Computing Optimal Transport Barycentres

Eloi Tanguy, Julie Delon, Nathaël Gozlan

MAP5, Université Paris-Cité

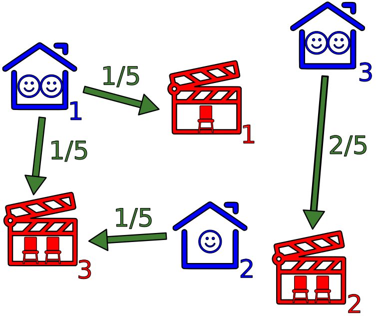
5th June 2025

1. Optimal Transport

2. Wasserstein Barycentres

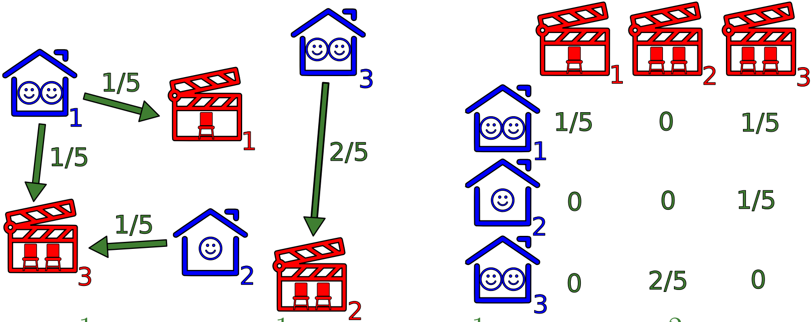
3. OT Barycentres

Introduction to Optimal Transport



	1	2	3
1	1/5	0	1/5
2	0	0	1/5
3	0	2/5	0

Introduction to Optimal Transport



$$\text{Cost} = \frac{1}{5} \times c(x_1, y_1) + \frac{1}{5} \times c(x_1, y_3) + \frac{1}{5} \times c(x_2, y_3) + \frac{2}{5} \times c(x_3, y_2).$$

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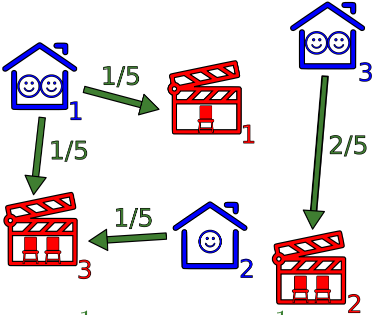

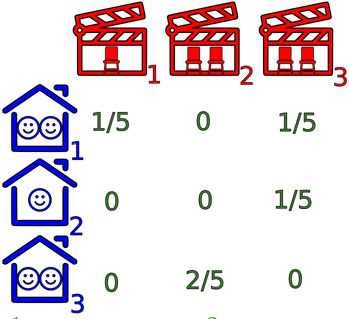

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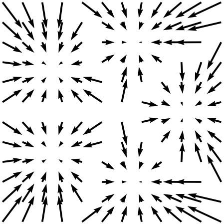
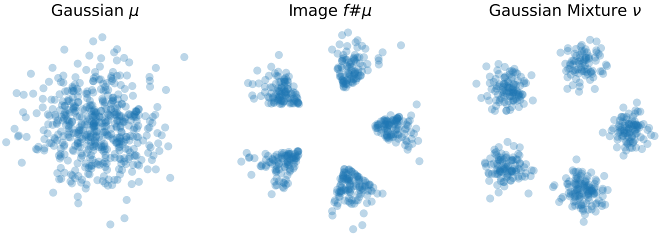
$$\mathcal{T}_c(\mu, \nu) = \inf_{\pi \in \Pi(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{Y}} c(x, y)\mathrm{d}\pi(x, y) = \inf_{X\sim\mu, Y\sim\nu} \mathbb{E}[c(X, Y)].$$

$$\mathrm{W}_2^2(\mu, \nu) = \inf_{\pi \in \Pi(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{Y}} \|x - y\|_2^2 \mathrm{d}\pi(x, y).$$

