Gromov-Wasserstein Distances: Entropic Regularization, Duality, and Sample Complexity

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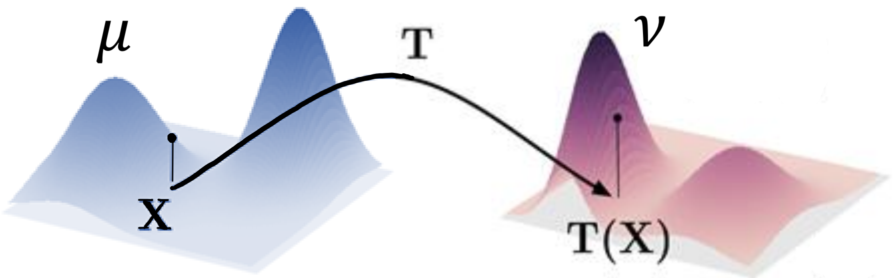
Primer:
Optimal Transport Theory

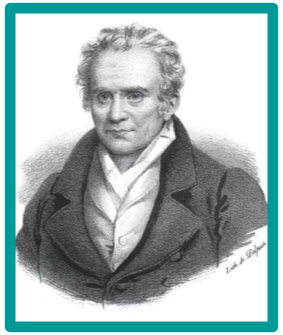
Why Optimal Transport?

Broad interest: Pure math, applied math, economics, comp. biology, machine learning…

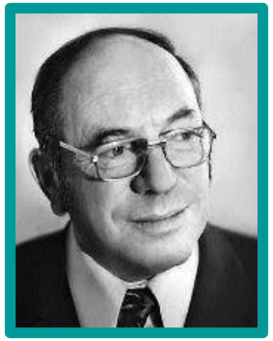


Rich history:

Monge

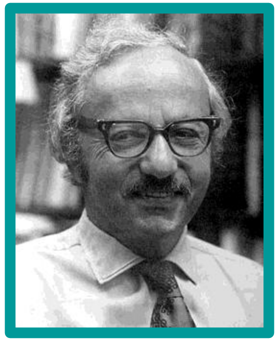


Kantorovich

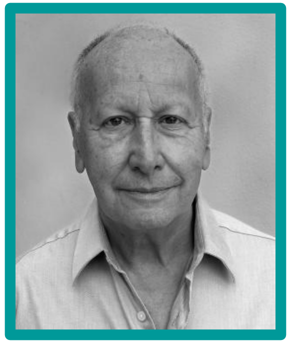


Koopmans

Dantzig



Caffarelli



Otto

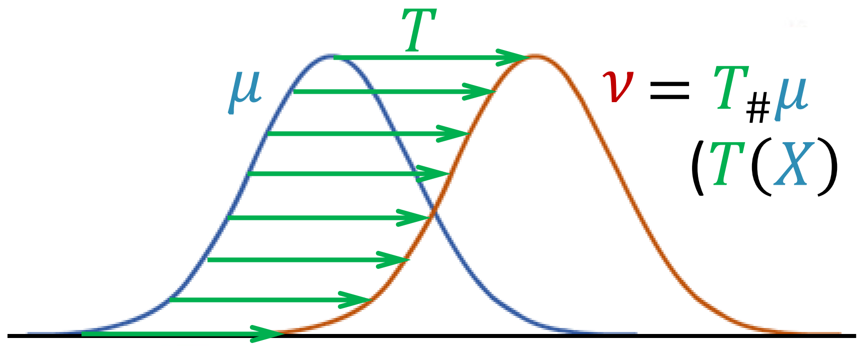
Villani

Figalli

Nobel ‘75 | NMoS ‘75 | Abel ‘23 | Liebniz ‘06 | Fields ‘10 | Fields ‘18

Has a bit of everything: Theory, statistics, algorithms, applications

Optimal Transport

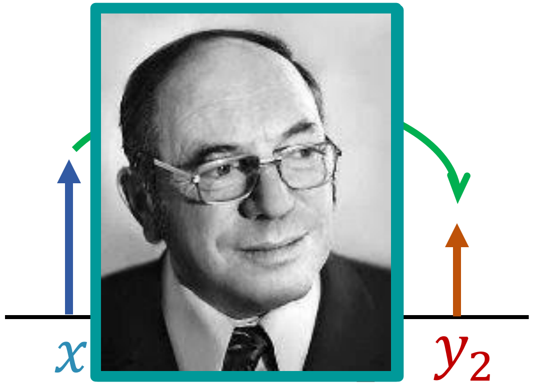


Distributions: $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$

Cost: $c\colon \mathbb{R}^d \times \mathbb{R}^d \to [0, \infty)$

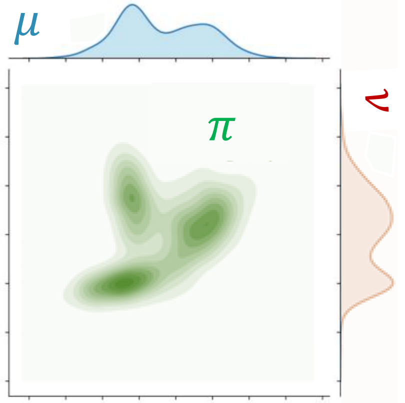
Transport map: $T\colon \mathbb{R}^d \to \mathbb{R}^d$ s.t. $T_{\#}\mu = \nu$

OT problem (Monge 1781): $\mathrm{M}_c(\mu, \nu) := \inf_{T:\, T_{\#}\mu = \nu} \int_{\mathbb{R}^d} c(x, T(x))\, d\mu(x)$



🚫 $\{T : T_{\#}\mu = \nu\}$ may be empty, not closed, non-linear problem, …

Coupling: $\Pi(\mu, \nu) = \{\pi \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d) \colon \pi(\cdot \times \mathbb{R}^d) = \mu,\ \pi(\mathbb{R}^d \times \cdot) = \nu\}$



