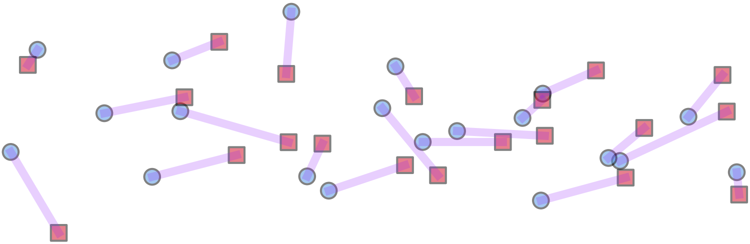
Theory and Computation of Optimal Transport Variants

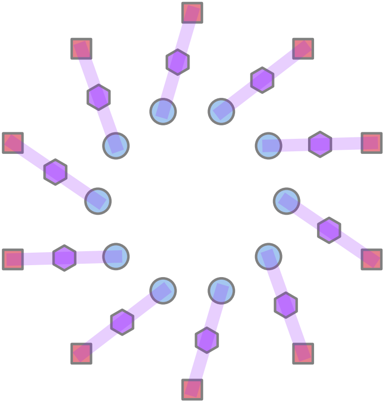
PhD Defence - supervision: Julie Delon and Agnès Desolneux

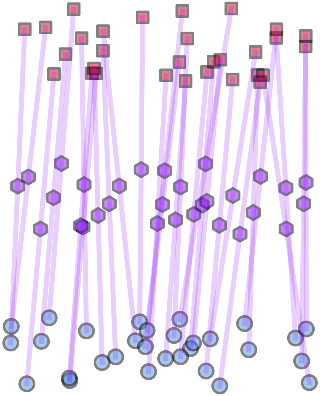


LABORATOIRE MAP5

Université Paris Cité

Discrete Monge Problem [Mon81]

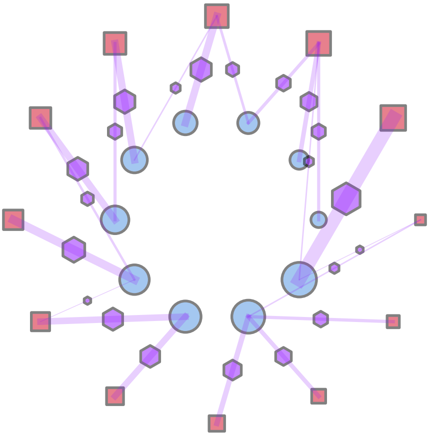


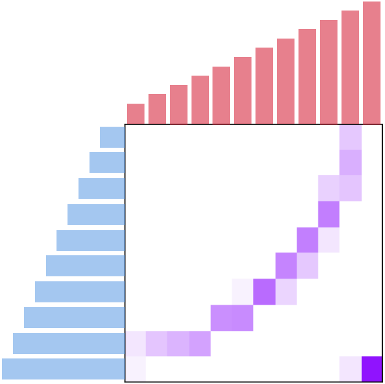


Discrete Monge Problem:

$$\min_{\sigma \in \mathfrak{S}_n} \frac{1}{n} \sum_{i=1}^{n} c(x_i, y_{\sigma(i)}).$$

Discrete Kantorovich Problem [Kan42]





Discrete Kantorovich Problem:

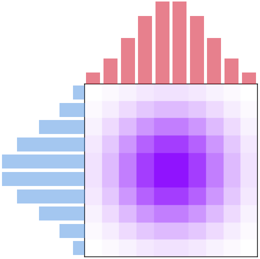
$$\min_{\substack{P \in \mathbb{R}_+^{n \times m} \\ P\mathbf{1}=a \\ P^\top \mathbf{1}=b}} \sum_{i=1}^{n} \sum_{j=1}^{m} c(x_i, y_j) P_{i,j}.$$

Comparing Measures with Optimal Transport

Discrete OT Cost

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

$$\mathcal{T}_c(\mu,\nu) := \min_{\substack{P\in\mathbb{R}_+^{n\times m}\\ P\mathbf{1}=a\\ P^\top\mathbf{1}=b}} \sum_{i=1}^n\sum_{j=1}^m c(x_i,y_j)P_{i,j}.$$



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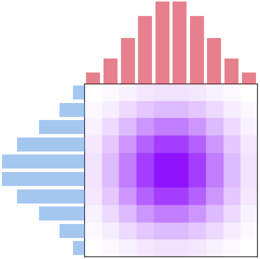
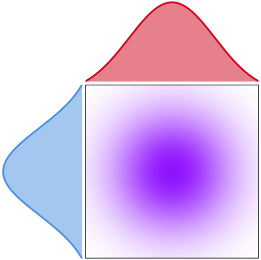


OT Cost $\mu \in \mathcal{P}(\mathcal{X}),\ \nu \in \mathcal{P}(\mathcal{Y})$

$$\mathcal{T}_c(\mu, \nu) := \inf_{\substack{\pi \in \mathcal{P}(\mathcal{X}\times\mathcal{Y}) \\ \pi_{\mathcal{X}} = \mu \\ \pi_{\mathcal{Y}} = \nu}} \int_{\mathcal{X}\times\mathcal{Y}} c(x, y) \mathrm{d}\pi(x, y).$$



Comparing Measures with Optimal Transport

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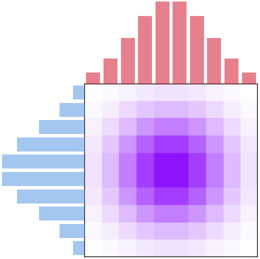

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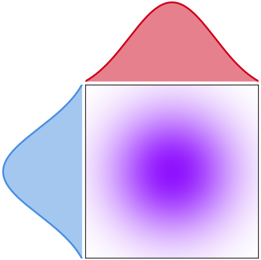


p-Wasserstein Distance: $\mathcal{X} = \mathcal{Y}$ and $c(x, y) = d_\mathcal{X}(x, y)^p$.

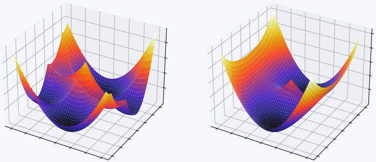
Random Variable Formulation: $\mathcal{T}_c(\mu, \nu) = \inf_{(X,Y):\ X \sim \mu, Y \sim \nu} \mathbb{E}\left[c(X, Y)\right].$

Part A: Optimal Transport Discrepancies as Losses

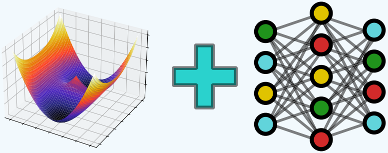
Chapter A.I: Reconstructing Discrete Measures from Projections [TFD24b].

$$\left\{\gamma \in \mathcal{P}(\mathbb{R}^d) : \forall i \in [\![p]\!],\ P_i\#\gamma = P_i\#\gamma_Z\right\}.$$

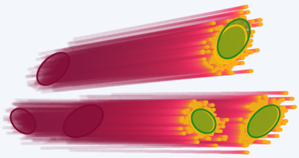
Chapter A.II: Properties of Discrete Sliced Wasserstein Losses [TFD24a].



