UNBALANCED OPTIMAL TRANSPORT

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CEREMADE
Université Paris Dauphine

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Introduction

Motivations

Image matching, Machine learning, Economics, Gradient flows...

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Static relaxed marginal constraints ([Hanin, 1992], [Benamou, 2003])

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- Transport + variation of mass & exact marginal constraints .

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- Transport + variation of mass & exact marginal constraints .

Setting : Ω convex compact in $\mathbb{R}^n$.

Outline

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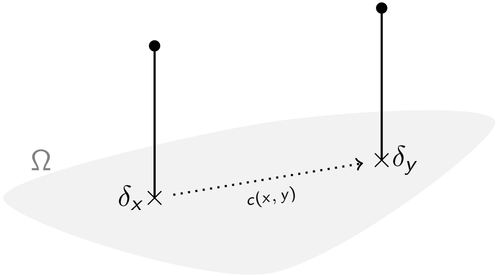
From standard OT...



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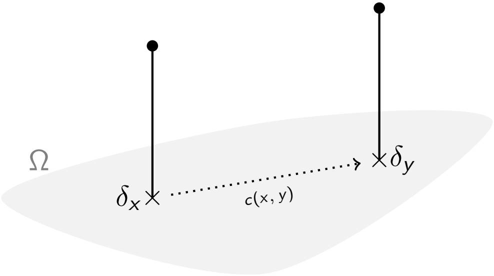

Assumptions on the cost:

- lower bounded;
- l.s.c.

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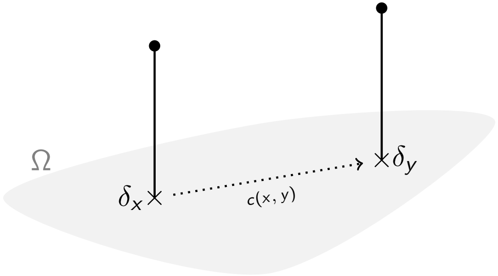

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Static formulation of OT:

$$\begin{aligned} \text{minimize } & \int_{\Omega^2} c(x,y)\,\mathrm{d}\gamma(x,y) \\ \text{subject to } & (\mathrm{proj}_x)_{\#}\gamma = \rho_0 \\ & (\mathrm{proj}_y)_{\#}\gamma = \rho_1 \end{aligned}$$

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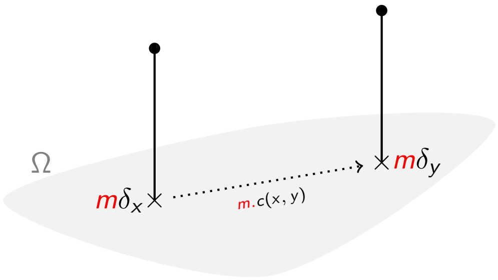

Assumptions on the cost:

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also linear in m.

Static formulation of OT:

$$\text{minimize } \int_{\Omega^2} c\left(\frac{\mathrm{d}\gamma}{\mathrm{d}\lambda}, x, y\right)\mathrm{d}\lambda(x,y) \qquad (\gamma \ll \lambda)$$

$$\text{subject to } (\mathrm{proj}_x)_{\#}\gamma = \rho_0$$

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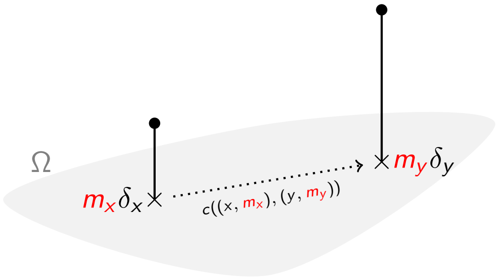
...to Unbalanced OT



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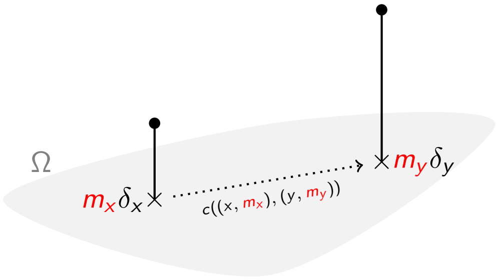

The cost function is

- pos. homogeneous in (m_x, m_y);