Optimal Transport (Kantorovich '42)

$$\mathrm{OT}_c(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \int_{\mathbb{R}^d \times \mathbb{R}^d} c(x, y)\, d\pi(x, y)$$

The Wasserstein Distance

Construction: Kantorovich OT with distance cost (or power thereof) $c(x,y) = \|x-y\|^p$

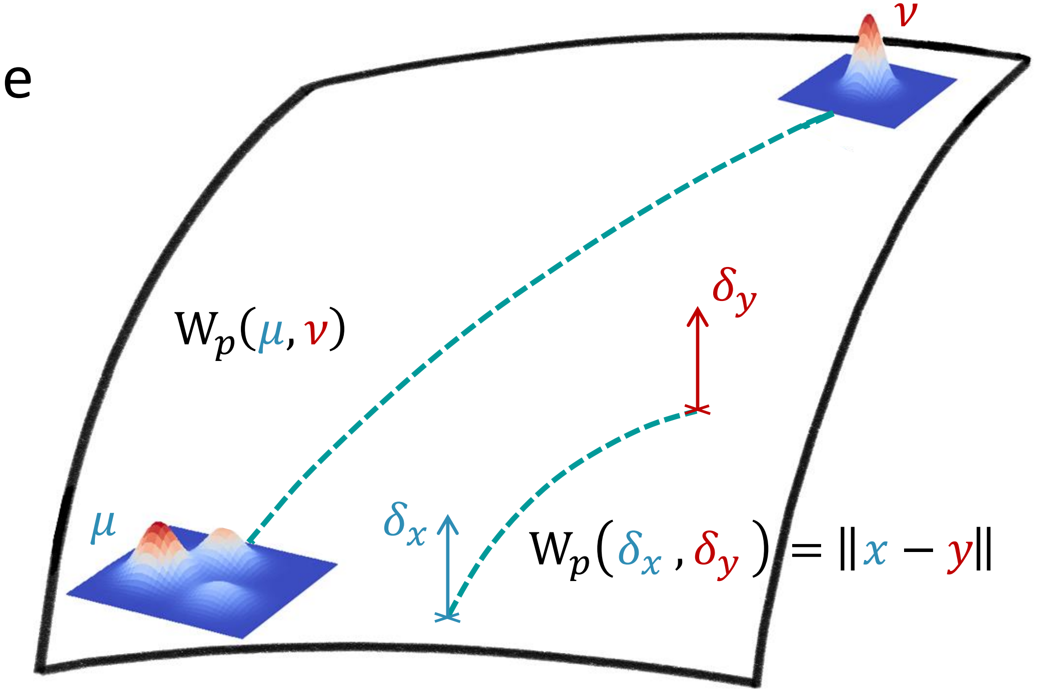
p-Wasserstein Distance

For $p \in [1,\infty)$ and $\mu,\nu \in \mathcal{P}_p(\mathbb{R}^d)$: $\mathrm{W}_p(\mu,\nu) := \inf_{\pi\in\Pi(\mu,\nu)} \left(\int_{\mathbb{R}^d\times\mathbb{R}^d} \|x-y\|^p d\pi(x,y)\right)^{1/p}$

Wasserstein space: $\mathfrak{W}_p = \left(\mathcal{P}_p(\mathbb{R}^d), \mathrm{W}_p\right)$ metric space

Wasserstein geometry:

- Euclidean geometry
- Geodesic curves (shortest paths)
- Barycenters (averages)
- Gradient flows



The Wasserstein Metric: Difficulties

$$\mathrm{W}_p(\mu,\nu) := \inf_{\pi\in\Pi(\mu,\nu)} \left(\int_{\mathbb{R}^d\times\mathbb{R}^d} \|x-y\|^p d\pi(x,y)\right)^{1/p}$$

Statistical: Data $\Longrightarrow$ $\hat{\mu}_n := \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$ & $\hat{\nu}_n := \frac{1}{n}\sum_{i=1}^n \delta_{Y_i}$ $\Longrightarrow$ $\mathrm{W}_p(\mu,\nu) \approx \mathrm{W}_p(\hat{\mu}_n,\hat{\nu}_n)$?

Theorem (Dudley '69, Boissard-Le Gouic '14, Fournier-Guillin '14,…)

For $\mu,\nu \in \mathcal{P}_p(\mathbb{R}^d)$ and $d > 2p$: $\mathbb{E}\left[\left|\mathrm{W}_p(\mu,\nu) - \mathrm{W}_p(\hat{\mu}_n,\hat{\nu}_n)\right|\right] \asymp n^{-\frac{1}{d}}$

🛇 **Too slow** for $d \gg 1$

Computational: Kantorovich OT is LP $\Longrightarrow$

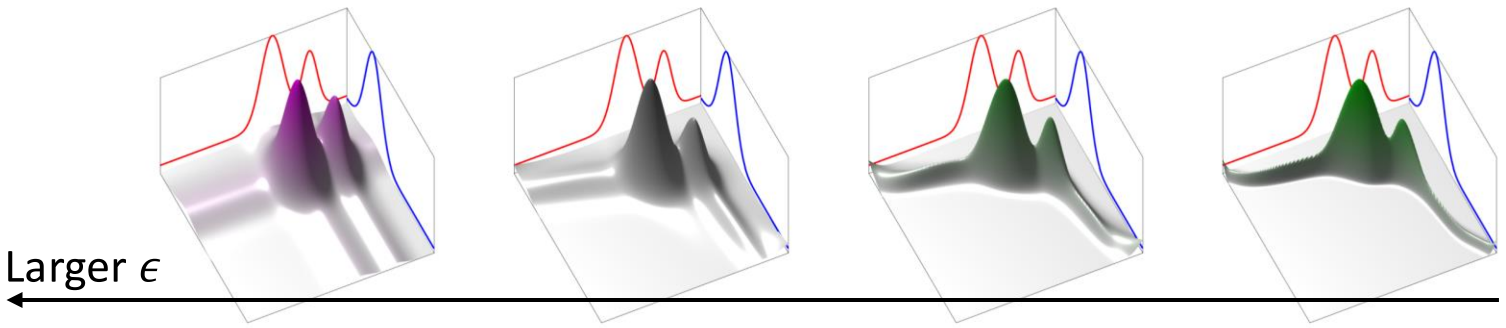
🛇 **Infeasible** for large scale problems

