UNBALANCED OPTIMAL TRANSPORT

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joint work with F-X. Vialard, G. Peyré & B. Schmitzer

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Optimal transport

Given

- (μ, ν) two probability measures on a space Ω
- a cost function $c : \Omega^2 \to \mathbb{R}$

compute

$$C(\mu,\nu) \overset{\text{def.}}{=} \inf_{\gamma \in \mathcal{P}(\Omega^2)} \left\{ \int_{\Omega^2} c(x,y) \mathrm{d}\gamma(x,y) : (\text{proj}_x)_\# \gamma = \mu, (\text{proj}_y)_\# \gamma = \nu \right\}$$

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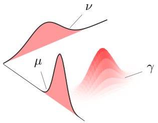

Figure: Independant coupling (here $\Omega = [0, 1]$)

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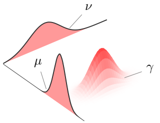

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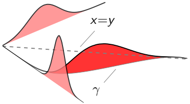

Figure: Best coupling for $c(x,y) = |x-y|^2$

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Interest

- **Optimal transport plan** γ_{opt}
- **Optimal cost** $C(\mu, \nu)$

Example of application (1)

$(g_{ij})_{ij} \in (\mathbb{R}^3)^{N_x \times N_y}$

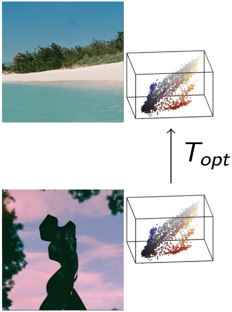

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Figure: Optimal transport for color transfer

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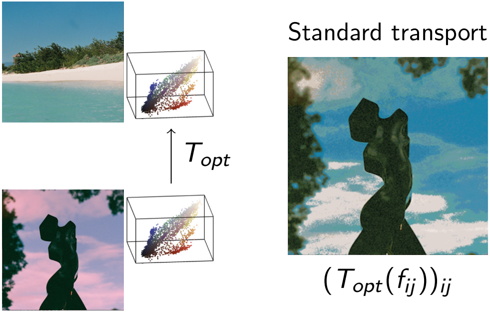

$(T_{opt}(f_{ij}))_{ij}$

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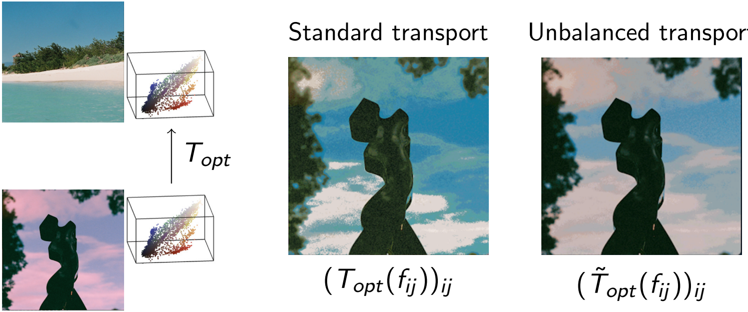

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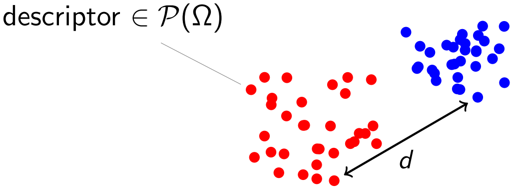

Figure: Machine learning: data described by empirical measures or histograms (text, image)

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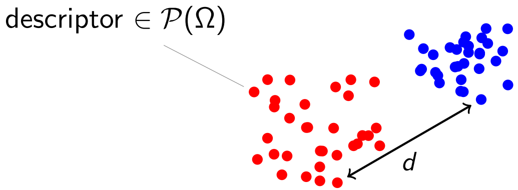

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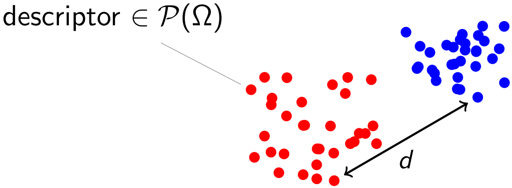

Figure: Machine learning: data described by empirical measures or histograms (text, image)

$\Rightarrow$ Conservation of mass sometimes undesirable...