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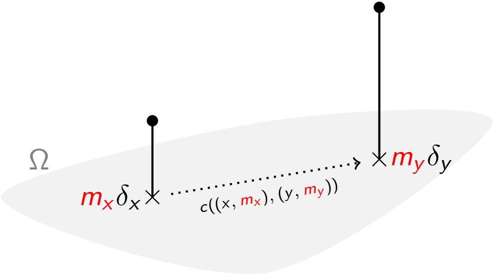

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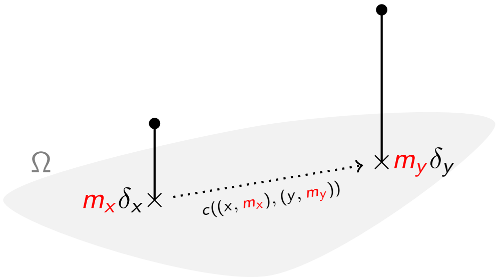

The cost function is

- pos. homogeneous in (m_x, m_y);
- subadditive in (m_x, m_y);
- nonnegative;

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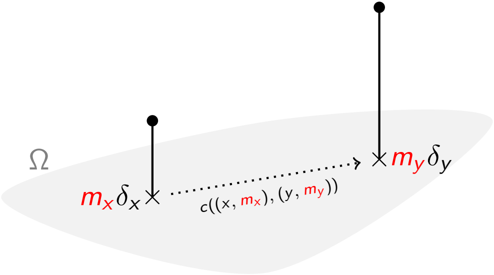

The cost function is

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- m_x or m_y negative $\Rightarrow c = +\infty$;

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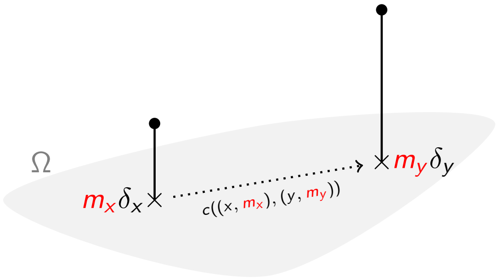

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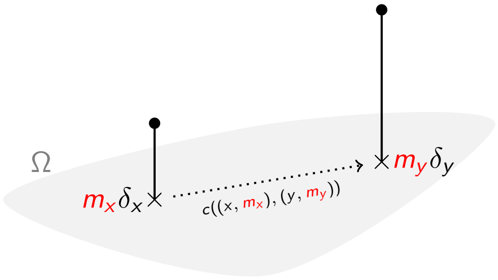

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Static formulation of Unbalanced OT

$$C(\rho_0, \rho_1) := \text{minimize} \int_{\Omega^2} c((x, \frac{\mathrm{d}\gamma_0}{\mathrm{d}\gamma}), (y, \frac{\mathrm{d}\gamma_1}{\mathrm{d}\gamma}))\mathrm{d}\gamma(x, y)$$

$$\text{subject to } (\pi_x)_\#\gamma_0 = \rho_0$$

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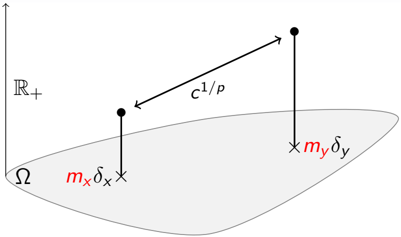
Properties



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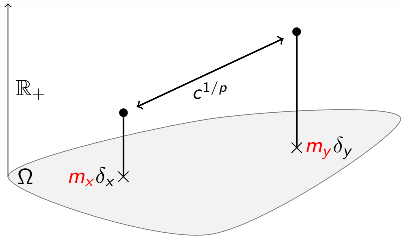

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Theorem (Metric property)

If $c^{1/p}$ is a metric on Cone(Ω) then $C^{1/p}$ is a metric on $\mathcal{M}_+(\Omega)$.

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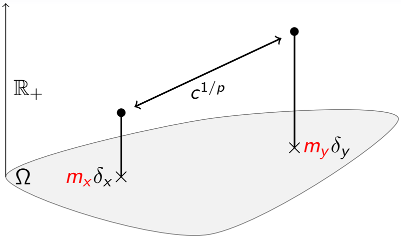

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For all $(x, y) \in \Omega^2$, $c(x, \cdot, y, \cdot)$ is the support function of a closed convex nonempty set $Q(x, y) \subset \mathbb{R}^2$.

