Computing Optimal Transport Barycentres

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1 Optimal Transport

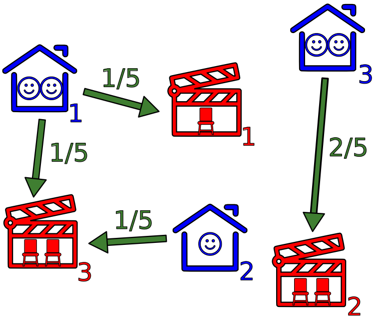
2 Wasserstein Barycentres

3 OT Barycentres

4 Discrete Case and Numerics

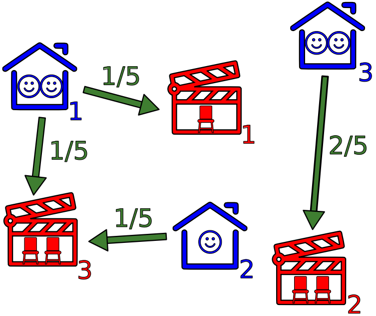
5 Application to GMMs

Discrete Optimal Transport



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

Discrete Optimal Transport



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

Assignment Cost:

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

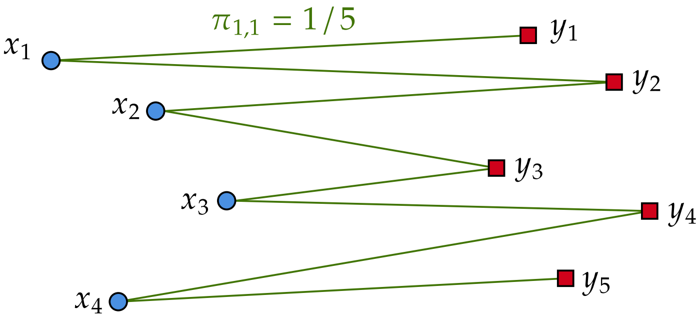
Constraints on $\pi \in \mathbb{R}_+^{3\times 3}$: $\pi \mathbf{1} = (2/5, 1/5, 2/5)$, $\pi^\top \mathbf{1} = (1/5, 2/5, 2/5)$.

$$\text{Optimal Transport Cost :} \quad \min_\pi \sum_{i,j} c(x_i, y_j)\pi_{i,j}.$$

OT between discrete measures

$$\mu = \sum_{i=1}^{n} a_i \delta_{x_i}, \ \nu = \sum_{j=1}^{m} b_j \delta_{y_j}$$

$$\mathcal{T}_c(\mu, \nu) = \inf_{\pi \in \Pi(a,b)} \sum_{i,j} c(x_i, y_j) \pi_{i,j}.$$



OT Cost and 2-Wasserstein Distance

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

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

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Bures-Wasserstein

$$\mathrm{W}_2^2(\mathcal{N}(m_1,S_1),\mathcal{N}(m_2,S_2))$$
$$= \|m_1 - m_2\|_2^2$$
$$+\mathrm{Tr}\left(S_1 + S_2 - 2(S_1^{1/2} S_2 S_1^{1/2})^{1/2}\right)$$

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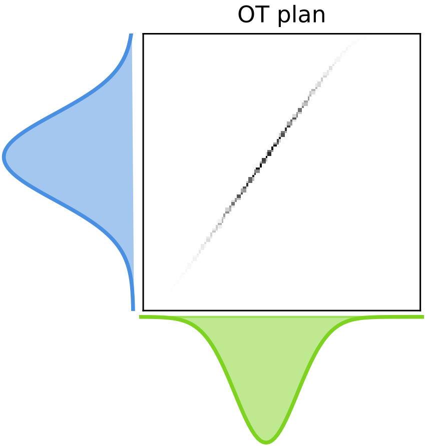
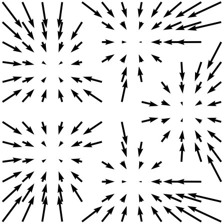
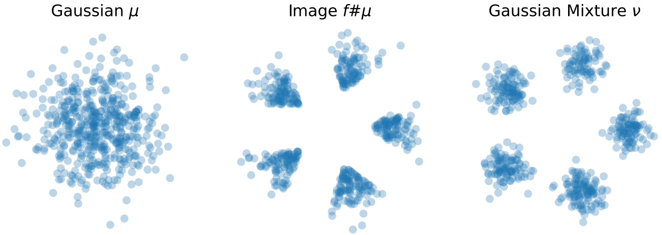


Push-forward measures and OT maps

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





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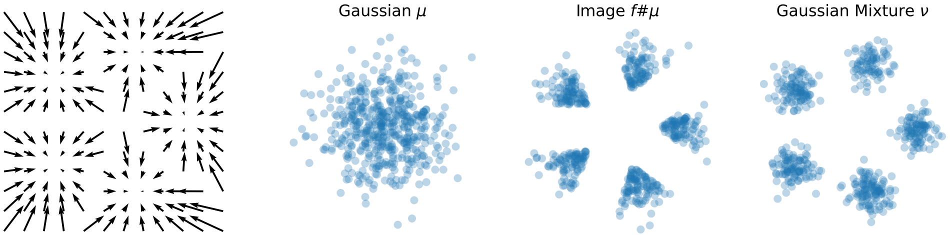