Also: gradient flows, shape matching, economics...

Beyond probability measures

Specific models:

Static [Hanin, 1992], [Benamou, 2003]

Dynamic [Piccoli and Rossi, 2013], [Mass et al., 2015], [Lombardi and Maitre, 2013]

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General framework:

- Static formulation
- Dynamic formulation
- Efficient algorithms

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- Static formulation
- Dynamic formulation
- Efficient algorithms

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

Outline

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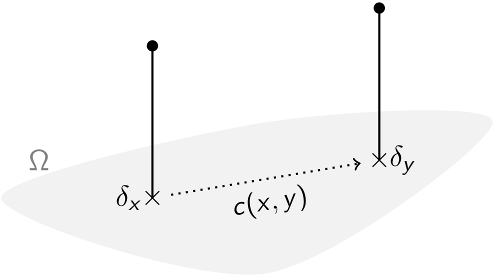
Static Formulation

Dynamic Formulation

Examples & Numerics

From standard OT...



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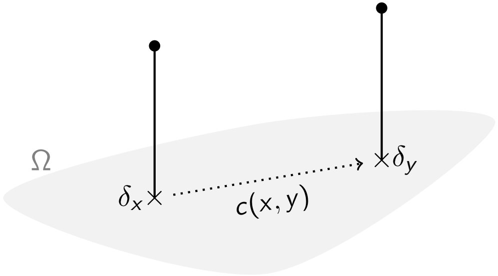

In general, c is assumed :

- lower bounded;
- l.s.c.

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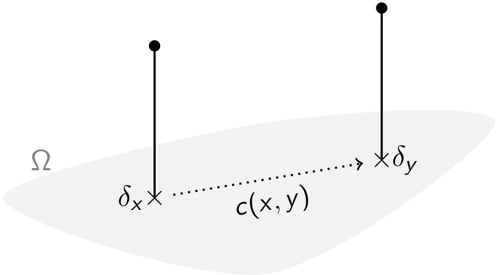

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Static formulation of OT:

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

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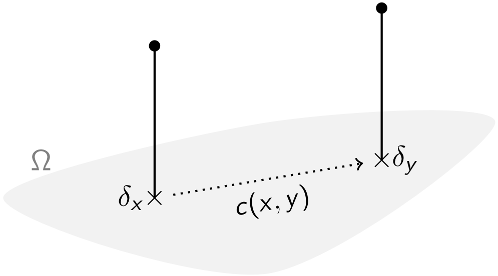

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Static formulation of OT:

$$\text{minimize} \int_{\Omega^2} c(x,y)m(x,y)\mathrm{d}\lambda_{ref} \qquad (\gamma = m\lambda_{ref})$$

$$\text{subject to } (\mathrm{proj}_x)_\# m = \mu \qquad \text{(abuse of notation)}$$

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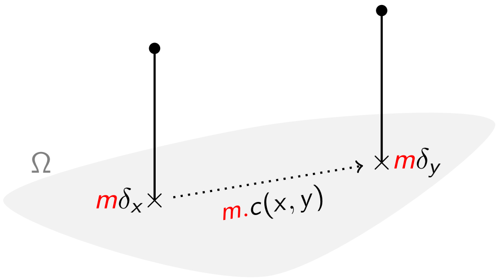

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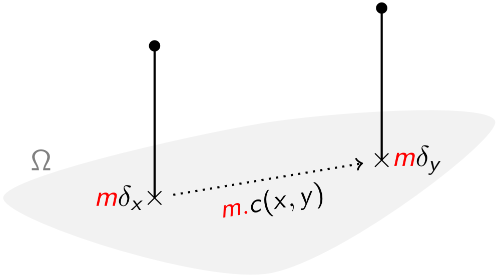