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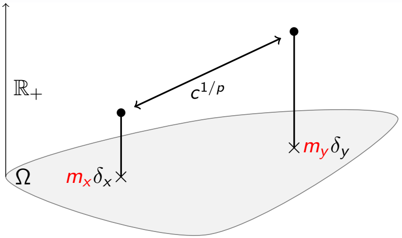

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If $c^{1/p}$ is a metric on Cone(Ω) then $C^{1/p}$ is a metric on $\mathcal{M}_+(\Omega)$.

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For all $(x, y) \in \Omega^2$, $c(x, \cdot, y, \cdot)$ is the support function of a closed convex nonempty set $Q(x, y) \subset \mathbb{R}^2$. If Q is l.s.c. in the sense of multifunctions, then

$$C(\rho_0, \rho_1) = \sup_{\phi,\psi \in C(\Omega)} \int_\Omega \phi(x)\mathrm{d}\rho_0(x) + \int_\Omega \psi(y)\mathrm{d}\rho_1(y)$$

subject to $(\phi(x), \psi(y)) \in Q(x, y)$ for all $(x, y) \in \Omega^2$.

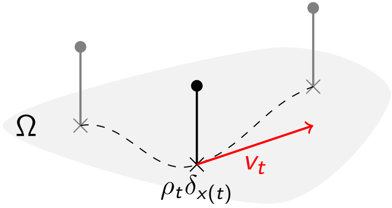
Outline

Static Formulation

Dynamic Formulation

Examples & Numerics

A dynamic approach: standard OT



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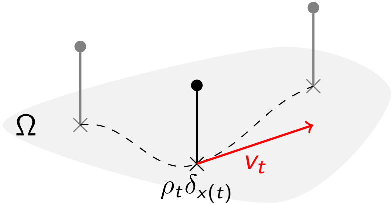

Change of variables: $\omega = \rho v$
Infinitesimal cost : $f(x, \rho, \omega)$

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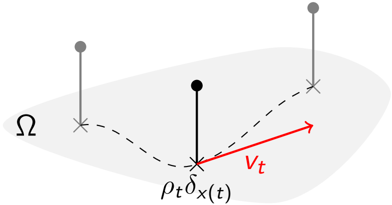

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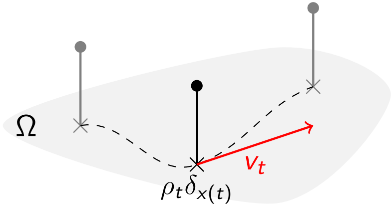

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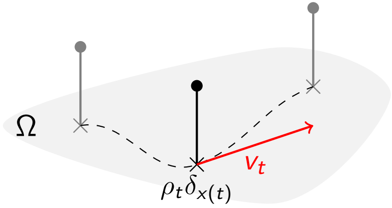

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Standard dynamic formulation

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&\text{minimize} && \int_0^1 \int_\Omega f(x, \frac{\mathrm{d}\rho}{\mathrm{d}\mu}, \frac{\mathrm{d}\omega}{\mathrm{d}\mu})\mathrm{d}\mu && (\rho, |\omega| \ll \mu) \\
&\text{subject to} && \partial_t \rho + \nabla \cdot \omega = 0 && \text{(weakly)} \\
& && (\mathrm{proj}_{t=0})_\# \rho = \rho_0 \quad , \quad (\mathrm{proj}_{t=1})_\# \rho = \rho_1 \,.
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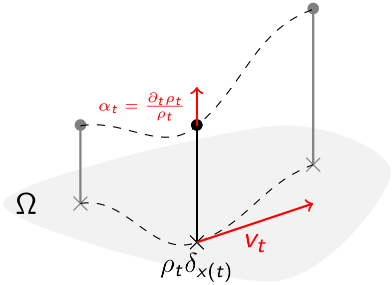

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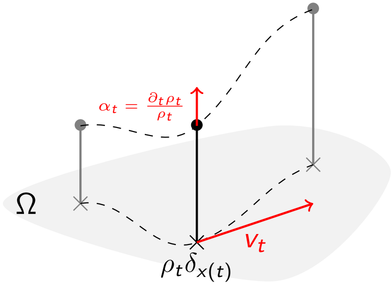