Entropic Optimal Transport

Entropic Optimal Transport

For $\epsilon > 0$: $\mathrm{EOT}_{\epsilon,c}(\mu,\nu) \coloneqq \inf_{\pi\in\Pi(\mu,\nu)} \mathbb{E}_\pi[c(X,Y)] - \epsilon \mathrm{H}(\pi)$

- **Entropic penalty:** Encourage randomness of π



[Peyré-Cuturi ’19]

- **Approximation error:** $\left|\mathrm{EOT}_{\epsilon,c}(\mu,\nu) - \mathrm{OT}_c(\mu,\nu)\right| \lesssim \epsilon \log(1/\epsilon)$

$\Longrightarrow$ **Strongly convex** optimization problem with a **unique** and **smooth solution**

Entropic Optimal Transport: Estimation

Setting: $\hat{\mu}_n = \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$ & $\hat{\nu}_n = \frac{1}{n}\sum_{i=1}^n \delta_{Y_i} \implies \mathrm{EOT}_{\epsilon,c}(\mu,\nu) \approx \mathrm{EOT}_{\epsilon,c}(\hat{\mu}_n,\hat{\nu}_n)$?

Duality: $$\mathrm{EOT}_{\epsilon,c}(\mu,\nu) := \sup_{(\varphi,\psi)\in L^1(\mu)\times L^1(\nu)} \int \varphi d\mu + \int \psi d\nu - \underbrace{\epsilon\left(\int e^{\frac{\varphi(x)+\psi(y)-c(x,y)}{\epsilon}} d\mu\otimes\nu - 1\right)}_{=0 \text{ for optimal } (\varphi,\psi)}$$

Empirical convergence analysis: Standard technique

1. **Regularity of EOT potentials:** $(\varphi,\psi)\in\mathcal{F}_s\times\mathcal{G}_s$ for Hölder classes of arbitrary smoothness
2. **Suprema of emp. process:** Decompose

$$\mathbb{E}\left[\left|\mathrm{EOT}_{\epsilon,c}(\mu,\nu) - \mathrm{EOT}_{\epsilon,c}(\hat{\mu}_n,\hat{\nu}_n)\right|\right] \le \mathbb{E}\left[\sup_{\varphi\in\mathcal{F}_s}\left|\mathbb{E}_\mu[\varphi] - \frac{1}{n}\Sigma_{i=1}^n\varphi(X_i)\right|\right] + \mathbb{E}\left[\sup_{\psi\in\mathcal{G}_s}\left|\mathbb{E}_\mu[\psi] - \frac{1}{n}\Sigma_{i=1}^n\psi(Y_i)\right|\right]$$

$\boxed{\text{Bound Dudley entropy integral of } \mathcal{F}_s \text{ and } \mathcal{G}_s \text{ (Hölder) with } s = \left\lceil \frac{d_x}{2}\right\rceil + 1}$

Entropic Optimal Transport: Computation

Setting: Compute EOT between discrete measures $\mu = \frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}$ & $\nu = \frac{1}{n}\sum_{i=1}^{n} \delta_{y_i}$

$$\boxed{\mathrm{EOT}_{\epsilon,c}(\mu,\nu) = \min_{\pi \in \Pi(\mu,\nu)} \langle \pi, C \rangle - \epsilon \mathrm{H}(\pi)}$$

Coupling matrix $[\pi]_{i,j} = \pi(x_i, y_j)$ Cost matrix $[C]_{i,j} = c(x_i, y_j)$

Proposition

Optimal $\pi_\epsilon^\star \in \Pi(\mu,\nu)$ is unique & $!\exists \boldsymbol{a}, \boldsymbol{b} \in \mathbb{R}^n_{\geq 0}$ s.t $\pi_\epsilon^\star = \mathrm{diag}(\boldsymbol{a}) K \mathrm{diag}(\boldsymbol{b})$, $[K]_{i,j} = e^{-\frac{[C]_{i,j}}{\epsilon}}$

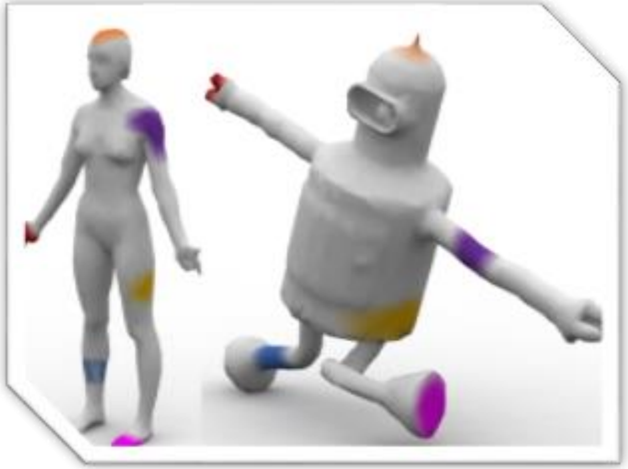
$$\pi_\epsilon^\star \in \Pi(\mu,\nu) \quad \Longleftrightarrow \quad \begin{cases} \boldsymbol{a} = \mu / K\boldsymbol{b} \\ \boldsymbol{b} = \nu / K\boldsymbol{a} \end{cases}$$