Push-forward measures and OT maps

Image Measure: $f\#\mu := \mathrm{Law}_{X\sim\mu}[f(X)]$





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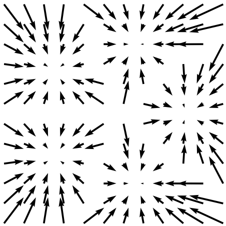

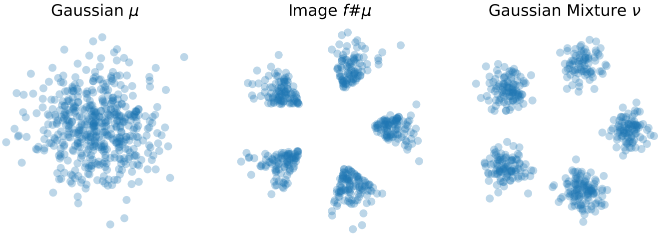

Brenier's Theorem

If $c(x,y) = \|x-y\|_2^2$, and $\mu \ll \mathscr{L}^d$, then there is a unique solution $\pi^* = (I, \nabla\varphi)\#\mu$, with φ convex.

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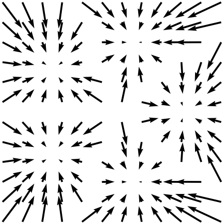

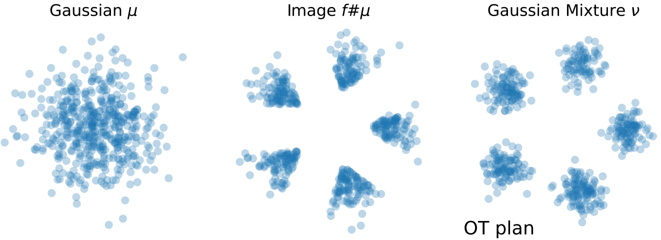

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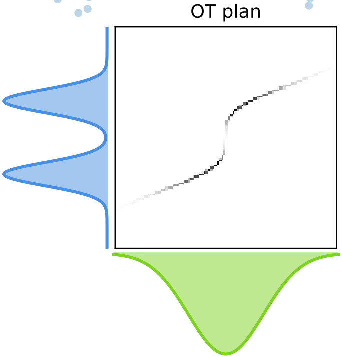


1. Optimal Transport

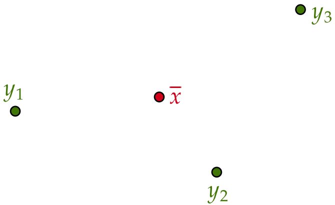
2. Wasserstein Barycentres

3. OT Barycentres

From Euclidean Combinations to Fréchet Means

$$\overline{x} = \sum_{k=1}^{K} \lambda_k y_k$$

$$\overline{x} = \underset{x \in \mathbb{R}^d}{\operatorname{argmin}} \sum_{k=1}^{K} \lambda_k \|x - y_k\|_2^2$$



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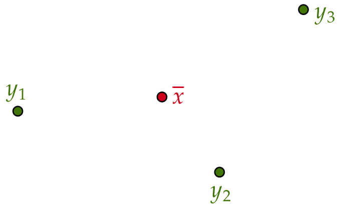

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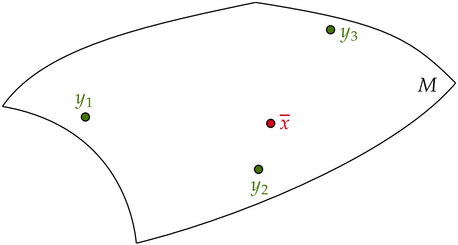
Fréchet mean:

$$\overline{x} \in \underset{x \in \mathcal{X}}{\mathrm{argmin}} \sum_{k=1}^{K} \lambda_k d(x, y_k)^2.$$



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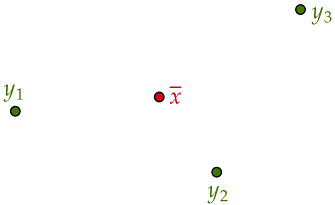