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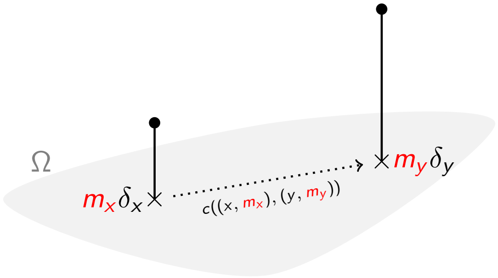

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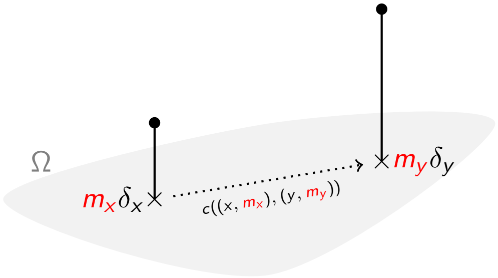

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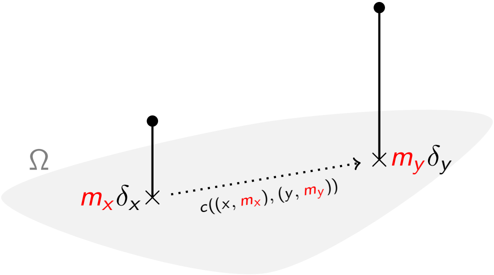

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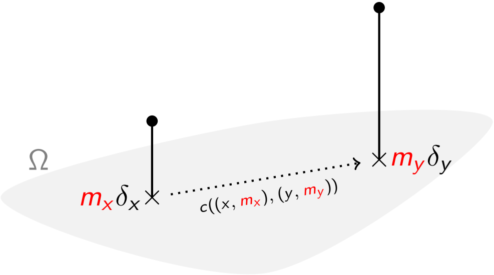

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- pos. homogeneous in (m_x, m_y);
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- nonnegative, l.s.c.

Static formulation of Unbalanced OT

$$C(\rho_0, \rho_1) \overset{\text{def.}}{=} \text{minimize} \int_{\Omega^2} c\big((x, m_\mu(x,y)), (y, m_\nu(x,y))\big) \mathrm{d}\lambda_{ref}$$

$$\text{subject to } (\text{proj}_x)_\# m_\mu = \mu$$

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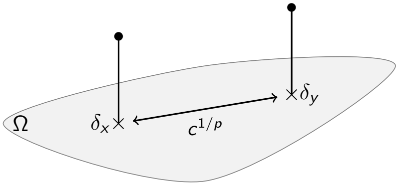
Properties



Theorem (Standard OT)

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

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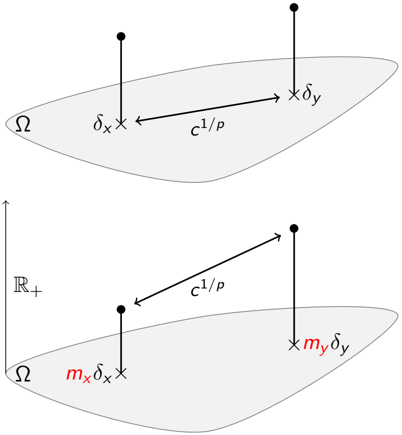

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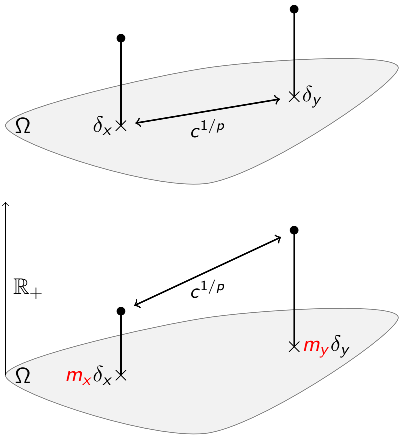