$\Longrightarrow$ **Fixed point (Sinkhorn) algorithm:** $O(n^2)$ time & highly parallelizable [Cuturi '13]

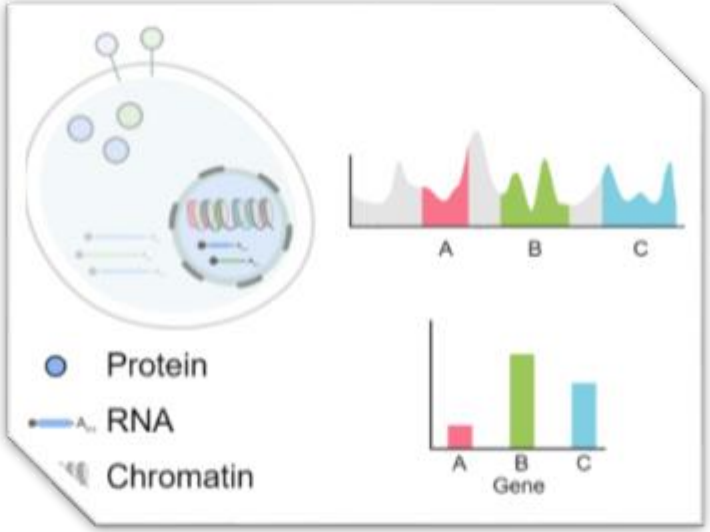
Gromov-Wasserstein Distance

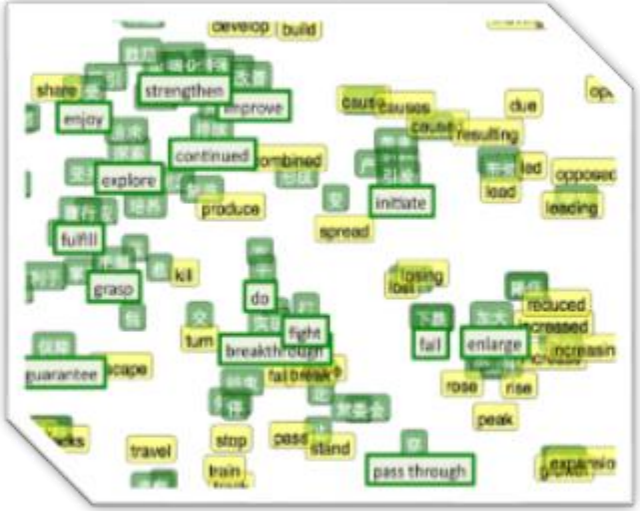
Heterogeneous & Structured Data

Dataset Matching: Various applications require matching heterogeneous **&** structured datasets



[Solomon-Peyré-Kim-Sra ’16]





Goals:
1. Compare how similar/different two datasets are
2. Obtain matching/alignment that respects individual structure

Gromov-Wasserstein Distance

- Datasets as metric measure spaces

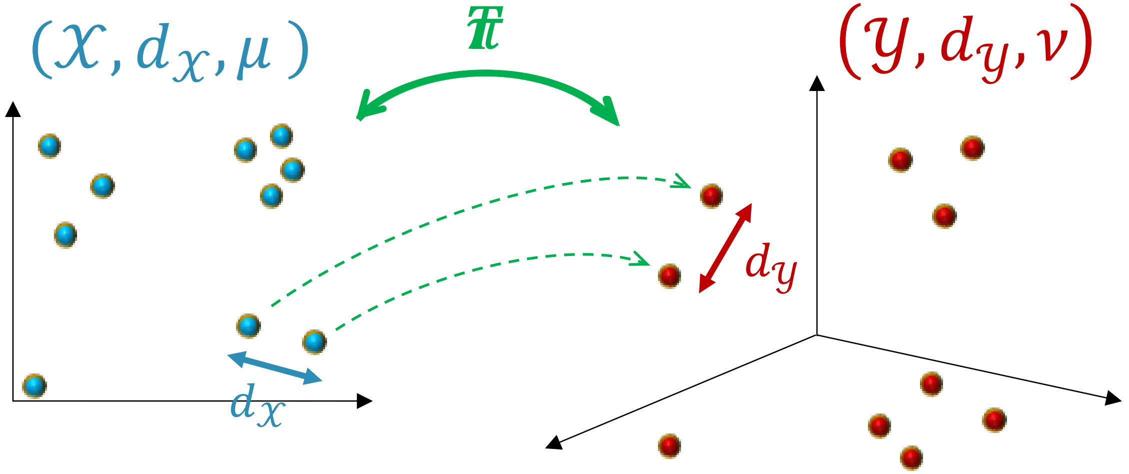
$\Longrightarrow$ $(\mathcal{X}, d_{\mathcal{X}}, \mu)$ & $(\mathcal{Y}, d_{\mathcal{Y}}, \nu)$

- Find matching (transport map) $T: \mathcal{X} \to \mathcal{Y}$

$\Longrightarrow$ $\nu = T_{\#}\mu$ (if $X \sim \mu$ then $T(X) \sim T_{\#}\mu$)

- Preserve distances (minimize distance distortion)

$\Longrightarrow$ cost $= \left| d_{\mathcal{X}}(x_i, x_j)^q - d_{\mathcal{Y}}\left(T(x_i), T(x_j)\right)^q \right|$



Gromov-Wasserstein Distance (Memoli '11)