Chapter A.III: Convergence of SGD for Training Neural Networks with Sliced Wasserstein Losses [Tan23].



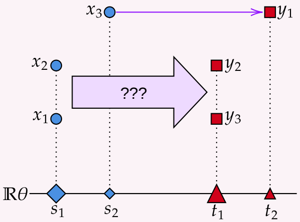
Chapter A.IV: Differentiable Expectation-Maximisation and Applications to Gaussian Mixture Model Optimal Transport [Boï+25].



Part B: Variants of Optimal Transport Maps and Plans

Chapter B.I: Constrained Approximate Optimal Transport Maps [TDD25] $\underset{g \in G}{\operatorname{argmin}} \mathcal{T}_c(g\#\mu, \nu)$.

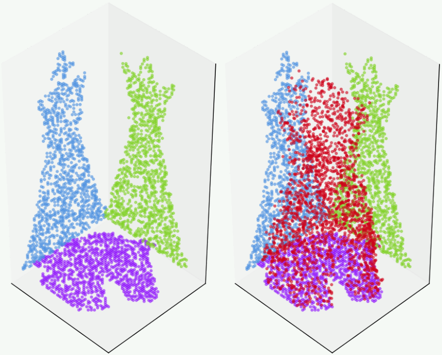
Chapter B.II: Sliced OT Plans [TCD25].



Chapter B.III: Sliced Gromov Wasserstein.

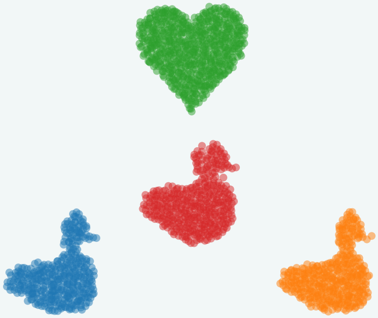
Part C: Optimal Transport Barycentres

Chapter C.I: (Blind) Generalised Wasserstein Barycentres.



Extends [DGS21].

Chapter C.II: Computing OT Barycentres [TDG24; TDG25].



Extends [CD14; Álv+16].

Part D: Some Contributions to Kernel Methods

Chapter D.I: A Gentle Introduction to RKHS.

Chapter D.II: On Gradients of Convex Functions in RKHS.

Chapter D.III: Explicit Universal and Approximate Universal Kernels on Compact Metric Spaces [Tan25].

List of Papers

Published works

[Tan23] **ET**. "Convergence of SGD for Training Neural Networks with Sliced Wasserstein Losses". *Transactions on Machine Learning Research* (Oct. 2023).

[TFD24a] **ET**, Rémi Flamary and Julie Delon. "Properties of Discrete Sliced Wasserstein Losses". *Mathematics of Computation* (Jun. 2024).

[TFD24b] **ET**, Rémi Flamary and Julie Delon. "Reconstructing discrete measures from projections. Consequences on the empirical Sliced Wasserstein Distance". *Comptes Rendus. Mathématique* 362 (Jun. 2024), pp. 1121-1129.

[TDD25] **ET**, Agnès Desolneux, and Julie Delon. "Constrained Approximate Optimal Transport Maps". *ESAIM: Control, Optimisation and Calculus of Variations*. (Aug. 2025)

Pre-prints

[TDG24] **ET**, Julie Delon and Nathaël Gozlan. "Computing Barycentres of Measures for Generic Transport Costs". *arxiv preprint* 2501.04016 (Dec. 2024).

[Tan25] **ET**. "Explicit Universal and Approximate-Universal Kernels on Compact Metric Spaces". *arxiv preprint* 2506.03661 (Jun. 2025).

[TCD25] **ET**, Laetitia Chapel and Julie Delon. "Sliced Optimal Transport Plans". *arxiv preprint* 2508.01243 (Aug. 2025).

[Boï+25] Samuel Boïté*, **ET***, Julie Delon, Agnès Desolneux and Rémi Flamary. "Differentiable Expectation-Maximisation and Applications to Gaussian Mixture Model Optimal Transport". *arxiv preprint* 2509.02109 (Sept. 2025). (*: equal contribution)

[Sis+25] Keanu Sisouk, **ET**, Julie Delon and Julien Tierny. "Robust Barycenters of Persistence Diagrams". *arxiv preprint* 2509.14904 (Sept. 2025).

Open-Source Code Contributions

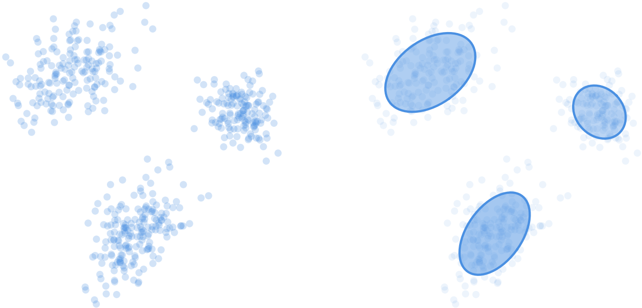
Github repositories:

- (Blind) generalised Wasserstein barycentres [DGS21]: eloitanguy/bgwb.
- OT barycentres [TDG24]: eloitanguy/ot_bar.
- GMM-OT toolbox [DD20; Boï+25] (WIP).

Contributions to the `POT` library [Fla+21]:

- Generalised Wasserstein barycentres [DGS21]: PR 372.
- Nearest Brenier potentials [PdC20; TDD25]: PR 526.
- GMM OT [DD20; Boï+25]: PR 649.
- Fixed-point solvers for OT barycentres [TDG24]: PR 715.
- Sliced OT plans [TCD25]: PR 767.

Differentiable EM and Applications to GMM OT [Boï+25]

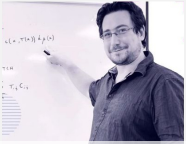


$$\text{Data } X \in (\mathbb{R}^d)^n \xmapsto{\ \nabla\ ?\ } \mathrm{EM}(X) : \text{GMM}$$