Brenier's Theorem

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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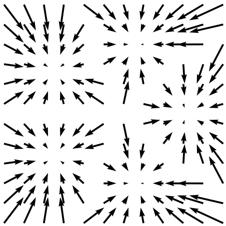

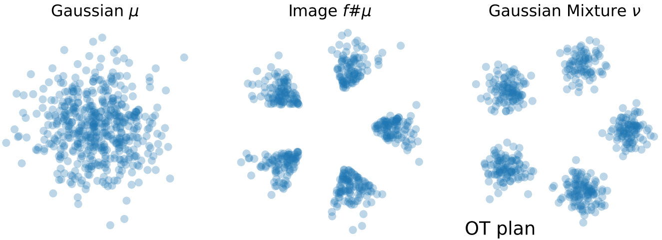

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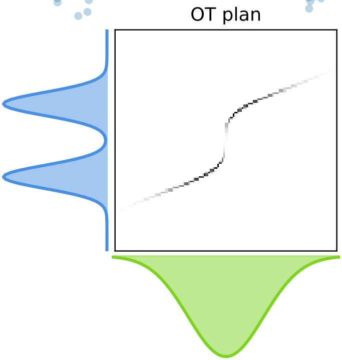

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2. **Wasserstein Barycentres**
3. OT Barycentres
4. Discrete Case and Numerics
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From Euclidean Combinations to Fréchet Means

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

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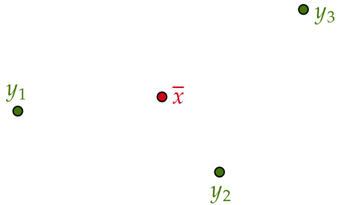

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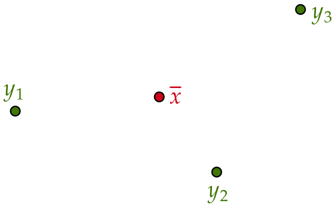

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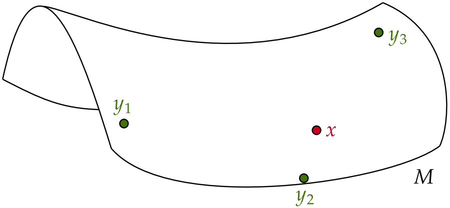
Fréchet mean:

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



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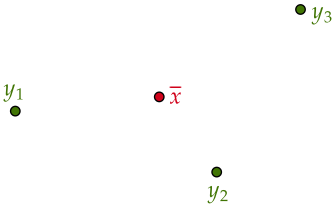

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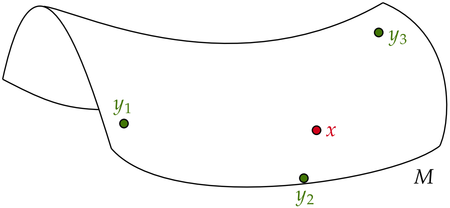
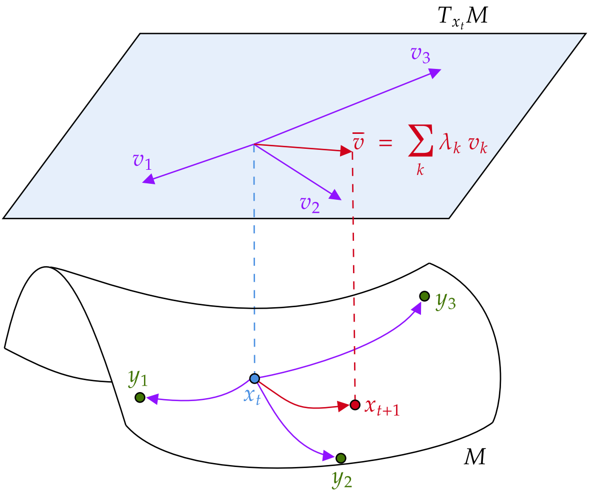


Generalisation: $\overline{x} \in \underset{x \in \mathcal{X}}{\operatorname{argmin}} \sum_{k=1}^{K} c_k(x, y_k).$

Fixed-Point Algorithm for Fréchet Means on Manifolds



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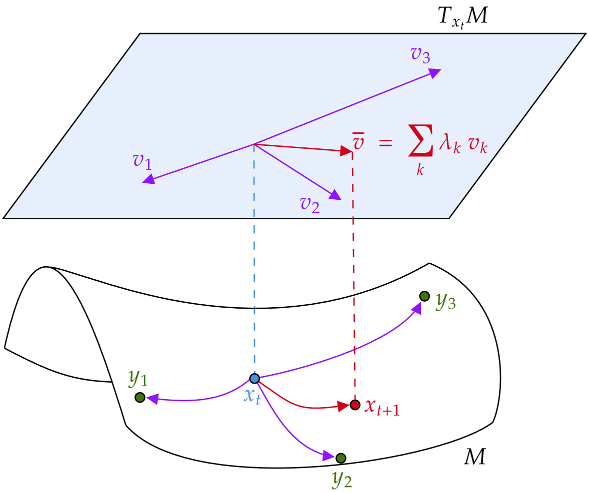