The (p,q)-GW distance between mm spaces $(\mathcal{X}, d_{\mathcal{X}}, \mu)$ and $(\mathcal{Y}, d_{\mathcal{Y}}, \nu)$ is

$$\mathrm{D}_{p,q}(\mu,\nu) := \inf_{\pi \in \Pi(\mu,\nu)} \left(\mathbb{E}_{\substack{(X,Y)\sim\pi \\ (X',Y')\sim\pi}} \left[\left| d_{\mathcal{X}}(X,X')^q - d_{\mathcal{Y}}(Y,Y')^q \right|^p \right] \right)^{1/p}$$

Gromov-Wasserstein Distance

$$\mathrm{D}_{p,q}(\mu,\nu) \coloneqq \inf_{\pi\in\Pi(\mu,\nu)} \left(\mathbb{E}_{\substack{(X,Y)\sim\pi \\ (X',Y')\sim\pi}} \left[\left| d_{\mathcal{X}}(X,X')^q - d_{\mathcal{Y}}(Y,Y')^q \right|^p \right] \right)^{1/p}$$

Comments: Relaxation of Gromov-Hausdorff distance between metric spaces ($p=\infty, q=1$)

- **Finiteness:** $\mathrm{D}_{p,q}(\mu,\nu) < \infty \; \forall \mu,\nu$ with $\int_{\mathcal{X}\times\mathcal{X}} d_{\mathcal{X}}(x,x')^{pq}\, d\mu\otimes\mu(x,x') < \infty$ & resp. for ν
- **Identification:** $\mathrm{D}_{p,q}(\mu,\nu) = 0 \iff \exists$ isometry $T:\mathcal{X}\to\mathcal{Y}$ with $T_\#\mu = \nu$ (invariances)
- **Metric:** Metrizes space of equivalence classes of mm spaces with finite size
- **Computation:** $\mathrm{D}_{p,q}\left(\frac{1}{n}\sum_{i=1}^n \delta_{x_i}, \frac{1}{n}\sum_{i=1}^n \delta_{y_i}\right)^p = \frac{1}{n^2}\min_{\sigma\in S_n} \sum_{i,j=1}^n \left| d_{\mathcal{X}}(x_i,x_j)^q - d_{\mathcal{Y}}\left(y_{\sigma(i)}, y_{\sigma(j)}\right)^q \right|^p$

Quadratic assignment problem (non-convex) [Commander '05] $\Longrightarrow$

Entropic GW vs. Computational Hardness

Approach: Explore variants of the GW problem for computational tractability

- **Sliced GW**: Avg/max of GW btw low-dimensional projections [Vayer-Flamary-Tavenard '20]
- **Unbalanced GW:** Relax marginal constraints via f-div. penalty [Séjourné-Vialard-Peyré '23]
- **Entropic GW:** Add entropic penalty to GW cost [Peyré-Cuturi-Solomon '16]

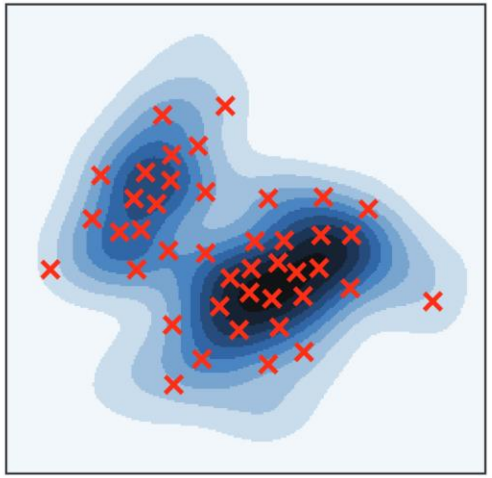
Entropic Gromov-Wasserstein Distance

$$\mathrm{S}_{p,q}^{\epsilon}(\mu,\nu) := \inf_{\pi\in\Pi(\mu,\nu)} \iint \left|d_{\mathcal{X}}(x,x')^q - d_{\mathcal{Y}}(y,y')^q\right|^p d\pi\otimes\pi(x,y,x',y') + \epsilon \mathrm{D}_{\mathrm{KL}}(\pi\|\mu\otimes\nu)$$

⊛ Computed via mirror-descent w/ Sinkhorn iterations [Solomon *et al* '16]

↳ Sinkhorn algorithm time complexity is $\tilde{O}(n^2/\epsilon^2)$ (highly parallelizable) [Lin *et al* '22]

A Statistical Question



Question: μ, ν are unknown; we sample $X_1, \dots, X_n \sim \mu$ **&** $Y_1, \dots, Y_n \sim \nu$

- **Empirical measures:** $\hat{\mu}_n := \frac{1}{n}\sum_{i=1}^{n} \delta_{X_i}$ and $\hat{\nu}_n := \frac{1}{n}\sum_{i=1}^{n} \delta_{Y_i}$

$\Longrightarrow$ Can we approximate $\mathrm{D}_{p,q}(\mu, \nu) \approx \mathrm{D}_{p,q}(\hat{\mu}_n, \hat{\nu}_n)$?

… $\mathrm{S}_{p,q}^{\epsilon}(\mu, \nu) \approx \mathrm{S}_{p,q}^{\epsilon}(\hat{\mu}_n, \hat{\nu}_n)$?

Asymptotic Ans: **Yes!** For μ, ν w/ finite pq–size, $\mathrm{D}_{p,q}(\hat{\mu}_n, \hat{\nu}_n) \to \mathrm{D}_{p,q}(\mu, \nu)$ a.s. [Mémoli '11]

Non-Asymptotic Regime: What is the **rate** at which $\mathbb{E}\left[\left|\mathrm{D}_{p,q}(\mu, \nu) - \mathrm{D}_{p,q}(\hat{\mu}_n, \hat{\nu}_n)\right|\right]$ decays?