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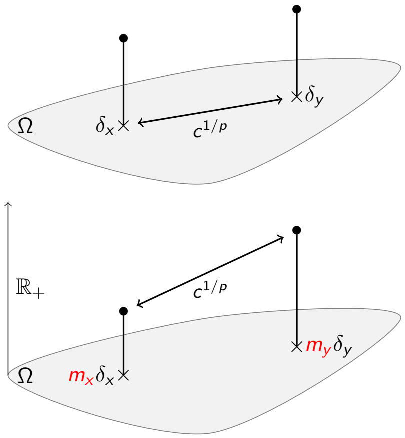

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Also: Duality, weak* continuity...

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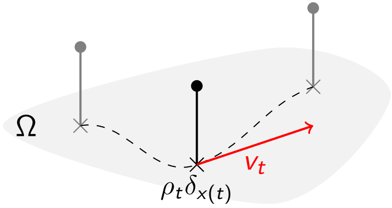
Static Formulation

Dynamic Formulation

Examples & Numerics

A dynamic approach: standard OT



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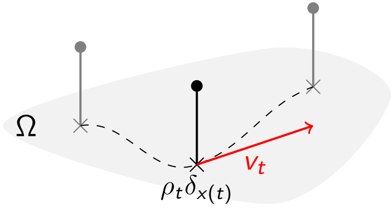

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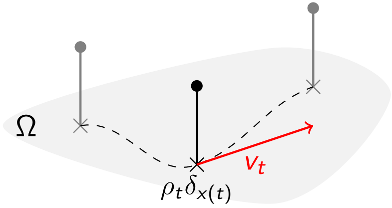

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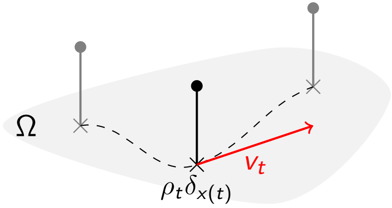

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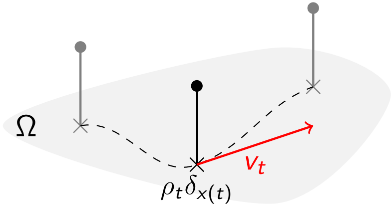

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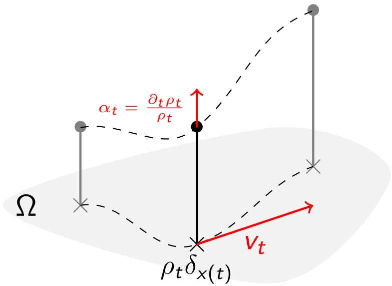

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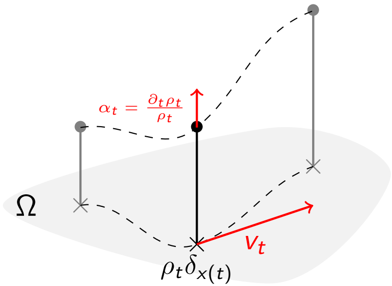

Variables: $\omega = \rho v$, $\zeta = \rho\alpha$
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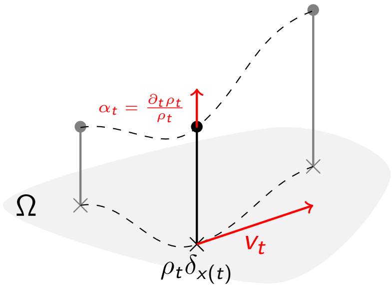

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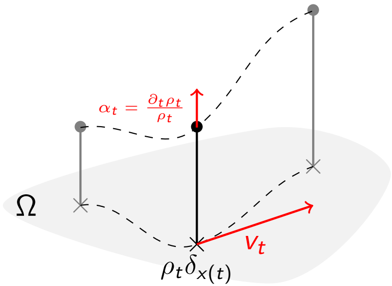