Samuel Boïté

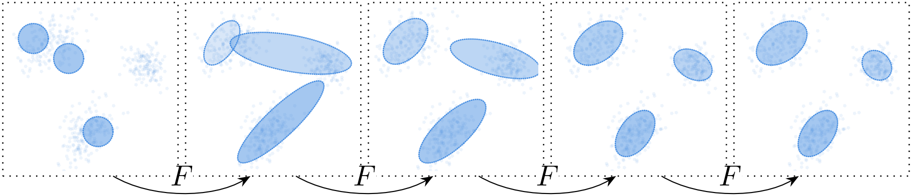
Julie Delon

Agnès Desolneux



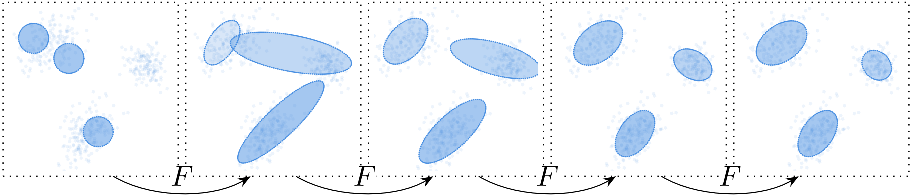
Rémi Flamary

Expectation-Maximisation as a Fixed-Point Algorithm



$$\boxed{\theta_t = F(\theta_{t-1}, X) = F_X^t(\theta_0).}$$

Expectation-Maximisation as a Fixed-Point Algorithm

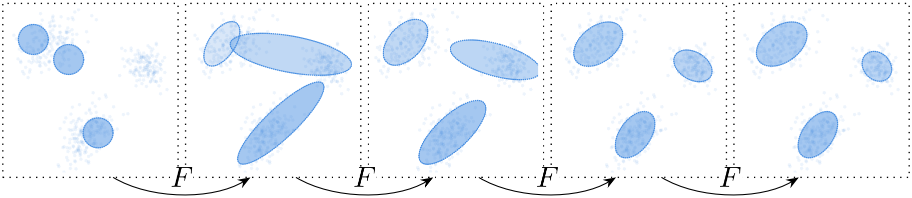


$$\boxed{\theta_t = F(\theta_{t-1}, X) = F_X^t(\theta_0).}$$

Differentiation methods:

- Automatic: $\dfrac{\partial \theta_T}{\partial X} = \dfrac{\partial}{\partial X}\left[F_X^T(\theta_0)\right].$

Expectation-Maximisation as a Fixed-Point Algorithm



$$\boxed{\theta_t = F(\theta_{t-1}, X) = F_X^t(\theta_0).}$$

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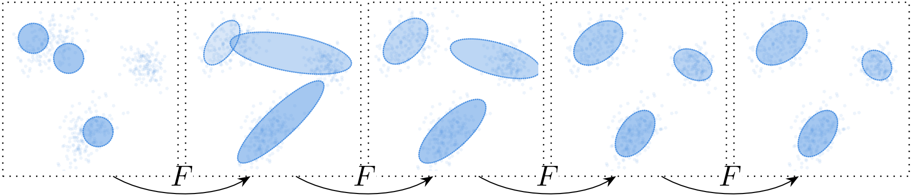
$$F(\theta_\infty, X) = \theta_\infty.$$

Expectation-Maximisation as a Fixed-Point Algorithm



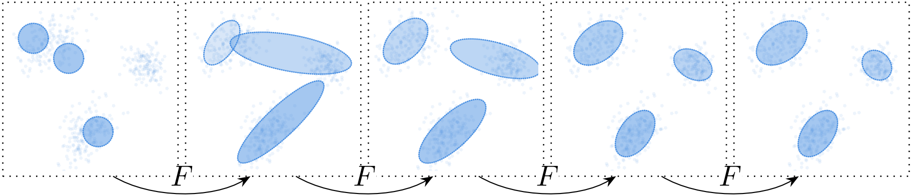
$$\boxed{\theta_t = F(\theta_{t-1}, X) = F_X^t(\theta_0).}$$

Differentiation methods:

- Automatic: $\dfrac{\partial \theta_T}{\partial X} = \dfrac{\partial}{\partial X}\left[F_X^T(\theta_0)\right].$

$$\frac{\partial}{\partial X}\Big[F(\theta_\infty, X)\Big] = \frac{\partial \theta_\infty}{\partial X}.$$

Expectation-Maximisation as a Fixed-Point Algorithm



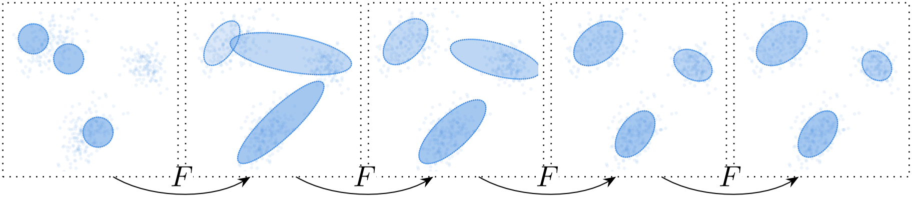
$$\theta_t = F(\theta_{t-1}, X) = F_X^t(\theta_0).$$

Differentiation methods:

- Automatic: $\dfrac{\partial \theta_T}{\partial X} = \dfrac{\partial}{\partial X}\left[F_X^T(\theta_0)\right].$

$$\frac{\partial F}{\partial \theta}(\theta_\infty, X)\frac{\partial \theta_\infty}{\partial X} + \frac{\partial F}{\partial X}(\theta_\infty, X) = \frac{\partial \theta_\infty}{\partial X}.$$

Expectation-Maximisation as a Fixed-Point Algorithm



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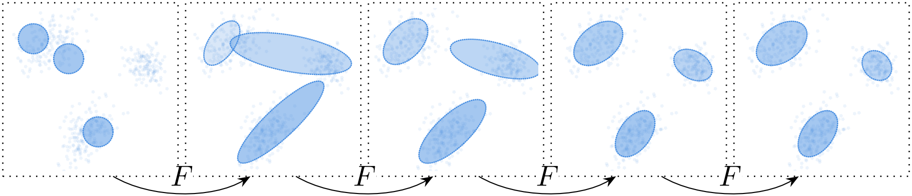
Differentiation methods:

- Automatic: $\dfrac{\partial \theta_T}{\partial X} = \dfrac{\partial}{\partial X}\left[F_X^T(\theta_0)\right].$

$$\frac{\partial \theta_\infty}{\partial X} = \left(I - \frac{\partial F}{\partial \theta}(\theta_\infty, X)\right)^{-1} \frac{\partial F}{\partial X}(\theta_\infty, X).$$

Expectation-Maximisation as a Fixed-Point Algorithm

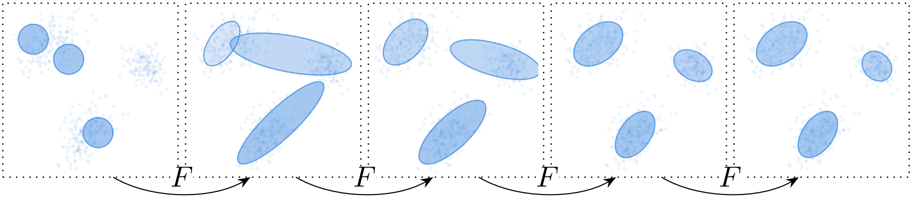


$$\theta_t = F(\theta_{t-1}, X) = F_X^t(\theta_0).$$

Differentiation methods:

- Automatic: $\dfrac{\partial \theta_T}{\partial X} = \dfrac{\partial}{\partial X}\left[F_X^T(\theta_0)\right].$
- Implicit: $\dfrac{\partial \theta_T}{\partial X} \approx \left(I - \dfrac{\partial F}{\partial \theta}(\theta_T, X)\right)^{-1} \dfrac{\partial F}{\partial X}(\theta_T, X).$