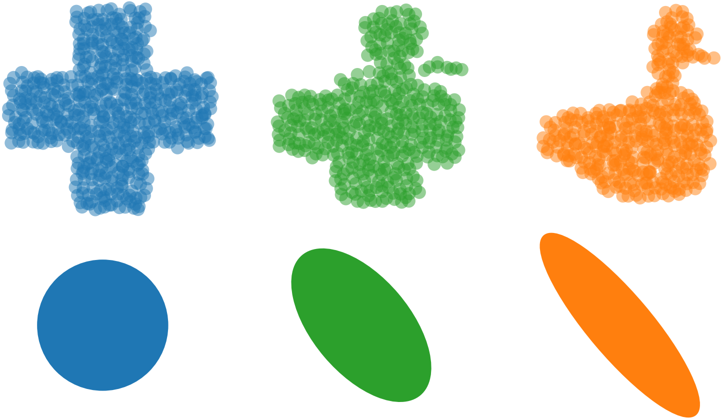
$$V(x) = \sum_{k=1}^{K} \lambda_k d(x, y_k)^2.$$

$$\nabla V(x) = -2 \sum_{k=1}^{K} \lambda_k \mathrm{Log}_x(y_k).$$

$$x_{t+1} = \mathrm{Exp}_{x_t}\left(-\frac{1}{2}\nabla V(x_t)\right).$$

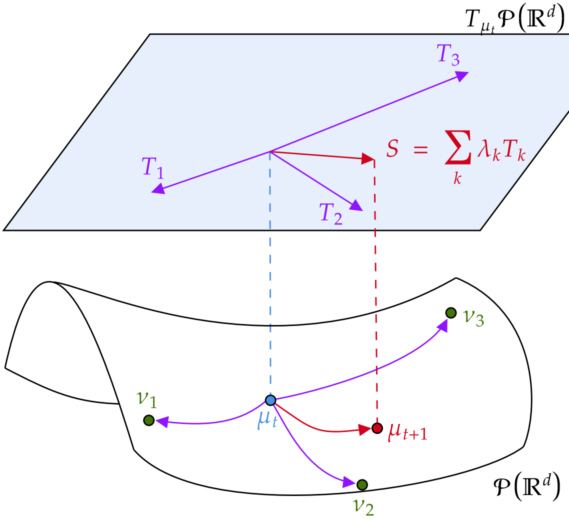
2-Wasserstein Barycentres (Agueh & Carlier 2011 [1])

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



Fixed-Point Method (Alvarez-Esteban et al. 2016 [3])

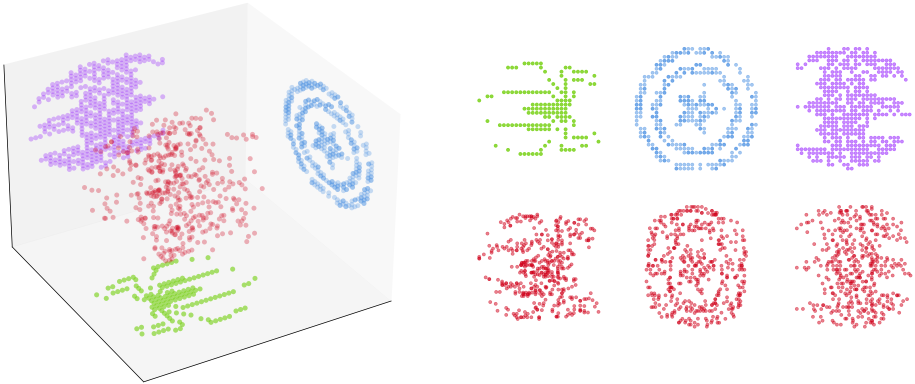
Assumptions: $c(x, y) = \|x - y\|_2^2$, AC measures on $\mathbb{R}^d$.



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 $\nu_k \in \mathcal{P}(\mathbb{R}^2)$.



Generalises Delon et al. 2021 [5] where $c_k(x,y) = \|P_k(x)-y\|_2^2$.

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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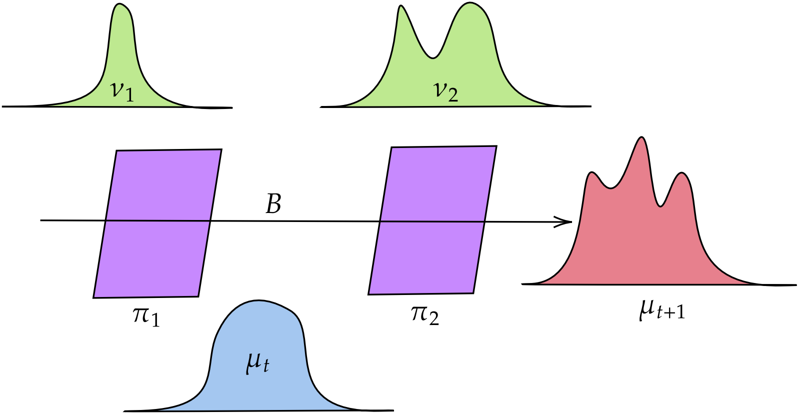
Assumption: The ground barycenter function

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

is well-defined.

