathcal{X}) + \nu(\mathcal{X})$$

- distance named *Wasserstein-Fisher-Rao* (C. *et al.*), or *Hellinger-Kantorovich* (Liero *et al.*)
- the analog of W_2 on $M_+(\mathcal{X})$

Case $p = 1$

$$L(v, g) = |v| + |g|$$

Proposition

The metric $\widehat{W}_1$ is the *bounded Lipschitz* metric on $M_+(\mathcal{X})$:

$$\widehat{W}_1(\mu, \nu) = \sup_{\varphi : \mathcal{X} \to \mathbb{R}} \left\{ \int_{\mathcal{X}} \varphi d(\mu - \nu) \; ; \; \|\varphi\|_\infty \leq 1, \mathrm{Lip}(\varphi) \leq 1 \right\}$$

Optimal partial transport

Theorem (Piccoli et Rossi, C. *et al.*)

For a Lagrangian of the form

$$L(v, g) = \tilde{L}(v) + |g|,$$

the equivalent static problem is a formulation of the optimal partial transport.

Optimal partial transport

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Optimal *partial* transport

Let $\mu, \nu \in M_+(\mathcal{X})$ be such that $m \leq \mu(\mathcal{X}), \nu(\mathcal{X})$. Find the optimal way to move a quantity m of mass among the available mass.

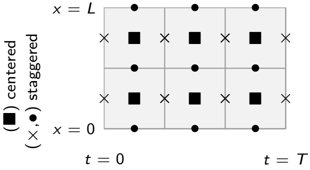
(Benamou *et al.*)

Content

Discretization

$$\min_{\rho,v,g} \left\{ \int_0^1 \int_\Omega L(v,g) d\rho \; ; \; \partial_t \rho + \mathrm{div}(\rho v) = g\rho \text{ and } (\rho_0, \rho_1) = (\mu, \nu) \right\}$$

- in variables $(\rho, \omega, \zeta) = (\rho, v\rho, g\rho)$
  $\Rightarrow$ convex functional, linear constraints
- $X, \tilde{X}$ discretized densities on centered and staggered grids



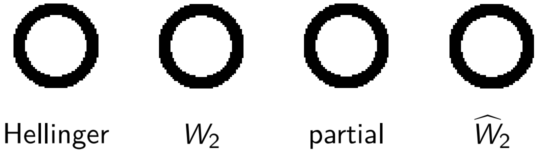
Finite dimensional non-smooth convex problem

$$\min_{X,\tilde{X}} \left\{ F(X) \; ; \; A(\tilde{X}) = b \text{ et } X = \mathrm{interp}(\tilde{X}) \right\}$$

Dynamic approach

- solve with *proximal* algorithms, adapted from (Papadakis *et al.*)
- proximal operators computable in quasi-linear complexity

Figure: Geodesics for densities on $\mathbb{R}^2$



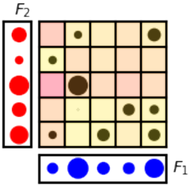
Content

Generic formulation

- cost function $c : \mathcal{X}^2 \to \mathbb{R}$
- marginal functions F_1, F_2 convex

Solve

$$\min_{\gamma \in M_+(\mathcal{X}^2)} \int_{\mathcal{X}^2} c \cdot d\gamma + F_1(\pi^1_{\#}\gamma) + F_2(\pi^2_{\#}\gamma)$$



- classical optimal transport
- entropy-transport problems
- barycentres, gradient flows...

Entropic regularization

Following (Cuturi),

$$\min_{\gamma \in M_+(\mathcal{X}^2)} \int_{\mathcal{X}^2} c \cdot d\gamma + F_1(\pi^1_\# \gamma) + F_2(\pi^2_\# \gamma) + \epsilon \mathcal{H}(\gamma)$$

where $\epsilon > 0$ is the *strength* of the regularization and $\mathcal{H}$ is minus the entropy.