Open question: No available results for either $\mathrm{D}_{p,q}$ or $\mathrm{S}_{p,q}^{\epsilon}$

↳ **Statistical implications:** Principled sample-size selection + further stat. advancements

↳ **Computational implications:** Time complexity depends on sample size

From Duality to Empirical Convergence Rates

Optimal Transport: For $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ and a cost function c, define

$$\mathrm{OT}_c(\mu,\nu) = \inf_{\pi\in\Pi(\mu,\nu)} \int c(x,y)d\pi(x,y)$$

Kantorovich Dual: $\mathrm{OT}_c(\mu,\nu) = \sup_{(\varphi,\psi)\in\Phi_c} \int \varphi d\mu + \int \psi d\nu$

where $\Phi_c \coloneqq \left\{(\varphi,\psi) \in C_b(\mathbb{R}^d) \times C_b(\mathbb{R}^d) \colon \varphi(x) + \psi(y) \le c(x,y) \;\; \forall x,y\right\}$

Empirical Convergence Analysis: Follow these steps

1. **Potentials:** Find regular classes $\mathcal{F}_c, \mathcal{G}_c$ containing optimal potentials $\Longrightarrow$

2. **Suprema of emp. process:** Decompose

$$\mathbb{E}[|\mathrm{OT}_c(\mu,\nu) - \mathrm{OT}_c(\hat{\mu}_n,\hat{\nu}_n)|] \le \mathbb{E}\left[\sup_{\varphi\in\mathcal{F}_c}|(\mu-\hat{\mu}_n)\varphi|\right] + \mathbb{E}\left[\sup_{\psi\in\mathcal{G}_c}|(\mu-\hat{\mu}_n)\psi|\right]$$

3. **Entropy integrals:** Use chaining to bound each term by entropy integral **&** obtain rates

Duality Theory for (Entropic) GW Distance

Setting: Quadratic cost over Euclidean spaces

- **mm-spaces:** $(\mathbb{R}^{d_x}, \|\cdot\|, \mu)$ and $(\mathbb{R}^{d_y}, \|\cdot\|, \nu)$ with $M_4(\mu) := \int \|x\|^4 d\mu(x)\,, M_4(\nu) < \infty$
- **Quadratic GW:** $\mathrm{S}_\epsilon(\mu,\nu) = \inf_{\pi\in\Pi(\mu,\nu)} \iint \left|\|x-x'\|^2 - \|y-y'\|^2\right|^2 d\pi\otimes\pi + \epsilon \mathrm{D}_{\mathrm{KL}}(\pi\|\mu\otimes\nu)$

Decomposition: Assume w.l.o.g. that μ,ν are centered (invariance to translation); then

$$\mathrm{S}_\epsilon(\mu,\nu) = \mathrm{S}_1(\mu,\nu) + \mathrm{S}_{2,\epsilon}(\mu,\nu)$$

where $\mathrm{S}_1(\mu,\nu) = \int \|x-x'\|^4 d\mu\otimes\mu + \int \|y-y'\|^4 d\nu\otimes\nu - 4\int \|x\|^2\|y\|^2 d\mu\otimes\nu$

$$\mathrm{S}_{2,\epsilon}(\mu,\nu) = \inf_{\pi\in\Pi(\mu,\nu)} \int -4\|x\|^2\|y\|^2 d\pi - 8\sum_{\substack{1\le i\le d_x\\ 1\le j\le d_y}} \left(\int x_i y_j d\pi\right)^2 + \epsilon \mathrm{D}_{\mathrm{KL}}(\pi\|\mu\otimes\nu)$$

$\Longrightarrow$ Derive a dual form for $\mathrm{S}_{2,\epsilon}(\mu,\nu)$!

Duality Theory for (Entropic) GW Distance

Approach: Linearize quadratic term using auxiliary variables

$$\mathsf{S}_{2,\epsilon}(\mu,\nu) = \inf_{\pi\in\Pi(\mu,\nu)} \int -4\|x\|^2\|y\|^2 d\pi - 8\sum_{\substack{1\le i\le d_x\\1\le j\le d_y}}\left(\int x_i y_j d\pi\right)^2 + \epsilon\mathrm{D}_{\mathrm{KL}}(\pi\|\mu\otimes\nu)$$

$$= \inf_{\pi\in\Pi(\mu,\nu)} \int -4\|x\|^2\|y\|^2 d\pi - 8\sum_{\substack{1\le i\le d_x\\1\le j\le d_y}} \inf_{-\frac{M_{\mu,\nu}}{2}\le a_{ij}\le\frac{M_{\mu,\nu}}{2}} \left(a_{ij}^2 - \int a_{ij}x_i y_j d\pi\right) + \epsilon\mathrm{D}_{\mathrm{KL}}(\pi\|\mu\otimes\nu)$$

$$= \inf_{\mathbf{A}\in\mathcal{D}_{M_{\mu,\nu}}} 32\|\mathbf{A}\|_{\mathrm{F}}^2 + \underbrace{\inf_{\pi\in\Pi(\mu,\nu)} \int \underbrace{\left(-4\|x\|^2\|y\|^2 - 32x^{\mathrm{T}}\mathbf{A}y\right)}_{=:\, c_{\mathbf{A}}(x,y)} d\pi + \epsilon\mathrm{D}_{\mathrm{KL}}(\pi\|\mu\otimes\nu)}_{=\,\mathrm{EOT}_{\epsilon,c_{\mathbf{A}}}(\mu,\nu)}$$

Optimality at $a_{ij}^*(\pi) = 0.5\int x_i y_j d\pi$ and define $M_{\mu,\nu} = \sqrt{M_2(\mu)M_2(\nu)}$

Theorem (Zhang-Goldfeld-Mroueh-Sriperumbudur '23)