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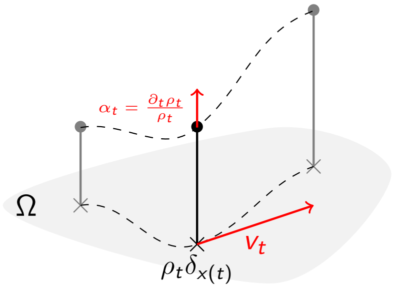

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Unbalanced dynamic formulation

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$$(\text{proj}_{t=0})_\# \rho = \mu \quad , \quad (\text{proj}_{t=1})_\# \rho = \nu \, .$$

Dynamic to Static : "Benamou-Brenier" formula

Costs between points in Cone(Ω) induced by f:

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

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 $C : \mathcal{M}_+(\Omega)^2 \to \mathbb{R}_+$ is weakly continuous, then $C = D$.*

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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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Static Formulation

Dynamic Formulation

Examples & Numerics

Partial OT / Wasserstein-TV

$$\text{minimize} \quad \int_0^1 \int_\Omega \Big(\underbrace{\frac{1}{p} \frac{|\omega_t(x)|^p}{\rho_t(x)^{p-1}}}_{\text{Wasserstein}} + \underbrace{\delta|\zeta_t(x)|}_{\text{TV of source}} \Big) \mathrm{d}x\mathrm{d}t$$

$$\text{subject to} \quad \partial_t \rho + \nabla \cdot \omega = \zeta$$

$$(\text{proj}_{t=0})_{\#}\rho = \mu \quad , \quad (\text{proj}_{t=1})_{\#}\rho = \nu \, .$$

[Piccoli and Rossi, 2013] , [C. et al, 2015b]

Partial OT / Wasserstein-TV

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- "Lagrangian" formulation of partial OT : $m \leftrightarrow \delta$;
- $C^{1/p}$ defines a metric on $\mathcal{M}_+(\Omega)$;

Partial OT / Wasserstein-TV

$$\text{minimize} \quad \int_0^1 \int_\Omega \Big(\underbrace{\frac{1}{p} \frac{|\omega_t(x)|^p}{\rho_t(x)^{p-1}}}_{\text{Wasserstein}} + \underbrace{\delta |\zeta_t(x)|}_{\text{TV of source}} \Big) \mathrm{d}x\mathrm{d}t$$

$$\text{subject to} \quad \partial_t \rho + \nabla \cdot \omega = \zeta$$

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

[Piccoli and Rossi, 2013] , [C. et al, 2015b]

- "Lagrangian" formulation of partial OT : $m \leftrightarrow \delta$;
- $C^{1/p}$ defines a metric on $\mathcal{M}_+(\Omega)$;
- $p = 1$ gives the so-called *bounded Lipschitz* metric.

Wasserstein-Fisher-Rao : *WF*

$$\text{minimize} \quad \int_0^1 \int_\Omega \Big(\underbrace{\frac{|\omega_t(x)|^2}{\rho_t(x)}}_{\text{Wasserstein cost}} + \underbrace{\frac{\zeta_t(x)^2}{\rho_t(x)}}_{\text{Fisher-Rao cost}} \Big) \mathrm{d}x\mathrm{d}t$$

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- *WF* defines a Riemannian-like metric on $\mathcal{M}_+(\Omega)$;
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- alternative formulation :

$$\inf_\gamma \int_{\Omega^2} \tilde{c}(x, y) \mathrm{d}\gamma(x, y) + \underbrace{KL((\mathrm{proj}_x)_\# \gamma | \mu) + KL((\mathrm{proj}_y)_\# \gamma | \nu)}_{\text{relaxed marginal constraints}}$$