Fixed-Point Algorithm: Intuition



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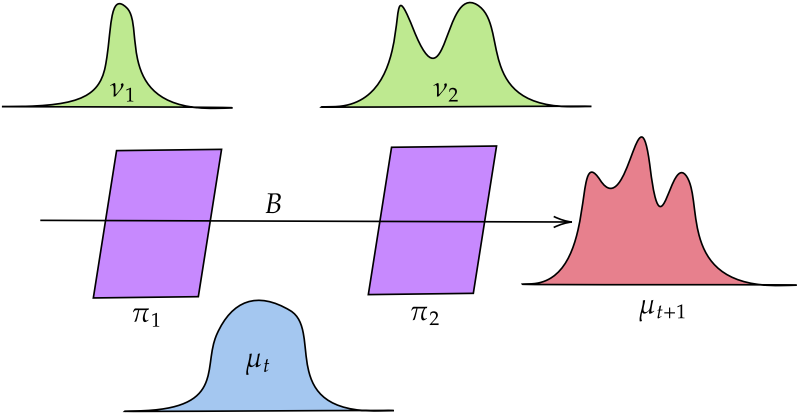
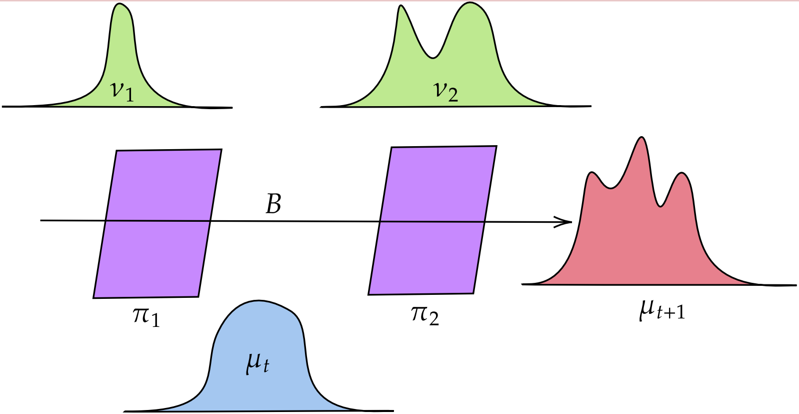


General Idea

Let $(X_t, Y_1, \cdots, Y_K)$ RVs such that $X_t \sim \mu_t$, $Y_k \sim \nu_k$ and $(X_t, Y_k) \sim \pi_k \in \Pi^*_{c_k}(\mu_t, \nu_k)$. Take $X_{t+1} = B(Y_1, \cdots, Y_K)$.

If $\Pi^*_{c_k}(\mu_t, \nu_k) = \{(I, T_k)\#\mu_t\}$ then $\mu_{t+1} = B(T_1, \cdots, T_K)\#\mu_t$.

Fixed-point Algorithm: (more) formal definition



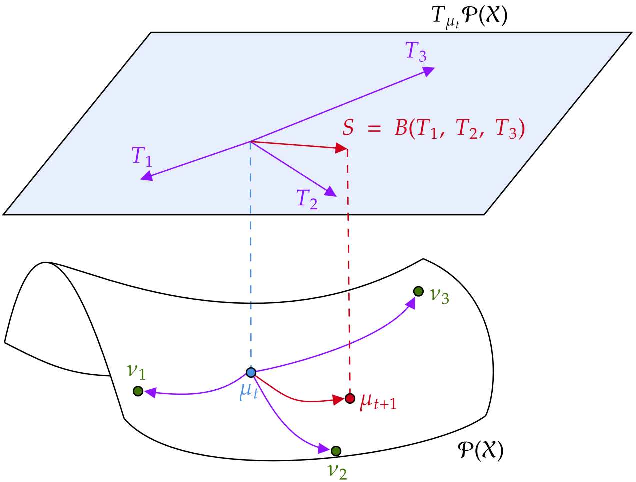
$$\Gamma(\mu) := \left\{ \gamma \in \mathcal{P}(\mathcal{X} \times \mathcal{Y}_1 \cdots \times \mathcal{Y}_K) : \ \forall k \in [\![1, K]\!], \ \gamma_{0,k} \in \Pi^*_{c_k}(\mu, \nu_k) \right\},$$

$$G := \left\{ \begin{array}{ccc} \mathcal{P}(\mathcal{X}) & \rightrightarrows & \mathcal{P}(\mathcal{X}) \\ \mu & \mapsto & B\#\Gamma(\mu) \end{array} \right. , \quad \mu_{t+1} \in G(\mu_t).$$

$$B\#\Gamma(\mu) := \{B\#\gamma, \ \gamma \in \Gamma(\mu)\}, \ B\#\gamma = \mathrm{Law}_{(X, Y_1, \cdots, Y_K) \sim \gamma} B(Y_1, \cdots, Y_K).$$

Relation to Alvarez-Esteban et al. 2016 [3]

Dream case: $\mathcal{X} = \mathcal{Y}_1 = \cdots = \mathcal{Y}_K$ and maps exist.