Fix $\epsilon > 0$, $(\mu,\nu) \in \mathcal{P}_4(\mathbb{R}^{d_x}) \times \mathcal{P}_4(\mathbb{R}^{d_y})$, and any $M \ge \sqrt{M_2(\mu)M_2(\nu)}$, we have

$$\mathsf{S}_{2,\epsilon}(\mu,\nu) = \inf_{\mathbf{A}\in\mathcal{D}_M} 32\|\mathbf{A}\|_{\mathrm{F}}^2 + \sup_{(\varphi,\psi)\in L^1(\mu)\times L^1(\nu)} \int\varphi d\mu + \int\psi d\nu - \epsilon\int e^{\frac{\varphi(x)+\psi(y)-c_{\mathbf{A}}(x,y)}{\epsilon}} d\mu\otimes\nu + \epsilon$$

Sample Complexity of Entropic GW

Theorem (Zhang-Goldfeld-Mroueh-Sriperumbudur '23)

Fix $\epsilon > 0$ and let $(\mu, \nu) \in \mathcal{P}(\mathbb{R}^{d_x}) \times \mathcal{P}(\mathbb{R}^{d_y})$ be $\overbrace{\text{4-sub-Weibull with param. } \sigma^2 > 0}^{\Leftrightarrow\ \|X\|^2, \|Y\|^2 \text{ are } \sigma^2\text{-sub-Gaussian}}$. Then

$$\mathbb{E}\left[\left|\mathsf{S}_\epsilon(\mu,\nu) - \mathsf{S}_\epsilon(\hat{\mu}_n, \hat{\nu}_n)\right|\right] \lesssim_{d_x, d_y} \underbrace{\frac{1+\sigma^4}{\sqrt{n}}}_{\substack{S_1 \text{ rate} \\ + \\ \text{centering bias}}} + \underbrace{\epsilon\left(1 + \left(\frac{\sigma}{\sqrt{\epsilon}}\right)^{9\lceil (d_x \vee d_y)/2 \rceil + 11}\right)\frac{1}{\sqrt{n}}}_{S_{2,\epsilon} \text{ rate}}$$

Comments:

- **Optimality:** Rate is parametric and hence minimax optimal
- **Entropic OT:** Rate matches that for EOT (assuming compact support or sub-Gaussianity)
- **Constants:** May not be optimal but matches best known dependence on ϵ, σ for EOT
- **One-sample:** When only μ is estimated, rate is similar but with d_x instead of $d_x \vee d_y$

Sample Complexity of Entropic GW: Proof Outline

Decomposition: Split S_ϵ into $\mathrm{S}_1 + \mathrm{S}_{2,\epsilon}$ and center empirical measures

$$\mathbb{E}[|\mathrm{S}_\epsilon(\mu,\nu) - \mathrm{S}_\epsilon(\hat{\mu}_n,\hat{\nu}_n)|] \leq \mathbb{E}[|\mathrm{S}_1(\mu,\nu) - \mathrm{S}_1(\hat{\mu}_n,\hat{\nu}_n)|] + \mathbb{E}\left[\left|\mathrm{S}_{2,\epsilon}(\mu,\nu) - \mathrm{S}_{2,\epsilon}(\hat{\mu}_n,\hat{\nu}_n)\right|\right] + \frac{\sigma^2}{\sqrt{n}}$$

S_1 Analysis: Involves only estimation of moments

$\mathrm{S}_{2,\epsilon}$ Analysis: Hinges on dual form + regularity analysis of optimal potentials

1. **EOT reduction:** $\left|\mathrm{S}_{2,\epsilon}(\mu,\nu) - \mathrm{S}_{2,\epsilon}(\hat{\mu}_n,\hat{\nu}_n)\right| \leq \sup_{\mathbf{A}\in\mathcal{D}_M} \left|\mathrm{EOT}_{\epsilon,c_{\mathbf{A}}}(\mu,\nu) - \mathrm{EOT}_{\epsilon,c_{\mathbf{A}}}(\hat{\mu}_n,\hat{\nu}_n)\right|$ ⊛
2. **Potentials:** For each $\mathbf{A} \in \mathcal{D}_M$: $|\varphi(x)| \leq C_{d_x,d_y}(1+\tilde{\sigma}^5)(1+\|x\|^4)$

   $|D^\alpha\varphi(x)| \leq C_{\alpha,d_x,d_y}\left(1+\tilde{\sigma}^{4.5|\alpha|}\right)\left(1+\|x\|^{3|\alpha|}\right), \forall\alpha \in \mathbb{N}_0^{d_x}$

$\Longrightarrow$ $\forall\mathbf{A} \in \mathcal{D}_M$ $(\varphi^*,\psi^*) \in \mathcal{F}_s \times \mathcal{G}_s$ for Hölder classes of arbitrary smoothness

3. **Reduction to emp. process:** $\mathbb{E}[⊛] \leq \mathbb{E}\left[\sup_{\varphi\in\mathcal{F}_s}|(\mu-\hat{\mu}_n)\varphi|\right] + \mathbb{E}\left[\sup_{\psi\in\mathcal{G}_s}|(\mu-\hat{\mu}_n)\psi|\right]$

$\Longrightarrow$ Partition $\mathbb{R}^{d_x}$ into compact sets **&** bound entropy int. of $\mathcal{F}_s$ (Hölder) with $s = \left\lceil\frac{d_x}{2}\right\rceil + 1$

Standard GW: Duality & Sample Complexity

Theorem (Zhang-Goldfeld-Mroueh-Sriperumbudur '23)

For $(\mu, \nu) \in \mathcal{P}_4(\mathbb{R}^{d_x}) \times \mathcal{P}_4(\mathbb{R}^{d_y})$ and any $M \geq \sqrt{M_2(\mu) M_2(\nu)}$, we have

$$\mathrm{S}_{2,\epsilon}(\mu, \nu) = \inf_{\mathbf{A} \in \mathcal{D}_M} 32\|\mathbf{A}\|_{\mathrm{F}}^2 + \sup_{\substack{(\varphi,\psi) \in C_b(\mathbb{R}^{d_x}) \times C_b(\mathbb{R}^{d_x}) \\ \varphi(x)+\psi(y) \leq c_{\mathbf{A}}(x,y)}} \int \varphi d\mu + \int \psi d\nu$$

where $\mathrm{c}_{\mathbf{A}}(x, y) \coloneqq -4\|x\|^2\|y\|^2 - 32 x^{\mathrm{T}} \mathbf{A} y$.