Expectation-Maximisation as a Fixed-Point Algorithm

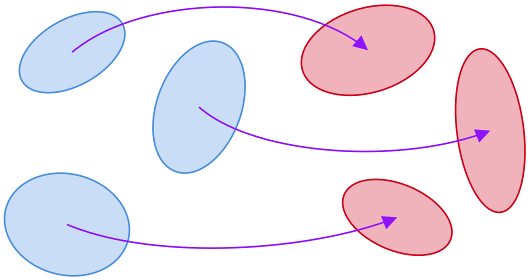


$$\theta_t = F(\theta_{t-1}, X) = F_X^t(\theta_0).$$

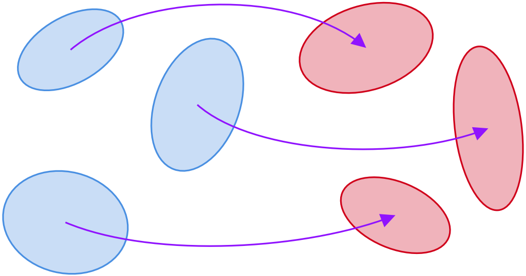
Differentiation methods:

- Automatic: $\dfrac{\partial \theta_T}{\partial X} = \dfrac{\partial}{\partial X}\left[F_X^T(\theta_0)\right].$
- Implicit: $\dfrac{\partial \theta_T}{\partial X} \approx \left(I - \dfrac{\partial F}{\partial \theta}(\theta_T, X)\right)^{-1} \dfrac{\partial F}{\partial X}(\theta_T, X).$
- One-Step: $\dfrac{\partial \theta_T}{\partial X} \approx \dfrac{\partial F}{\partial X}(\theta_T, X).$

Crash Course on GMMOT [DD20]



Crash Course on GMMOT [DD20]

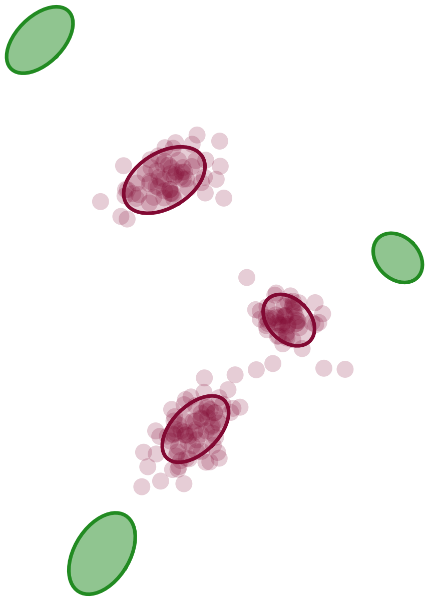


Mixture-Wasserstein Distance [DD20]

$$\mathrm{MW}_2^2(\mu_0,\mu_1) = \min_{P\in\Pi(w_0,w_1)} \sum_{k,\ell} P_{k\ell}\mathrm{W}_2^2(\mu_{0,k},\mu_{1,\ell})$$
$$= \min_{\pi\in\Pi(\mu_0,\mu_1)\cap\mathrm{GMM}} \int_{\mathbb{R}^{2d}} \|x_1 - x_2\|_2^2 \mathrm{d}\pi(x_1,x_2).$$

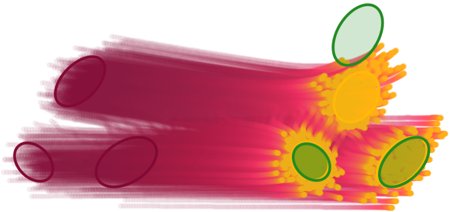
EM-MW2 as a Loss

Gradient Descent on $X \longmapsto \mathrm{MW}_2^2(\mu(F_X^T(\theta_0)), \nu)$.

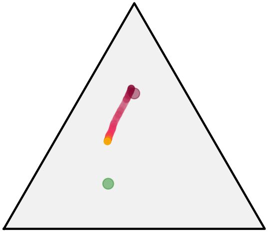


Fixing GMM Weights

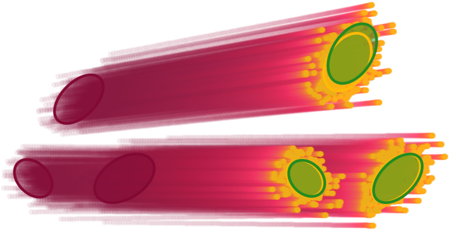
Gradient Descent on $X \longmapsto \mathrm{MW}_2^2(\mu(F_X^T(\theta_0)), \nu)$.



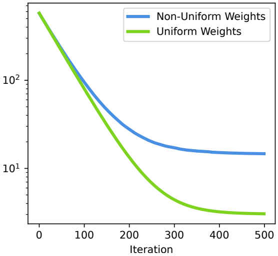
Particle flow (non-uniform).



Weight evolution (non-uniform).

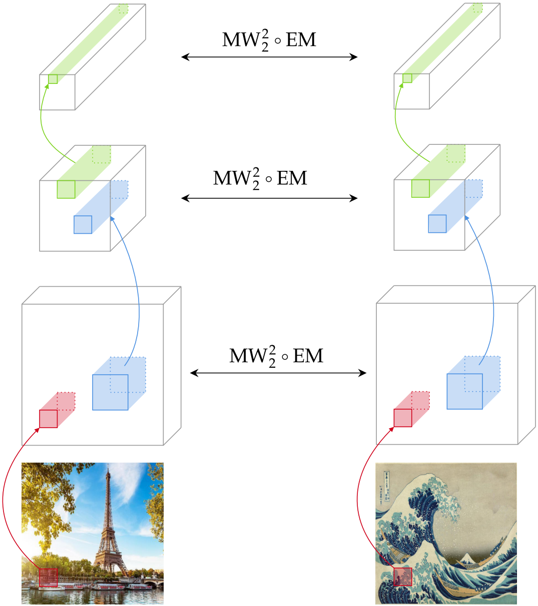


Particle flow (uniform).



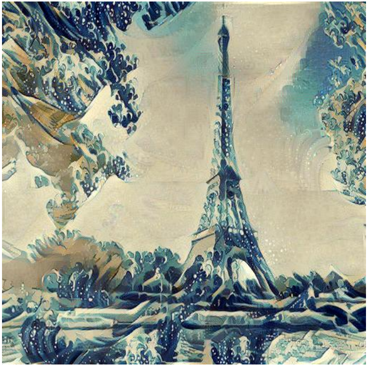
Energy evolutions.