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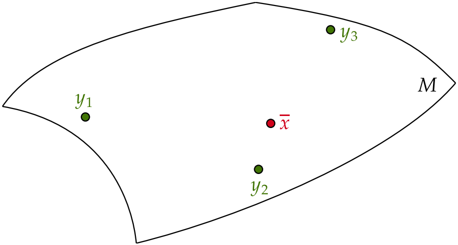
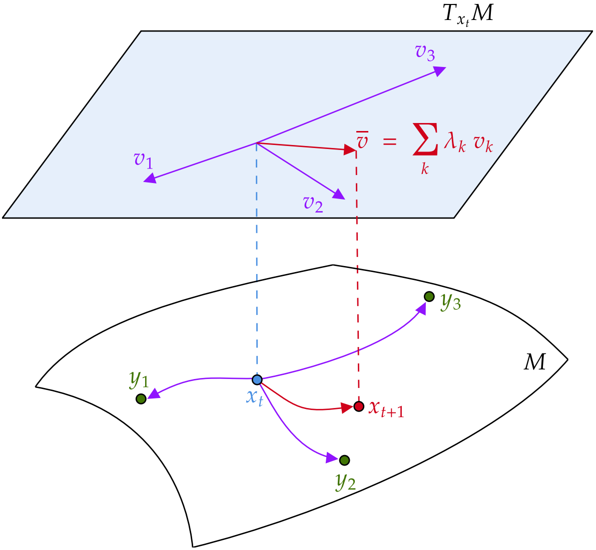


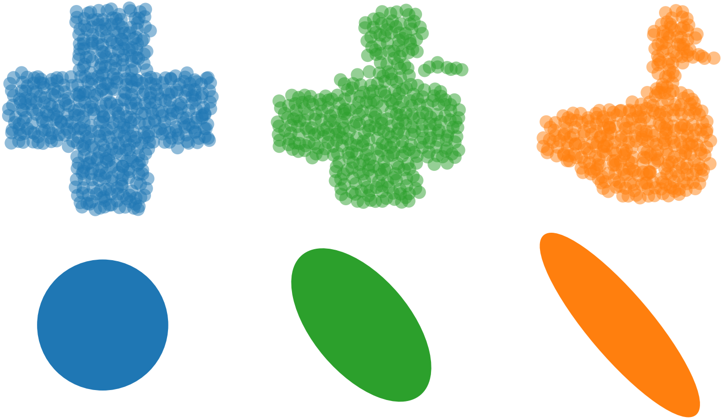
Generalisation: $\overline{x} \in \operatorname*{argmin}_{x \in \mathcal{X}} \sum_{k=1}^{K} c_k(x, y_k)$.

Fixed-Point Algorithm for Fréchet Means on Manifolds



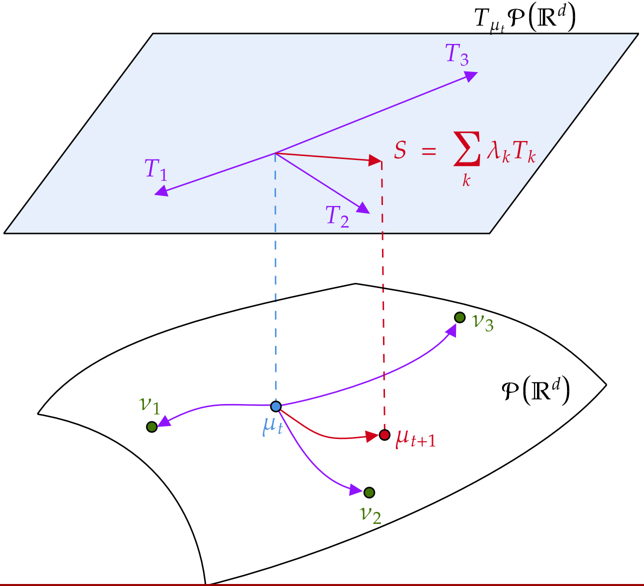
2-Wasserstein Barycentres (Agueh & Carlier 2011 [1])

$$\underset{\mu \in \mathcal{P}(\mathbb{R}^d)}{\operatorname{argmin}} \sum_{k=1}^{K} \lambda_k \mathrm{W}_2^2(\mu, \nu_k).$$