Proof: Same argument as before but apply **standard OT duality** in the last step

$$\mathrm{S}_{2,\epsilon}(\mu, \nu) = \cdots = \inf_{\mathbf{A} \in \mathcal{D}_{M_{\mu,\nu}}} 32\|\mathbf{A}\|_{\mathrm{F}}^2 + \boxed{\inf_{\pi \in \Pi(\mu,\nu)} \int \left(-4\|x\|^2\|y\|^2 - 32 x^{\mathrm{T}} \mathbf{A} y\right) d\pi}$$

$= \mathrm{OT}_{c_{\mathbf{A}}}(\mu, \nu)$

Standard GW: Duality & Sample Complexity

Theorem (Zhang-Goldfeld-Mroueh-Sriperumbudur '23)

Let $(\mu, \nu) \in \mathcal{P}(\mathbb{R}^{d_x}) \times \mathcal{P}(\mathbb{R}^{d_y})$ have compact support with diameter bounded by $R > 0$. Then

$$\mathbb{E}[|\mathrm{D}(\mu,\nu)^2 - \mathrm{D}(\hat{\mu}_n, \hat{\nu}_n)^2|] \lesssim_{d_x,d_y,R} \underbrace{\frac{R^4}{\sqrt{n}}}_{S_1 \text{ rate + centering bias}} + \underbrace{(1+R^4) n^{-\frac{2}{d_x \vee d_y \vee 4}} (\log n)^{\mathbb{1}_{\{d_x \vee d_y = 4\}}}}_{S_{2,0} \text{ rate}}$$

Proof: Similar argument using Lipschitness **&** concavity of optimal potentials (via cost concavity)

- **Low dimension:** Potential class is Donsker for $d_x \vee d_y \leq 3$ [Hundrieser *et al* '22]

Comments:

- **OT:** Rate is matches that for empirical OT with compact support [Manole-Niles Weed '22]
- **Unbdd. support:** [Manole-Niles Weed '22] have argument for OT under strong assumptions
- **Non-squared GW:** If $\mathrm{D}(\mu, \nu) > 0$ then the same rates hold for empirical D itself
- **One-sample:** When only μ is estimated, rate is similar but with d_x instead of $d_x \vee d_y$

Entropic GW: Stability Analysis

Question: Is entropic GW cost and coupling a good approximation of the GW ones?

Theorem (Zhang-Goldfeld-Mroueh-Sriperumbudur '23)

Let $p = q = 2$ and $(\mu, \nu) \in \mathcal{P}_4(\mathbb{R}^{d_x}) \times \mathcal{P}_4(\mathbb{R}^{d_y})$.

1. For any $\epsilon > 0$: $|\mathrm{S}_\epsilon(\mu,\nu) - \underbrace{\mathrm{S}_0(\mu,\nu)}_{= \mathrm{D}(\mu,\nu)^2}| \lesssim_{d_x, d_y, M_4(\mu), M_4(\nu)} \epsilon \log \frac{1}{\epsilon}$
2. Let $\epsilon_k \searrow \epsilon \geq 0$, and for each $k \in \mathbb{N}$, let $\pi_k \in \Pi(\mu,\nu)$ be optimal for $\mathrm{S}_{\epsilon_k}(\mu,\nu)$. Then $\pi_k \to \pi$ weakly (up to extracting subsequence) for some π optimal for $\mathrm{S}_\epsilon(\mu,\nu)$.

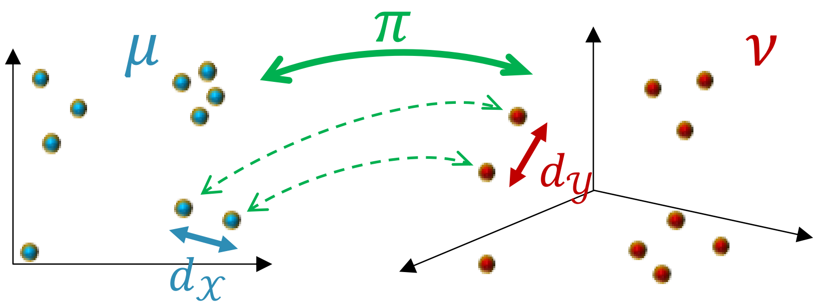
Comments: Stability of GW cost and coupling in regularization parameter

- **Entropic OT**: Matching bounds and similar convergence results
- **Proofs:**
  1. Discretization argument + maximum entropy bounds
  2. Γ-convergence of EGW functional

Summary

Gromov-Wasserstein Distance: Quantifies discrepancy between mm spaces

- Applications in ML and beyond for heterogeneous data
- Foundational statistical **&** computational questions open



Contributions: Duality and first steps towards statistical theory

- Dual form using auxiliary matrix-valued variable
- First sample complexity results for GW and EGW (quadratic cost over Euclidean spaces)
- Additional results: stability or GW cost and coupling in reg. parameter

Directions: New optimization algorithms, limit distribution theory, GW gradient flow, etc.

[∗] Zhang, Goldfeld, Mroueh, Sriperumbudur, “Gromov-Wasserstein distances: entropic regularization, duality, and sample complexity”, ArXiv: 2212.12848

Thank you!