Application: Style Transfer



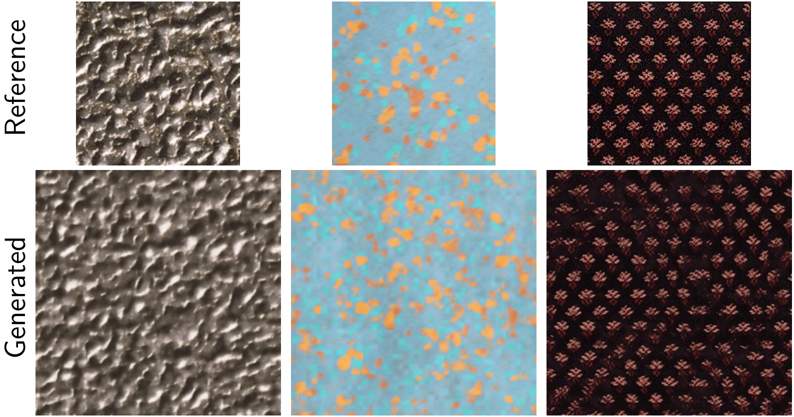
Optimised Image

Style Target

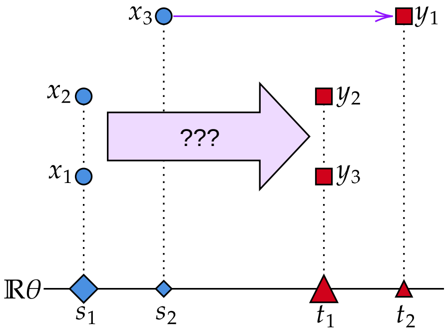


Application: Texture Synthesis

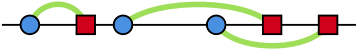
$$\min_X \sum_{\ell=1}^{L} \lambda_\ell \mathrm{MW}_2^2\Big(F^T \circ \mathrm{Patches}_{p\times p} \circ \mathrm{Downscale}_{s_\ell}(X), F^T \circ \mathrm{Patches}_{p\times p} \circ \mathrm{Downscale}_{s_\ell}(Y)\Big).$$



Sliced OT Plans [TCD25]

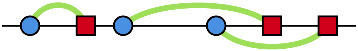


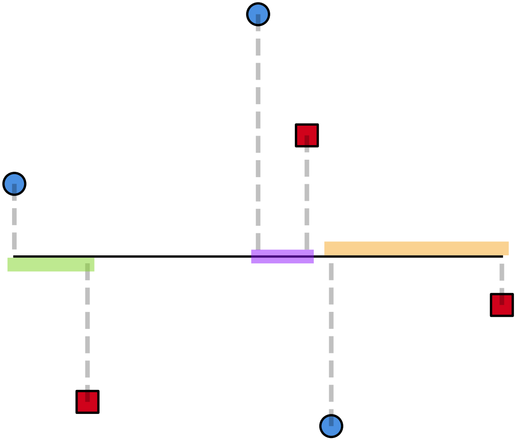
Sliced Wasserstein Distance [Rab+12]



Sliced Wasserstein Distance [Rab+12]

$$\mathrm{SW}_2^2(\mu_1, \mu_2) := \int_{\mathbb{S}^{d-1}} \mathrm{W}_2^2(P_\theta \# \mu_1, P_\theta \# \mu_2) \mathrm{d}\sigma(\theta).$$





Sliced Wasserstein Distance [Rab+12]

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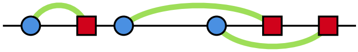
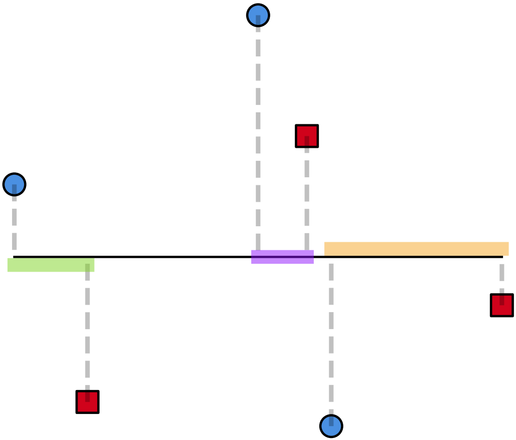
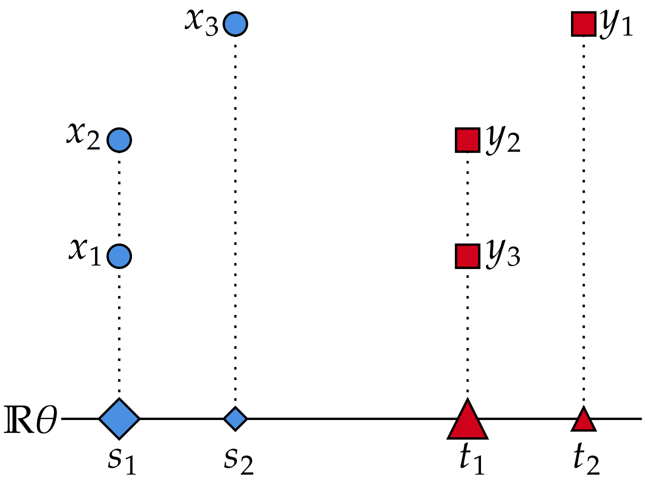




Sliced plan propositions:

- SWGG [Mah+23]
  ↳ Pivot-Sliced
- Expected SW [Liu+24]
  ↳ more theory

Pivot-Sliced: Definition and Reformulation



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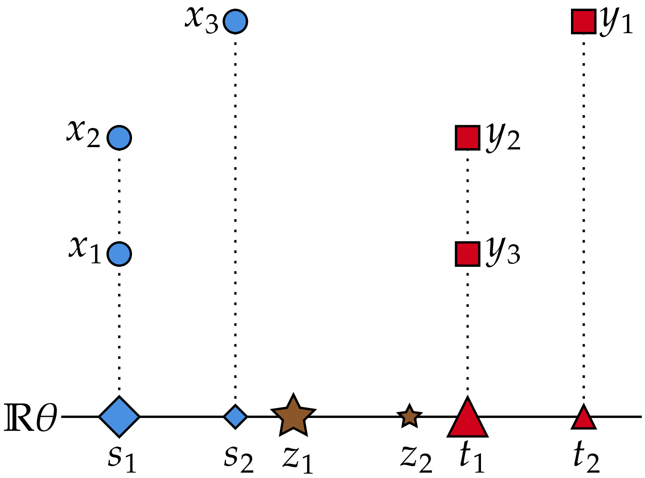

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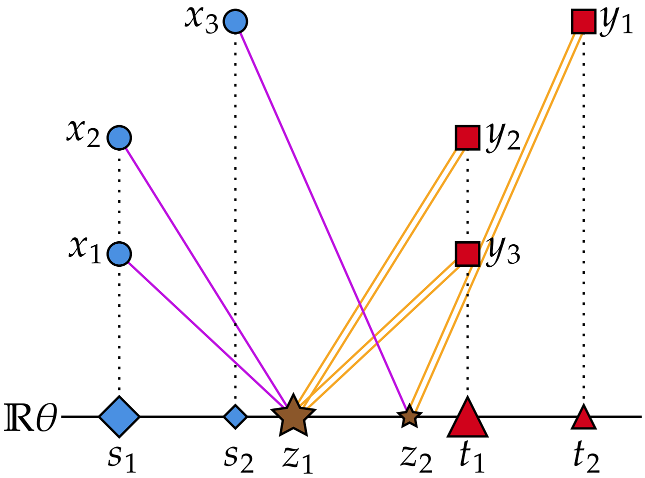