Fixed-Point Method (Alvarez-Esteban et al. 2016 [2])

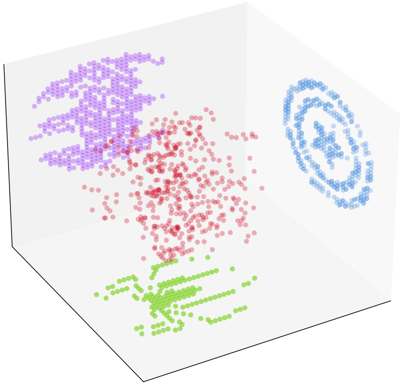
Assumptions: $c(x,y) = \|x-y\|_2^2$, AC measures on $\mathbb{R}^d$.

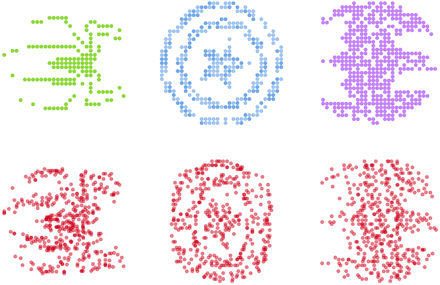


Motivation for OT barycenters with generic costs

$$\mathrm{W}_1(\mu, \nu) := \inf_{\pi \in \Pi(\mu,\nu)} \int \|x - y\|_2 \mathrm{d}\pi(x, y).$$

Find $\mu \in \mathcal{P}(\mathbb{R}^3)$ minimising $\sum_k \frac{1}{3}\mathrm{W}_1(P_k\#\mu, \nu_k)$ where $\nu_k \in \mathcal{P}(\mathbb{R}^2)$.





Generalising Wasserstein Barycentres

Setting:

- $(\mathcal{X}, d_{\mathcal{X}})$ compact metric space for barycentres.
- $(\mathcal{Y}_k, d_{\mathcal{Y}_k})$ compact metric spaces for measures ν_k.
- $c_k : \mathcal{X} \times \mathcal{Y}_k \longrightarrow \mathbb{R}_+$ continuous cost functions.

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$$\underset{\mu \in \mathcal{P}(\mathcal{X})}{\operatorname{argmin}} \ V(\mu), \quad V(\mu) := \sum_{k=1}^{K} \mathcal{T}_{c_k}(\mu, \nu_k).$$

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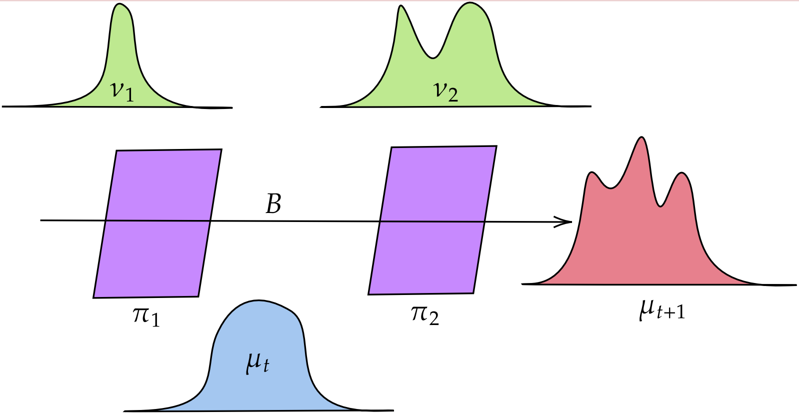
Assumption: The ground barycenter function

$$B(y_1, \cdots, y_K) := \underset{x \in \mathcal{X}}{\operatorname{argmin}} \sum_{k=1}^{K} c_k(x, y_k)$$

is well-defined.