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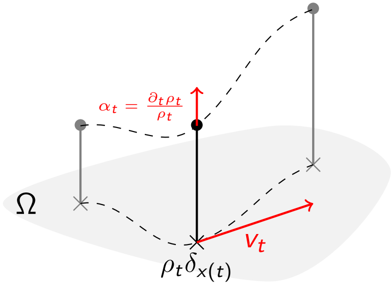

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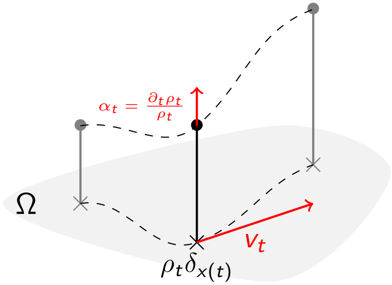

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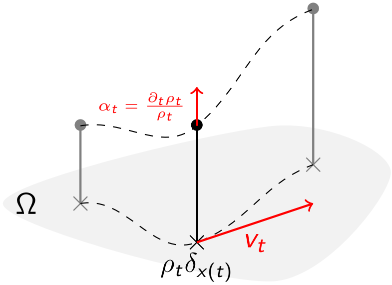

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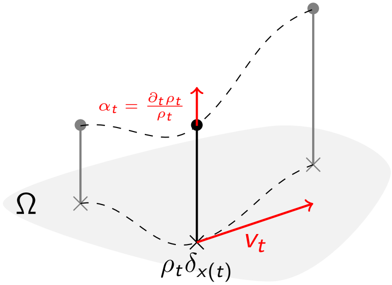

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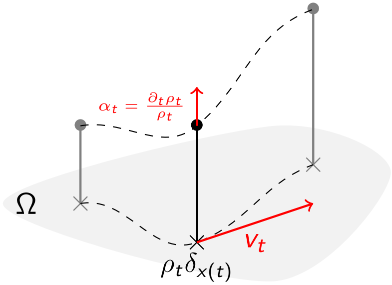

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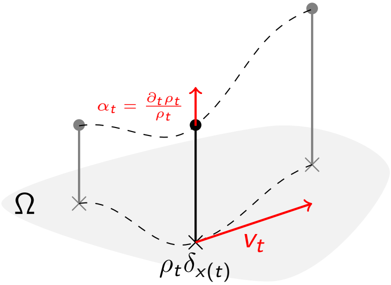

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Unbalanced dynamic formulation

$$C_D(\rho_0, \rho_1) := \text{minimize} \quad \int_0^1 \int_\Omega f(x, \frac{\mathrm{d}\rho}{\mathrm{d}\mu}, \frac{\mathrm{d}\omega}{\mathrm{d}\mu}, \frac{\mathrm{d}\zeta}{\mathrm{d}\mu}) \mathrm{d}\mu(t, x)$$

$$\text{subject to } \partial_t \rho + \nabla \cdot \omega = \zeta \qquad \text{(weakly)}$$

$$(\mathrm{proj}_{t=0})_\# \rho = \rho_0 \quad , \quad (\mathrm{proj}_{t=1})_\# \rho = \rho_1 \, .$$

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Theorem

Assume that Q is a l.s.c. multifunction. Then the minimum defining C_D is attained and

$$C_D(\rho_0, \rho_1) = \sup_{\varphi \in C^1([0,1]\times\Omega)} \int_\Omega \varphi(1, x)\mathrm{d}\rho_1(x) - \int_\Omega \varphi(0, x)\mathrm{d}\rho_0(x)$$

$$\textit{subject to } (\partial_t \varphi, \nabla\varphi, \varphi)(t, x) \in Q(x)\,.$$

Dynamic to Static : "Benamou-Brenier" formula

Costs between points in Cone(Ω):

Dirac-based cost c_d : $C_D(m_0\delta_{x_0}, m_1\delta_{x_1})$

Path-based cost c_p : infimum of the dynamic functional restricted to smooth, stable Dirac trajectories $m(t)\delta_{x(t)}$.

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Theorem (C. et al., 2015)

Let c be a cost function satisfying $c_d \leq c \leq c_p$. If the associated problem C is weakly continuous, then $C = C_D$ (and $c = c_d$).*

Note : c_d is *hard* to compute directly in general.