Reality:

$$\gamma : \gamma_{0,k} \in \Pi^*_{c_k}(\mu_t, \nu_k),$$

$$\mu_{t+1} = B\#\gamma.$$

Algorithm Convergence

Ground Barycentre Lemma

$$\sum_k c_k(x, y_k) \geq \sum_k c_k(B(y_1, \cdots, y_K), y_k) + \delta(x, B(y_1, \cdots, y_K)).$$

Case $\|x - y\|_2^2$: simply $\sum_k \lambda_k \|x - y_k\|_2^2 = \sum_k \|\overline{x} - y_k\|_2^2 + \|x - \overline{x}\|_2^2$.

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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 $G(\mu^*) = \{\mu^*\}$.

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Using arcane magic about the regularity of the multimap G:

Convergence

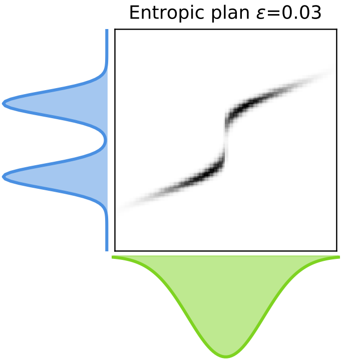
If μ is a subsequential limit of (μ_t) then $\mu \in G(\mu)$.

Entropic Barycentres

$$\mathcal{T}_{c,\varepsilon}(\mu,\nu) := \inf_{\pi\in\Pi(\mu,\nu)} \int_{\mathcal{X}\times\mathcal{Y}} c\mathrm{d}\pi + \varepsilon\,\mathrm{KL}(\pi|\mu\otimes\nu).$$

$$V_\varepsilon(\mu) := \sum_{k=1}^{K} \mathcal{T}_{c,\varepsilon}(\mu,\nu_k).$$

$$G_\varepsilon(\mu) := B\#\gamma,\ \text{with } \gamma_{0,k} = \Pi^*_{c_k,\varepsilon}(\mu,\nu_k).$$



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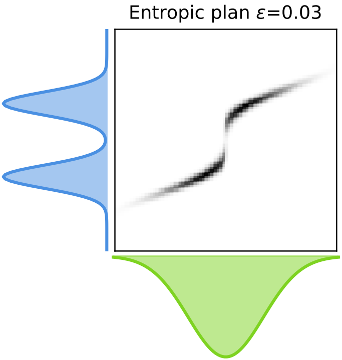


Decrease Property

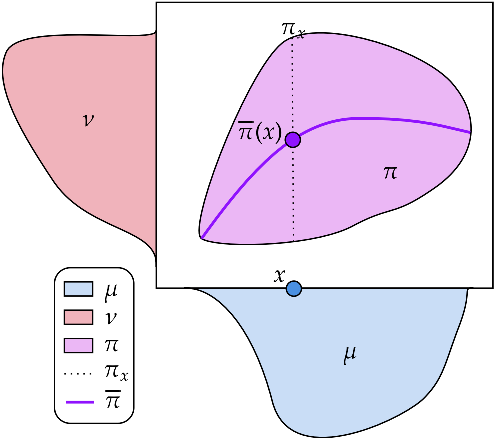
$V_\varepsilon(\mu) \geq V_\varepsilon(G_\varepsilon(\mu)) + \mathcal{T}_\delta(\mu, G_\varepsilon(\mu))$. If μ^* barycentre, $G_\varepsilon(\mu^*) = \mu^*$.

Convergence

If μ is a subsequential limit of (μ_t) then $\mu = G_\varepsilon(\mu)$.

Barycentric Projections

Replace a coupling π with a map $\overline{\pi}$.



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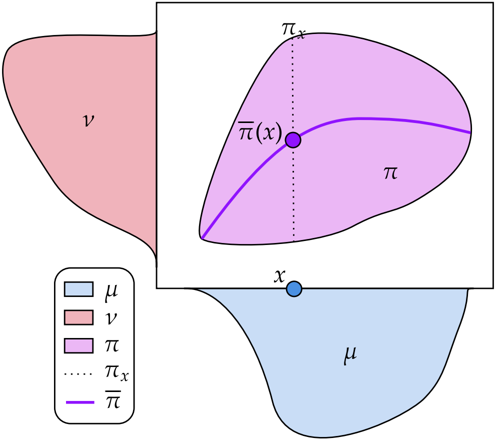

$$\overline{\pi}(x) = \int y \mathrm{d}\pi_x(y).$$

$$\overline{\pi}(x) = \mathbb{E}_{(X,Y)\sim\pi}[Y|X = x].$$

$$\overline{\pi} = \underset{f\in L^2(\mu)}{\mathrm{argmin}} \int \|f(x)-y\|_2^2 \mathrm{d}\pi(x,y).$$