Fixed-point Algorithm

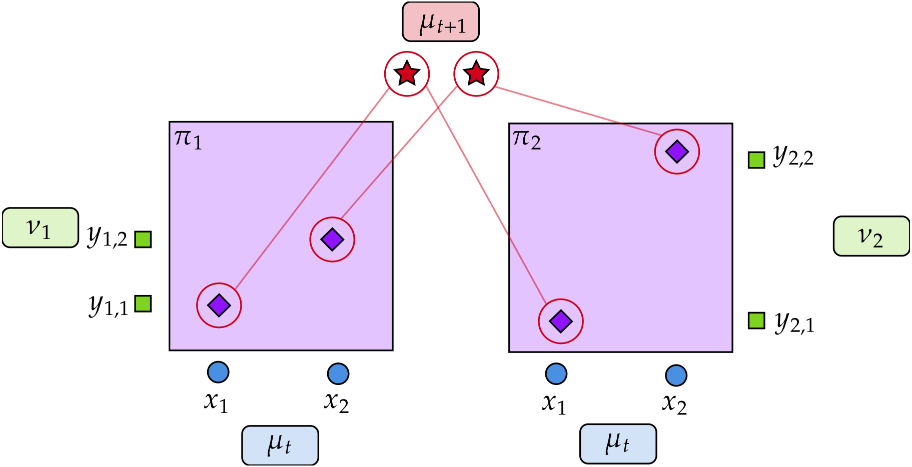


$$\Gamma(\mu) := \left\{(X, Y_1, \cdots, Y_K) \ : \ (X, Y_k) \in \Pi^*_{c_k}(\mu, \nu_k)\right\},$$

$$G := \begin{cases} \mathcal{P}(\mathcal{X}) & \rightrightarrows \quad \mathcal{P}(\mathcal{X}) \\ \mu & \mapsto \quad \{\mathrm{Law}\,[B(Y_1, \cdots, Y_K)] \ : (X, Y_1, \cdots, Y_K) \in \Gamma(\mu).\} \end{cases}$$

$$\mu_{t+1} \in G(\mu_t).$$

Discrete G (Simplified)



Algorithm Convergence

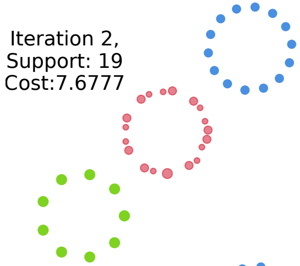
Decrease Property

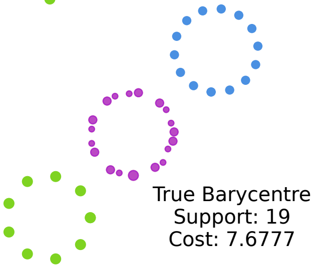
$$\forall \overline{\mu} \in G(\mu),\ V(\mu) \geq V(\overline{\mu}) + \mathcal{T}_\delta(\mu, \overline{\mu}).$$

If μ^* is a barycentre then $G(\mu^*) = \{\mu^*\}$.

Convergence

If μ is a subsequential limit of (μ_t) then $\mu \in G(\mu)$.





- Talk based on *ET, Julie Delon and Nathaël Gozlan (2024):* Computing Barycentres of Measures for Generic Transport Costs. arXiv preprint 2501.04016.
- All code at `https://github.com/eloitanguy/ot_bar`
- Functions (soon) released on `https://pythonot.github.io/`
- Slides at `https://eloitanguy.github.io/publications/`

Thanks!

[1] Martial Agueh and Guillaume Carlier.
Barycenters in the Wasserstein space.
SIAM Journal on Mathematical Analysis, 43(2):904–924, 2011.

[2] Pedro C Álvarez-Esteban, E Del Barrio, JA Cuesta-Albertos, and C Matrán.
A fixed-point approach to barycenters in Wasserstein space.
Journal of Mathematical Analysis and Applications, 441(2):744–762, 2016.