Numerics: dynamic

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

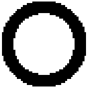


Figure: FR

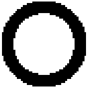


Figure: W_2

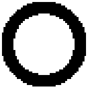
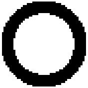


Figure: $W_2 - TV$



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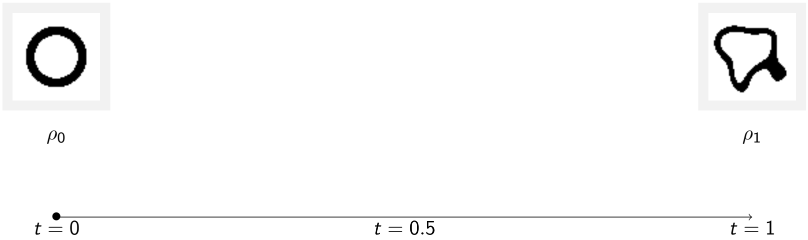

Figure: Geodesics between ρ_0 and ρ_1 for (1st row) Fisher-Rao (2nd row) W_2 (3rd row) partial OT (4th row) WF.

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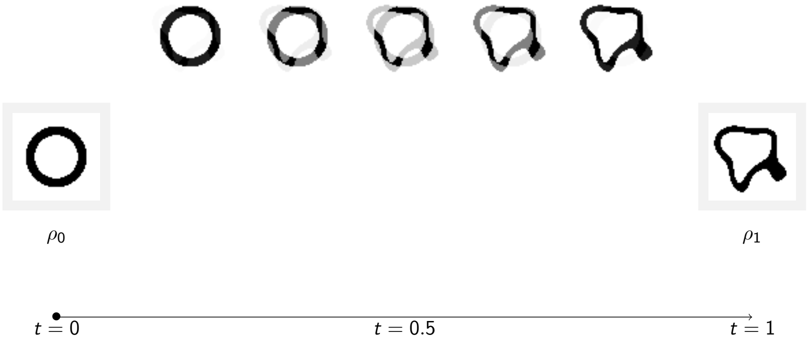

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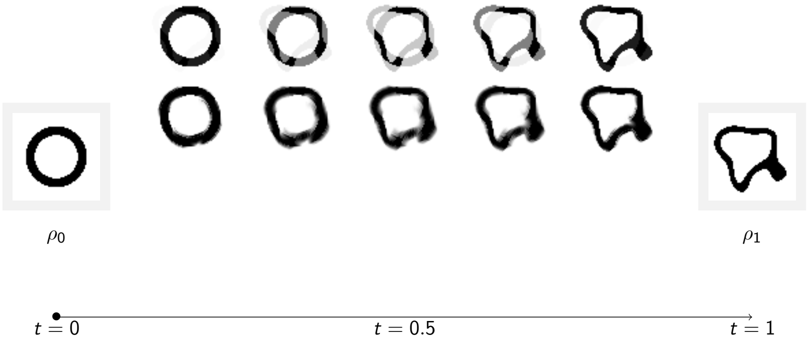

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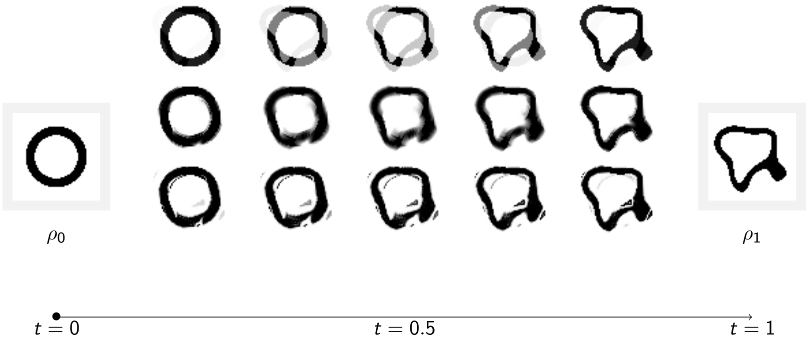