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Example

A good candidate is the convex regularization of c_p:

$$\inf_{\substack{m_0^a+m_0^b=m_0 \\ m_1^a+m_1^b=m_1}} c_p((x_0, m_0^a),(x_1, m_1^a)) + c_p((x_0, m_0^b),(x_1, m_1^b))$$

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Partial OT / Wasserstein-TV

Extend the results in [Piccoli and Rossi, 2013]

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Static

$$C := \min_{\tilde{\rho}_0, \tilde{\rho}_1} \frac{1}{p} W_p^p(\tilde{\rho}_0, \tilde{\rho}_1)$$
$$+ \delta \left(|\rho_0 - \tilde{\rho}_0|_{TV} + |\rho_1 - \tilde{\rho}_1|_{TV} \right)$$

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Dynamic

$$\min \quad \int_0^1 \int_\Omega \frac{1}{p} \frac{\omega^p}{\rho^{p-1}} + \delta|\zeta|$$
$$\text{s.t.} \quad \partial_t \rho + \nabla \cdot \omega = \zeta$$

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$$\min \int_0^1 \int_\Omega \frac{1}{p} \frac{\omega^p}{\rho^{p-1}} + \delta|\zeta| \quad \text{s.t.} \quad \partial_t \rho + \nabla \cdot \omega = \zeta$$

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- $C^{1/p}$ defines a metric on $\mathcal{M}_+(\Omega)$;
- geodesics are not absolutely continuous;
- dual formula : add the contraint "bounded by δ".

Wasserstein-Fisher-Rao : *WF*

Static

$$WF^2 := \min \Big\{ |\rho_0|_{TV} + |\rho_1|_{TV}$$
$$-2 \int_{\Omega^2} \cos\left(\frac{|y-x|}{2} \wedge \frac{\pi}{2} \right) \mathrm{d}\sqrt{\gamma_0 \gamma_1}(x,y) \Big\}$$
$$\text{s.t. } \mathrm{proj}_x \gamma_0 = \rho_0 \, , \, \mathrm{proj}_y \gamma_1 = \rho_1$$

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$$-2 \int_{\Omega^2} \cos\left(\frac{|y-x|}{2} \wedge \frac{\pi}{2} \right) \mathrm{d}\sqrt{\gamma_0 \gamma_1}(x,y) \Big\}$$
$$\text{s.t. } \mathrm{proj}_x \gamma_0 = \rho_0 \,,\ \mathrm{proj}_y \gamma_1 = \rho_1$$

Dynamic

$$\min \quad \frac{1}{4} \int_0^1 \int_\Omega \frac{|\omega|^2}{\rho} + \frac{\zeta^2}{\rho}$$
$$\text{s.t.} \quad \partial_t \rho + \nabla \cdot \omega = \zeta$$

Wasserstein-Fisher-Rao : *WF*

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- [Liero et al., 2015, Kondratyev et al., 2015, Chizat et al., 2015b] .

Numerics

Proximal splitting algorithms on the dynamic formulation :
`https://github.com/lchizat/optimal-transport`

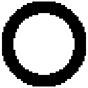

Figure: FR

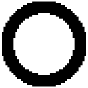

Figure: W_2

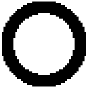

Figure: $W_2 - TV$

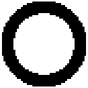

Figure: $W_2 - FR$

Conclusion

In progress

- Numerics on the relaxed marginal formulation

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- More applications

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Take home message

A unified framework for unbalanced OT allowing dynamic, static and dual formulations.

For Further Reading I

Chizat, L., Peyré, G., Schmitzer, B., and Vialard, F.-X. (2015a).
Unbalanced optimal transport: geometry and Kantorovich formulation.
arXiv preprint arXiv:1508.05216.

Chizat, L., Schmitzer, B., Peyré, G., and Vialard, F.-X. (2015b).
An interpolating distance between optimal transport and Fisher-Rao.
http://arxiv.org/abs/1506.06430.

Kondratyev, S., Monsaingeon, L., and Vorotnikov, D. (2015).
A new optimal transport distance on the space of finite Radon measures.
Technical report, Pre-print.

For Further Reading II

Liero, M., Mielke, A., and Savaré, G. (2015).
Optimal Entropy-Transport problems and a new Hellinger-Kantorovich distance between positive measures.
ArXiv e-prints.

Piccoli, B. and Rossi, F. (2013).
On properties of the Generalized Wasserstein distance.
arXiv:1304.7014. d