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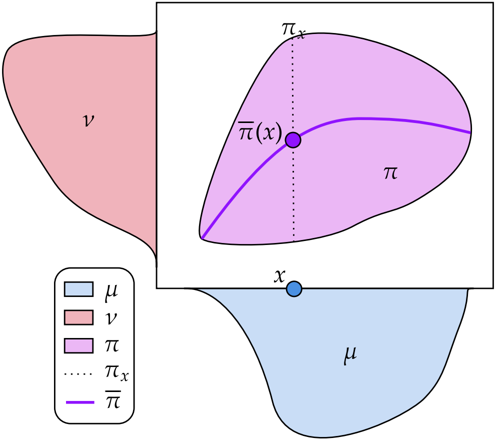

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$$H(\mu) = \left\{B(\overline{\pi_1}, \cdots, \overline{\pi_K})\#\mu,\ \pi_k \in \Pi^*_{c_k}(\mu, \nu_k)\right\}.$$

⚠ No guarantees.

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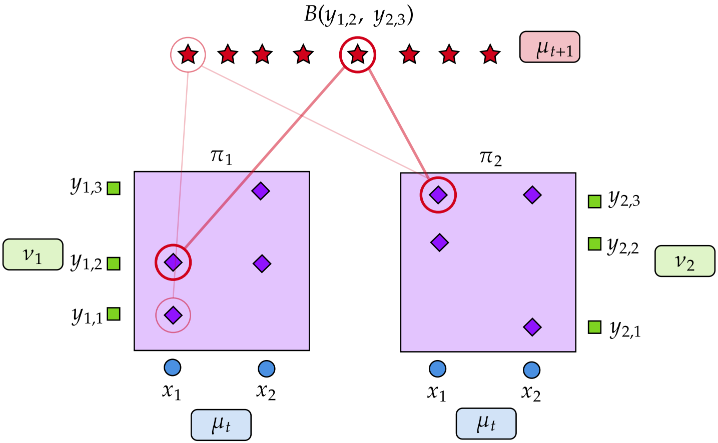
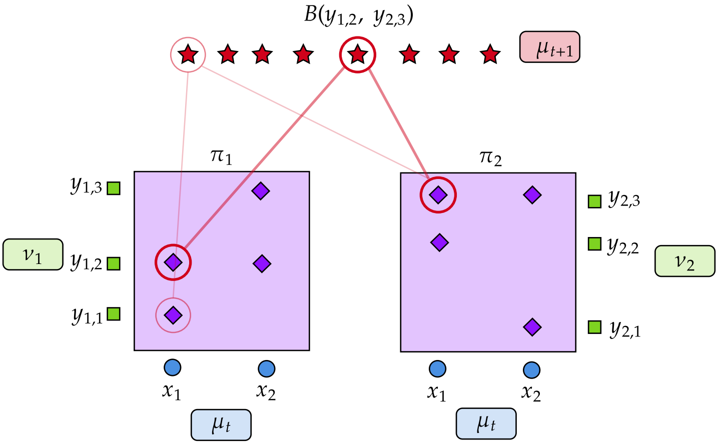
Discrete G



$$\mu = \sum_{i=1}^{n} a_i \delta_{x_i}$$

$$\nu_k = \sum_{j=1}^{n_k} b_{k,j} \delta_{y_{k,j}}$$

Discrete G



$$\mu = \sum_{i=1}^n a_i \delta_{x_i}$$

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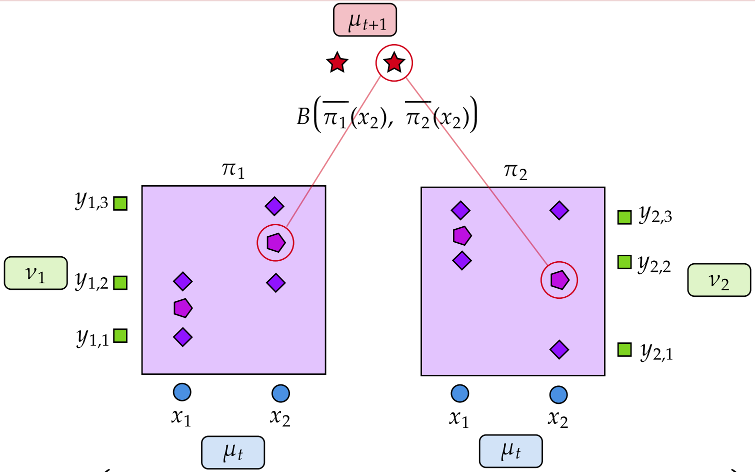
$$G(\mu) = \left\{ \sum_{j_1,\cdots,j_K} \left(\sum_{i=1}^n \frac{1}{a_i^{K-1}} \pi^{(1)}_{i,j_1} \times \cdots \times \pi^{(K)}_{i,j_K} \right) \delta\left(B(y_{1,j_1},\cdots,y_{K,j_K})\right), \quad \pi^{(k)} \in \Pi^*_{c_k}(\mu,\nu_k) \right\}.$$