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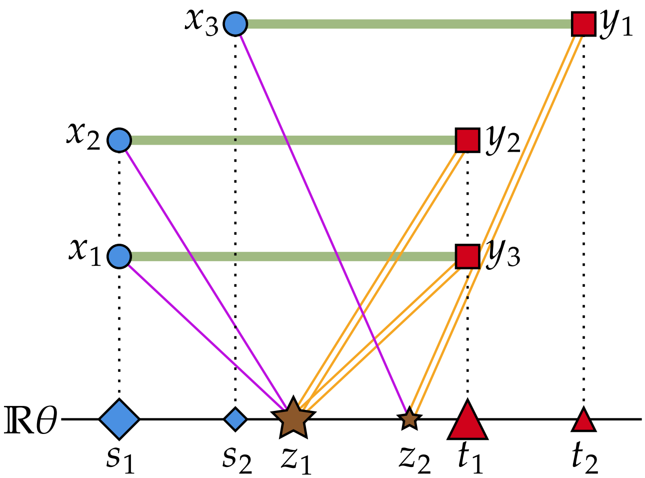

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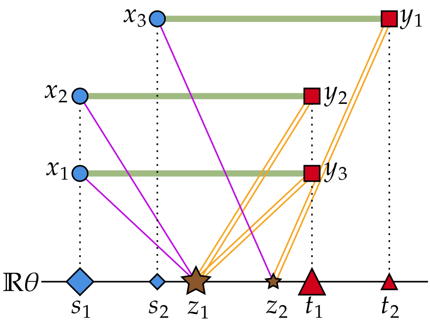

$$\Gamma(\nu, \mu_1, \mu_2) := \left\{\rho \in \mathcal{P}_2(\mathbb{R}^{3d}) : \rho_{0,1} \in \Pi^*(\nu, \mu_1) \text{ and } \rho_{0,2} \in \Pi^*(\nu, \mu_2)\right\}.$$

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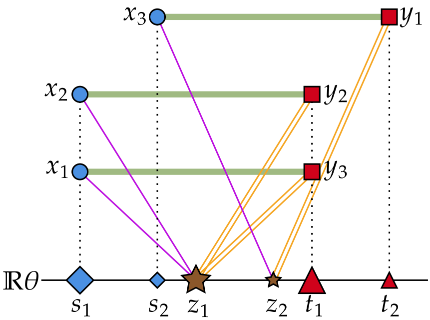

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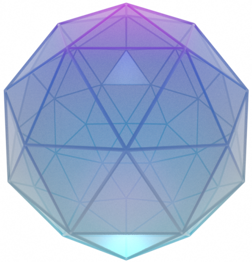
Equivalent Formulation

$$\mathrm{PS}_\theta^2(\mu_1, \mu_2) = \min_{\substack{\omega \in \Pi(\mu_1, \mu_2) \\ (P_\theta, P_\theta)\#\omega \in \Pi^*(P_\theta\#\mu_1, P_\theta\#\mu_2)}} \int_{\mathbb{R}^{2d}} \|x_1 - x_2\|_2^2 \mathrm{d}\omega(x_1, x_2).$$

Pivot-Sliced: Point Cloud Monge Formulation



Extreme Optimality [Thm 2.7 in BT97]

Let $\mathcal{P}$ be a convex and compact polytope.

$$\min_{x \in \mathcal{P}} c \cdot x = \min_{x \in \operatorname{Extr} \mathcal{P}} c \cdot x.$$

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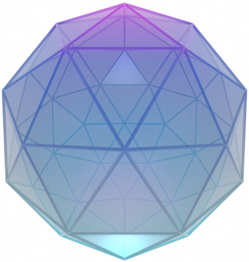

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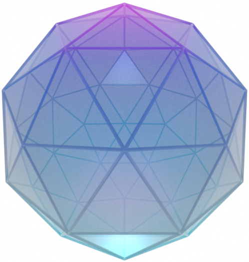

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LP formulation

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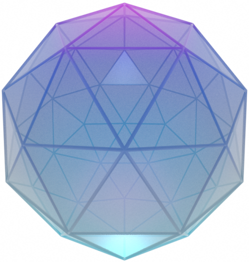

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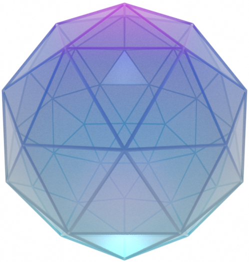

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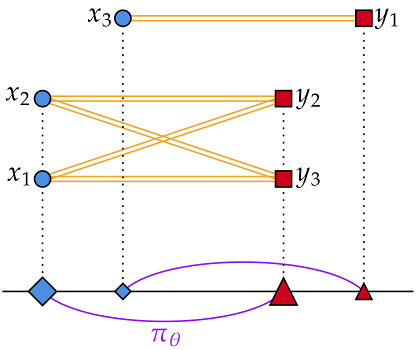
$\operatorname{Extr} \mathcal{P} = \cdots$

$$= \min_{(\sigma,\tau) \in \mathfrak{S}_\theta(X,Y)} \frac{1}{n} \sum_{i=1}^n \|x_{\sigma(i)} - y_{\tau(i)}\|_2^2.$$

Expected Sliced: Definition



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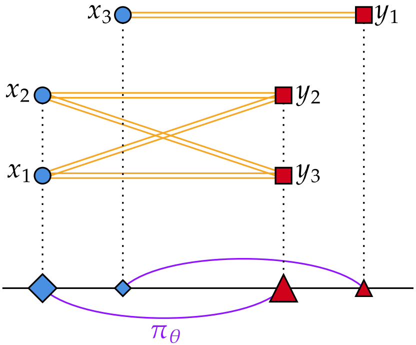

Definition of $\gamma_\theta[\mu_1, \mu_2]$

$$\int_{\mathbb{R}^{2d}} \phi(x_1, x_2) \mathrm{d}\gamma_\theta(x_1, x_2) = \int_{\mathbb{R}^2} \left(\int_{P_\theta^{-1}(s) \times P_\theta^{-1}(t)} \phi(x_1, x_2) \mathrm{d}\mu_1^s(x_1) \mathrm{d}\mu_2^t(x_2) \right) \mathrm{d}\pi_\theta(s, t).$$

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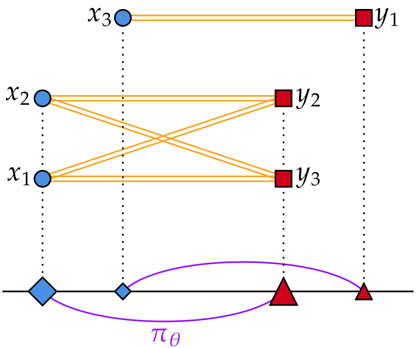

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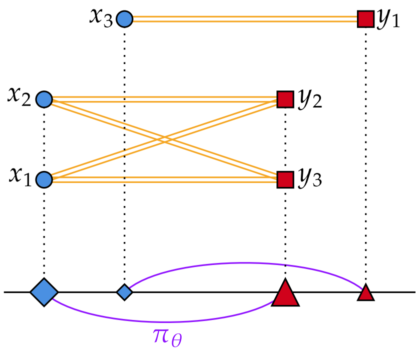

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$$\overline{\gamma}[\mu_1, \mu_2, \sigma] := \int_{\mathbb{S}^{d-1}} \gamma_\theta[\mu_1, \mu_2] \mathrm{d}\sigma(\theta); \quad \mathrm{ES}_\sigma^2(\mu_1, \mu_2) := \int_{\mathbb{R}^{2d}} \| \cdot - \cdot \|_2^2 \mathrm{d}\overline{\gamma}[\mu_1, \mu_2, \sigma].$$