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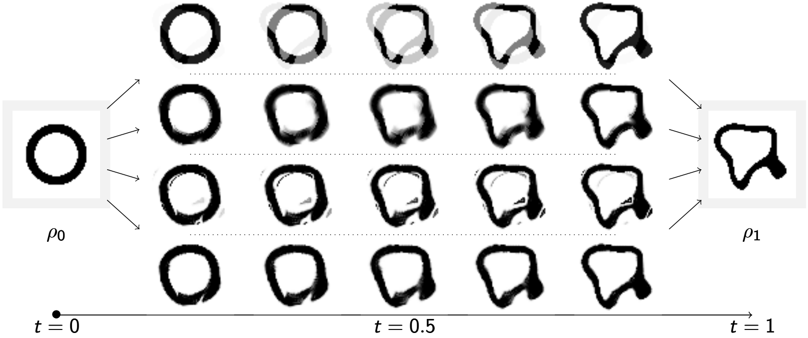

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Numerics: static

Entropy regularization on the static formulation : fast Sinkhorn-like algorithm

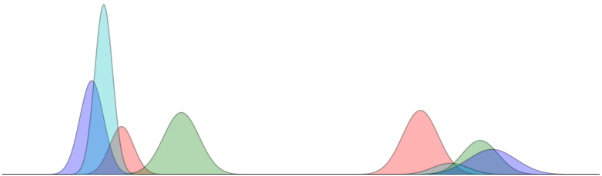

Figure: (top) 4 probability measures on $\Omega = [0, 1]$ with two bumps each

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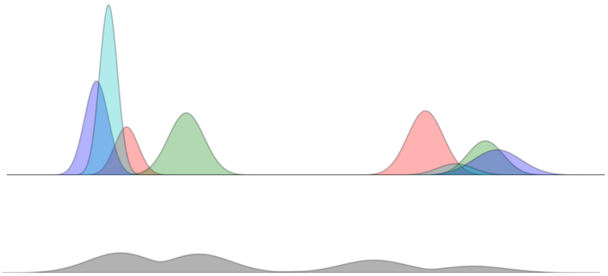

Figure: (top) 4 probability measures on $\Omega = [0, 1]$ with two bumps each (middle) W_2 barycenter

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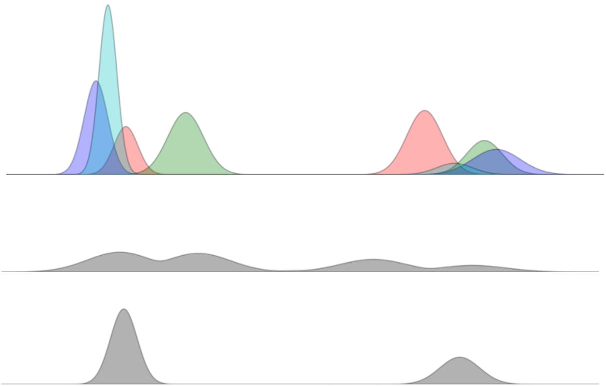

Figure: (top) 4 probability measures on $\Omega = [0, 1]$ with two bumps each (middle) W_2 barycenter (bottom) WF barycenter.

Conclusion

Take home messages

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Unbalanced optimal transport :

- **stabilizes** solutions and is **natural** in many applications ;
- admits **dynamic**, **static** and **dual** formulations ;
- can be solved by **fast algorithms** adapted from standard OT.

For Further Reading I

- Chizat, L., Peyré, G., Schmitzer, B., and Vialard, F.-X. (2015a).
  Unbalanced optimal transport: geometry and Kantorovich formulation.
- Chizat, L., Peyré, G., Schmitzer, B., and Vialard, F.-X. (2015b).
  An interpolating distance between optimal transport and Fisher-Rao.
- Liero, M., Mielke, A., and Savaré, G. (2015).
  Optimal Entropy-Transport problems and a new Hellinger-Kantorovich distance between positive measures.