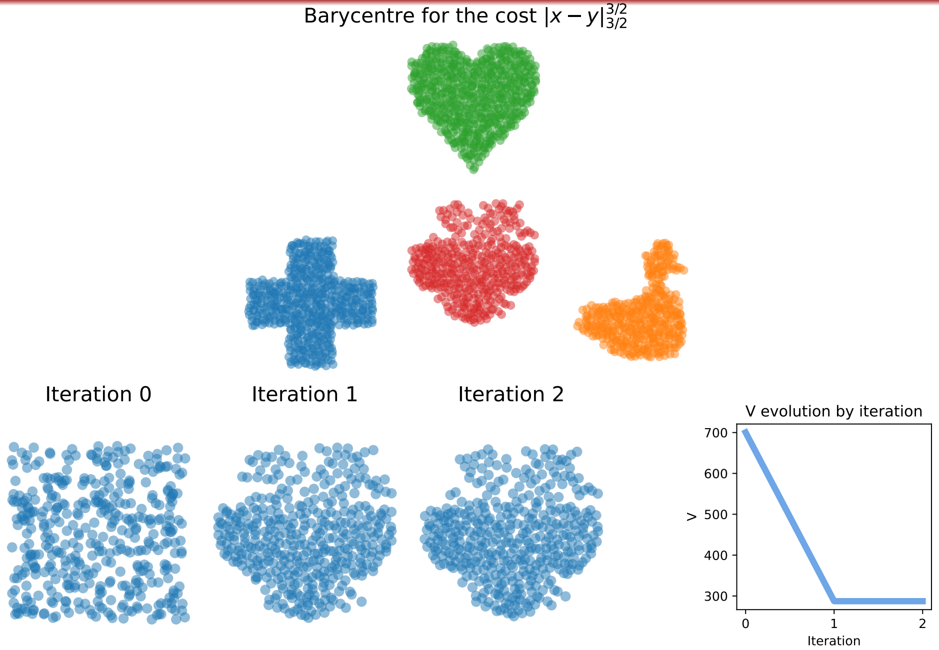
Discrete H (Generalises Cuturi & Doucet 2014 [4])



$$H(\mu) = \left\{ \sum_{i=1}^{n} a_i \delta \left(B \left(\overline{\pi}_1(x_i), \cdots, \overline{\pi}_K(x_i) \right) \right),\ \pi_k \in \Pi^*_{c_k}(\mu, \nu_k) \right\},$$

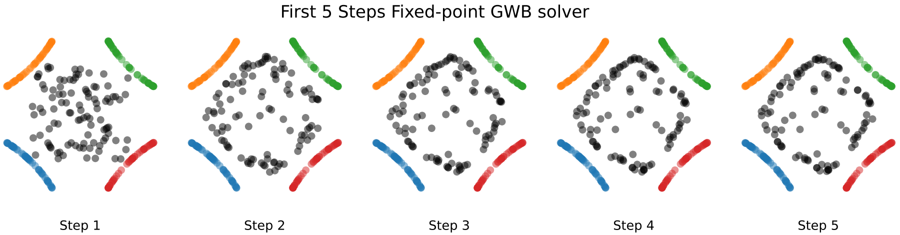
$$\overline{\pi}_k(x_i) = (1/a_i) \sum_{j=1}^{n_1} \pi^{(k)}_{i,j} y_{1,j}.$$

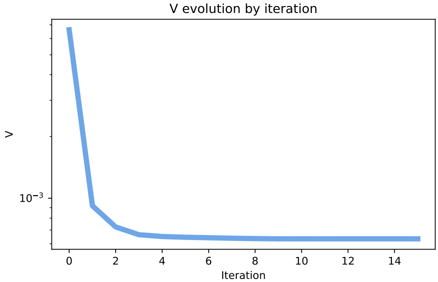
Illustration for $c(x, y) = \|x - y\|_{1.5}^{1.5}$



Non-linear Generalised Wasserstein Barycentre

$\text{argmin}_\mu \sum_{k=1}^4 \frac{1}{4} \mathrm{W}_2^2(P_k \# \mu, \nu_k)$ where P_k is the projection onto circle k.