Are (min)-Pivot-Sliced and Expected Sliced Distances?

$$\min \mathrm{PS}^2(\mu_1, \mu_2) := \min_{\theta \in \mathbb{S}^{d-1}} \mathrm{PS}_\theta^2(\mu_1, \mu_2);$$

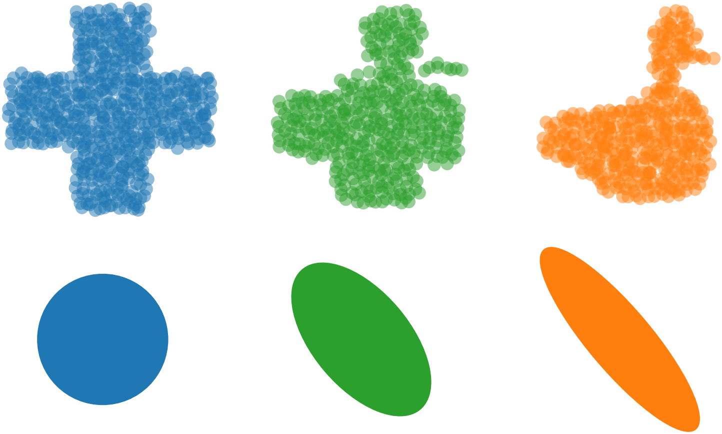
$$\mathrm{ES}_\varpi^2(\mu_1, \mu_2) := \int_{\mathbb{R}^{2d}} \| \cdot - \cdot \|_2^2 \mathrm{d}\overline{\gamma}[\mu_1, \mu_2, \varpi].$$

	PS_θ	$\min \mathrm{PS}$	LS_θ	ES_ϖ
$D(\mu_1, \mu_2) = 0 \implies \mu_1 = \mu_2$	✔	✔	✔	✔
$D(\mu, \mu) = 0$	✔	✔	✘ discrete only	✘
Triangle Inequality	✘ AC only	✘	✔	✔

Optimal Transport Barycentres [TDG24]

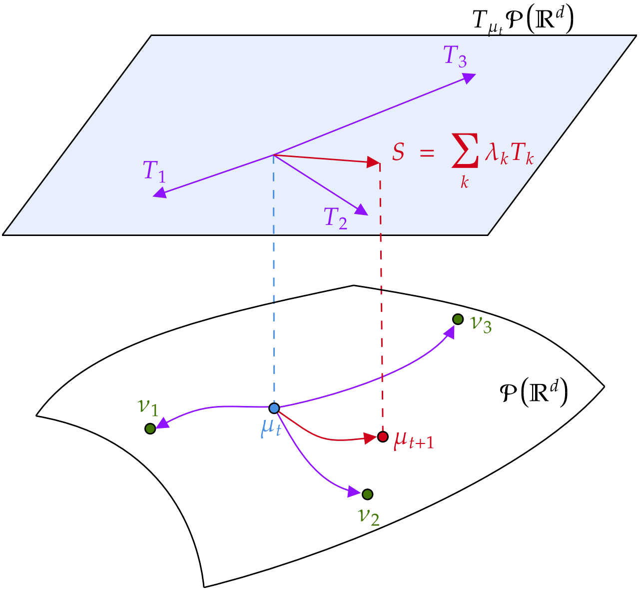
2-Wasserstein Barycentres [AC11]

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



Fixed-Point Method [Álv+16]

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



Generalising Wasserstein Barycentres

Setting:

- $(\mathcal{X}, d_{\mathcal{X}})$ compact metric space for barycentres μ.
- $(\mathcal{Y}_k, d_{\mathcal{Y}_k})$ 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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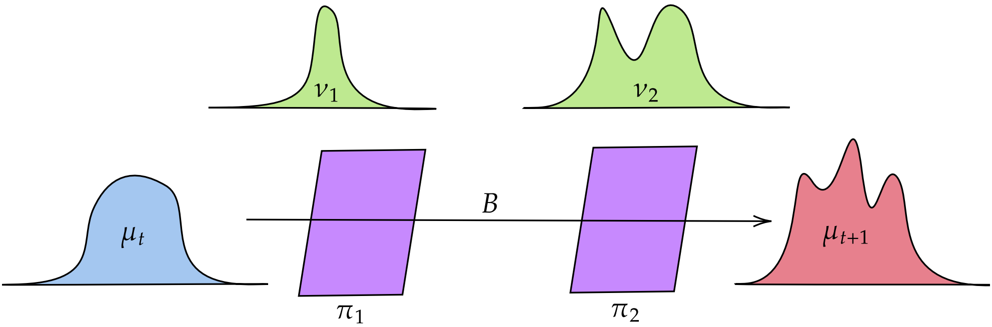
Assumption: The ground barycenter function

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

is well-defined.

Fixed-point Algorithm



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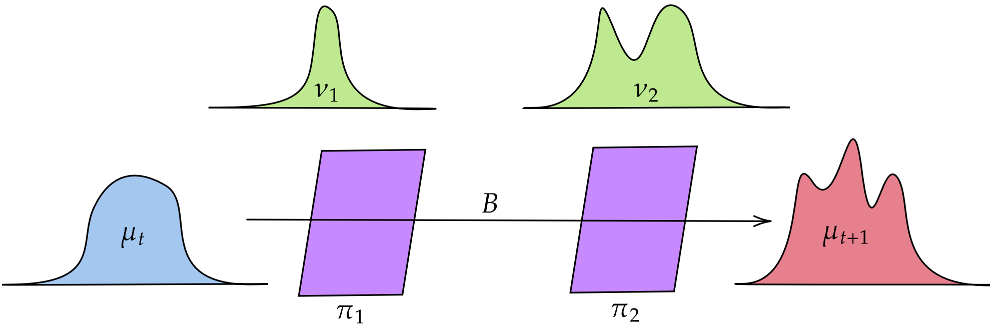

$$\Gamma(\mu) := \left\{(X, Y_1, \cdots, Y_K) \ : \ (X, Y_k) \in \Pi^*_{c_k}(\mu, \nu_k)\right\},$$

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

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

Algorithm Convergence

Ground Barycentre Inequality [Lemma 3.8 in TDG24]

$$\sum_k c_k(x, y_k) \geq \sum_k c_k(\overline{x}, y_k) + \delta(x, \overline{x}), \quad \overline{x} := B(y_1, \cdots, y_K).$$

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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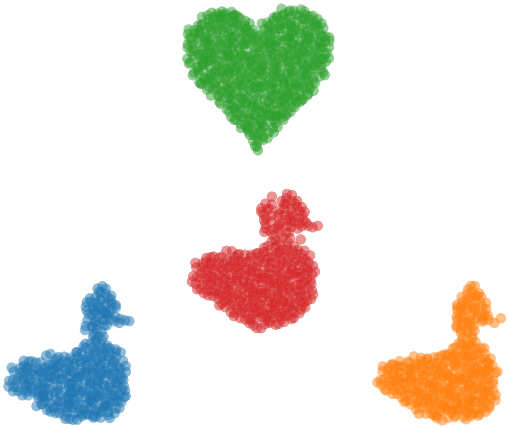
Convergence [Theorem 3.10 in TDG24]

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

Application: Barycentres for p-norms with power q

Cost: $c(x, y) = \|x - y\|_p^q$.