Scaling algorithms

Theorem (Optimality condition)

Consider the kernel $K(x,y) = \exp(-c(x,y)/\epsilon)$. *Under assumptions, there exists* $a : \mathcal{X} \to \mathbb{R}_+$ *and* $b : \mathcal{X} \to \mathbb{R}_+$ *such that at optimality*

$$\gamma_{\rm opt}(x,y) = a(x)K(x,y)b(y)$$

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Scaling algorithm (C. *et al.*)

1. initialize $b = 1_m$ and repeat until convergence
   1. $a \leftarrow \mathrm{prox}^{\mathcal{H}}_{F_1}(Kb) \oslash (Kb)$
   2. $b \leftarrow \mathrm{prox}^{\mathcal{H}}_{F_2}(K^T a) \oslash (K^T a)$
2. return $\gamma_{\mathrm{opt}} = (a_i K_{i,j} b_j)_{i,j}$.

$$\mathrm{prox}^{\mathcal{H}}_{F}(\bar{s}) := \arg\min\{F(s) + \epsilon\mathcal{H}(s|\bar{s})\}$$

Linear convergence

Hilbert metric on L^∞_{++}

$d_H(a,b) :=$

$\log(\sup(a/b)\sup(b/a))$

Proposition (Franklin, Lorenz)

Linear convergence of Sinkhorn iterates for d_H.

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Thompson's metric on L^∞_{++}

$$d_T(a,b) := \log\max(\sup(a/b), \sup(b/a))$$

Proposition (C. *et al.*)

$$s \mapsto \operatorname{prox}^{\mathcal{H}}_F(s)/s$$

is non-expansive for d_T and *contracting* if $F = \mathcal{H}$.

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Corollary

Global linear convergence of the iterates for d_T for the resolution of problems related to $\widehat{W}_2$. Holds in infinite dimension, under positivity conditions.

Content

Gradient flows (formal)

Reminder: W_2 gradient flow

For $F : P(\Omega) \to \bar{\mathbb{R}}$ et $\rho_0 \in P(\Omega)$,

$$\partial_t \rho_t = \mathrm{div}(\rho_t \nabla F'(\rho_t))$$

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$\widehat{W}_2$ gradient flow

For $F : M_+(\Omega) \to \bar{\mathbb{R}}$ et $\rho_0 \in M_+(\Omega)$,

$$\partial_t \rho_t = \mathrm{div}(\rho_t \nabla F'(\rho_t)) - 4\rho_t F'(\rho_t)$$

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- *splitting* scheme (Gallouet, Monsaingeon, Laborde)
- with Di Marino, analysis of a specific problem:
  - degenerate EDP of Hele-Shaw type
  - true gradient flow structure
  - similarity with (Roudneff-Chupin, Santambrogio, Maury)

Gradient flow in $M_+(\Omega)$

Theorem (Di Marino and C.)

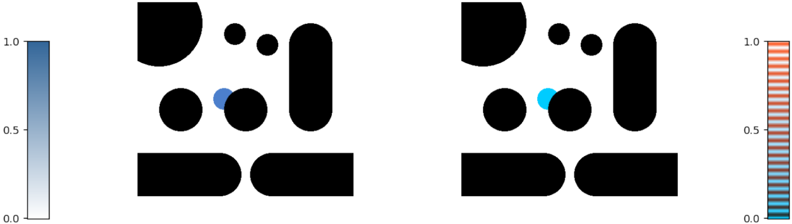
The tumor growth model of Hele-Shaw type (Perthame et al.)

$$\partial_t \rho_t + \mathrm{div}(\rho_t \nabla \mathrm{p}_t) = 4(1-\mathrm{p}_t)\rho_t$$
$$\mathrm{p}_t(1-\rho_t) = 0 \quad \textit{and} \quad \rho_t \leq 1$$

characterizes gradient flows for the metric $\widehat{W}_2$ of the function

$$G(\rho_t) = \begin{cases} -\rho_t(\Omega) & \textit{si } \rho_t \leq 1 \\ \infty & \textit{sinon.} \end{cases}$$

- existence of weak solutions through the JKO scheme
- uniqueness through the EVI characterization (for Ω convex)



ρ_t p_t

Conclusion

Unbalanced Optimal Transport :

- extension motivated by several applications
- unified theory including old and new models
- numerical complexity similar to standard optimal transport

Perspectives:

- transport of vector valued measures (matricial)