1. Optimal Transport

2. Wasserstein Barycentres

3. OT Barycentres

4. Discrete Case and Numerics

5. Application to GMMs

OT between GMMs

$$\mathrm{W}_2^2(\mathcal{N}(m_1, S_1), \mathcal{N}(m_2, S_2)) = \|m_1 - m_2\|_2^2 + \underbrace{\mathrm{Tr}\left(S_1 + S_2 - 2(S_1^{1/2} S_2 S_1^{1/2})^{1/2}\right)}_{d_{\mathrm{BW}}^2(S_1, S_2) :=}.$$

OT between GMMs

$$\mathrm{W}_2^2(\mathcal{N}(m_1, S_1), \mathcal{N}(m_2, S_2)) = \|m_1 - m_2\|_2^2 + \underbrace{\mathrm{Tr}\left(S_1 + S_2 - 2(S_1^{1/2} S_2 S_1^{1/2})^{1/2}\right)}_{d_{\mathrm{BW}}^2(S_1,S_2):=}.$$

Ground space: $(\mathcal{X}, d) = (\mathcal{Y}_k, d_{\mathcal{Y}_k}) = (\mathcal{N}, \mathrm{W}_2)$ with ground cost $c = \mathrm{W}_2^2$.

$$\mu = \sum_{i=1}^n a_i \delta_{\mathcal{N}(m_i, S_i)}, \ \nu = \sum_{j=1}^m b_j \delta_{\mathcal{N}(m_j', S_j')} \in \mathcal{P}(\mathcal{N});$$

$$\mathcal{T}_{\mathrm{W}_2^2}(\mu, \nu) = \min_{\pi \in \Pi(a,b)} \sum_{i,j} (\|m_i - m_j'\|_2^2 + d_{\mathrm{BW}}^2(S_i, S_j'))\pi_{i,j}.$$

Ground Barycentre Between Gaussians

Gaussian barycentres (Agueh & Carlier 2011 [1]).

$$B(\mathcal{N}(m_1, S_1), \cdots, \mathcal{N}(m_K, S_K)) = \mathcal{N}(\overline{m}, \overline{S}),$$

$$\overline{m} := \sum_{k=1}^{K} \lambda_k m_k, \ \overline{S} := \underset{S \in S_d^{++}(\mathbb{R})}{\operatorname{argmin}} \sum_{k=1}^{K} \lambda_k d_{\mathrm{BW}}^2(S, S_k).$$

Fixed-point computation for $\overline{S}$:

$$G_{\mathcal{N}}(S) = S^{-1/2} \left(\sum_{k=1}^{K} \lambda_k (S^{1/2} S_k S^{1/2})^{1/2} \right)^2 S^{-1/2}.$$

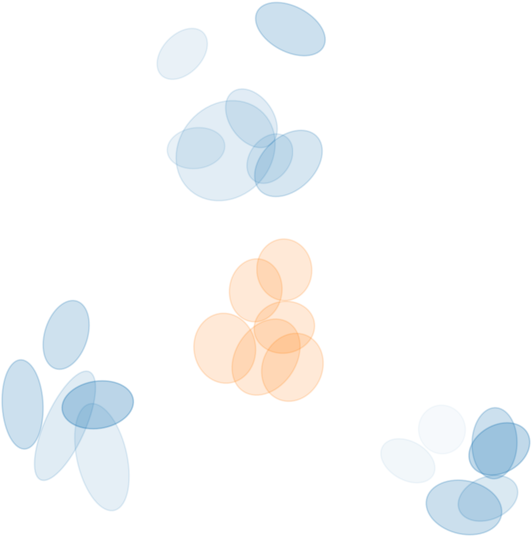
Riemannian gradient descent interpretation by Altschuler et al. 2021 [2].

GMM Barycentre

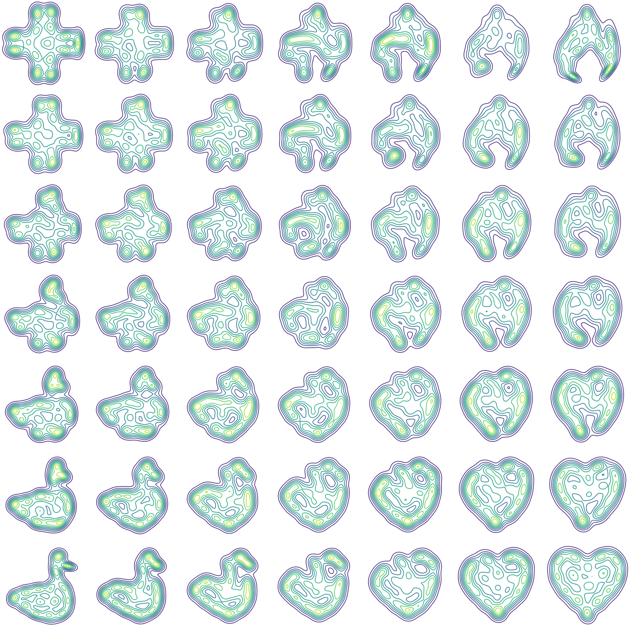
$$\mu = \sum_{i=1}^{n} a_i \delta_{\mathcal{N}(m_i, S_i)},$$

$$\nu_k = \sum_{j=1}^{n_k} b_k \delta_{\mathcal{N}(m_{k,j}, S_{k,j})},$$

$$V(\mu) = \sum_{k=1}^{K} \lambda_k \mathcal{T}_{\mathrm{W}_2^2}(\mu, \nu_k).$$



GMM Barycentre Example



- 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!

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