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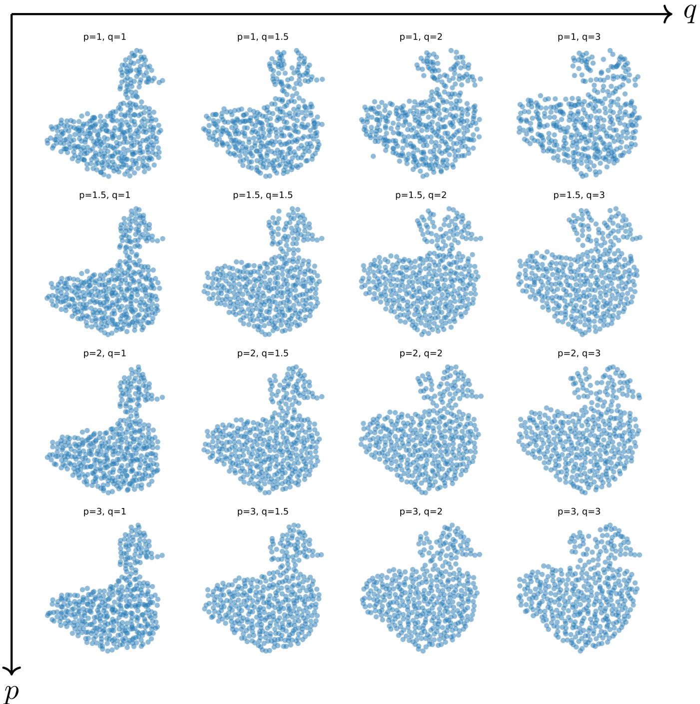


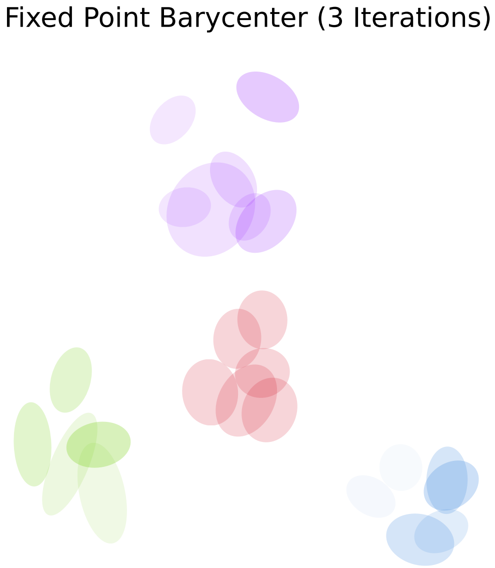
Application: GMM Barycentres

`ot.gmm.gmm_barycenter_fixed_point`

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

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

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



https://pythonot.github.io/auto_examples/barycenters/plot_gmm_barycenter.html

Conclusion and Outlook

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  ↳ Infinite mixtures?
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Thanks!

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EM Formulas

$$F(\theta, X) = (w', m', \Sigma') :$$

$$\gamma_{ik}(\theta) = \frac{w_k g_{m_k,\Sigma_k}(x_i)}{\sum_{\ell=1}^{K} w_\ell g_{m_\ell,\Sigma_\ell}(x_i)},$$

$$w'_k = \frac{1}{n}\sum_{i=1}^{n} \gamma_{ik}(\theta) ,$$

$$m'_k = \frac{\sum_{i=1}^{n} \gamma_{ik}(\theta) x_i}{\sum_{j=1}^{n} \gamma_{jk}(\theta)} ,$$

$$\Sigma'_k = \frac{\sum_{i=1}^{n} \gamma_{ik}(\theta)(x_i - m'_k)(x_i - m'_k)^\top}{\sum_{j=1}^{n} \gamma_{jk}(\theta)} .$$

Application: Colour Transfer

Gradient Descent on $X \in (\mathbb{R}^3)^{h \times w} \longmapsto \mathrm{MW}_2^2\left(\mu\left(F_X^T(\theta)\right), \mu\left(F_Y^T(\theta_0)\right)\right)$.

Source

Result

Target

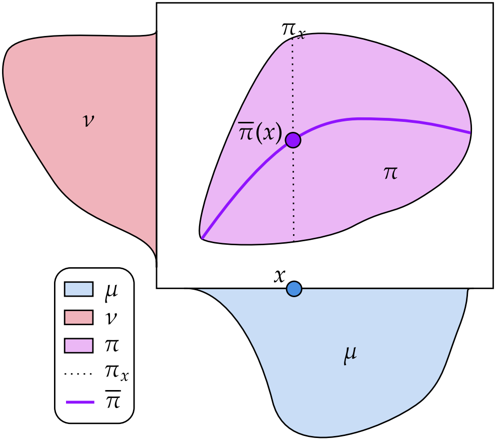
Balanced result

Unbalanced result

Corrupted target

Barycentric Projections

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



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

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

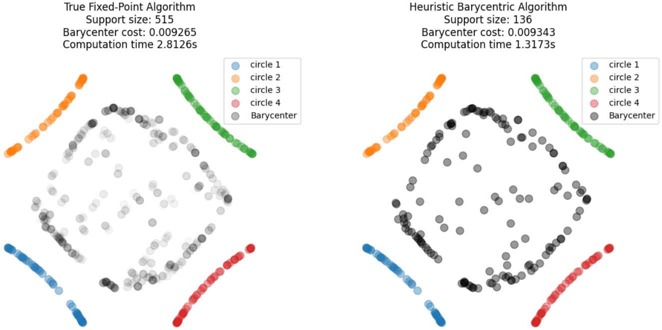
$$\overline{\pi} = \underset{f\in L^2(\mu)}{\mathrm{argmin}} \int \|f(x)-y\|_2^2 \mathrm{d}\pi(x,y).$$

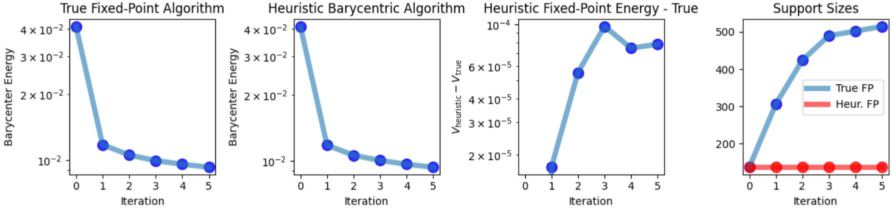
$$H(\mu) = \left\{ B(\overline{\pi_1}, \cdots, \overline{\pi_K})\#\mu,\ \pi_k \in \Pi^*_{c_k}(\mu, \nu_k) \right\}.$$

No guarantees... yet?

Illustration: $c_k(x, y) = \|P_{\text{circle}\#k}(x) - y\|_2^2$

`ot.lp.generalized_free_support_barycenter`





https://pythonot.github.io/auto_examples/barycenters/plot_free_support_barycenter_generic_cost.html