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

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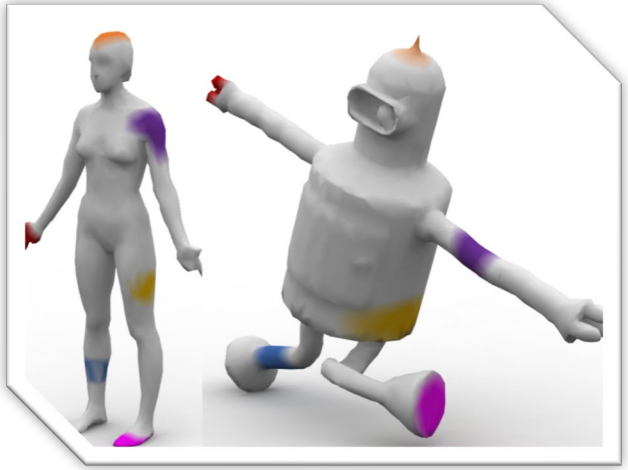
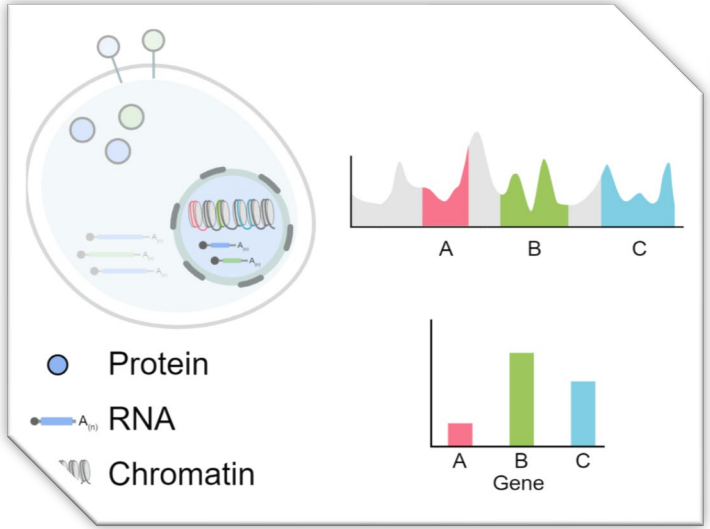
Information Systems Laboratory Colloquium, Stanford University
February 23rd, 2023

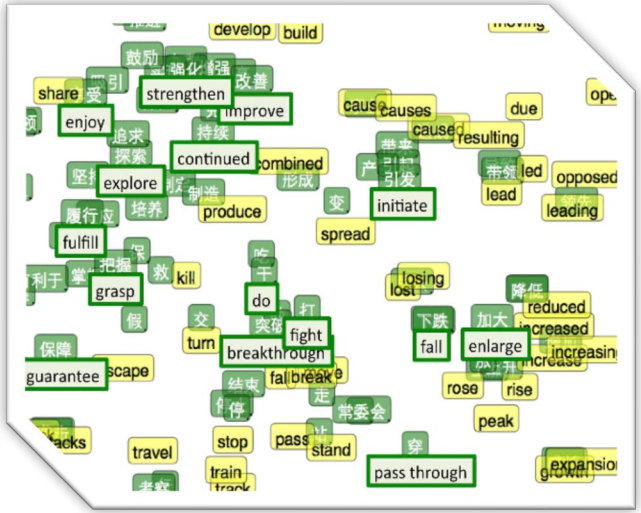
Heterogeneous & Structured Data

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



[Solomon-Peyré-Kim-Sra '16]





Garfield as an eldritch horror.

Goals:

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

The Gromov-Wasserstein Distance

Object matching: Correspondence between geometric objects

- Represent objects as metric measure spaces

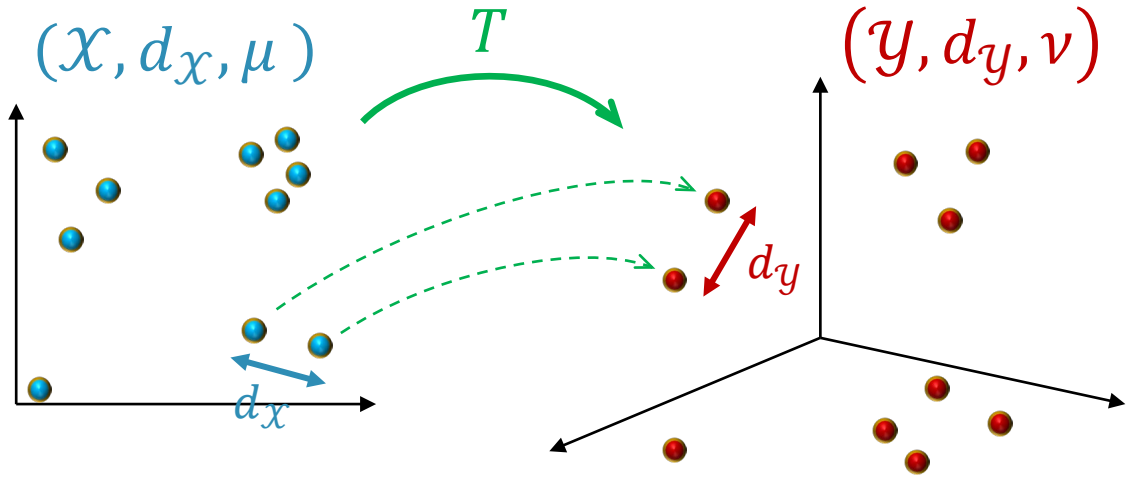
$\Longrightarrow$ $(\mathcal{X}, d_{\mathcal{X}}, \mu)$ & $(\mathcal{Y}, d_{\mathcal{Y}}, \nu)$

- 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 distortion)

$\Longrightarrow$ $\|x_i - x_j\| \approx \|T(x_i) - T(x_j)\|$



$$\Pi(\mu, \nu) = \{\pi \in \mathcal{P}(\mathcal{X} \times \mathcal{Y}) : \pi(\cdot \times \mathcal{Y}) = \mu, \pi(\mathcal{X} \times \cdot) = \nu\}$$

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

$$\mathrm{D}_{p,q}(\mu, \nu) := \inf_{\pi \in \Pi(\mu,\nu)} \left(\int_{\mathcal{X}\times\mathcal{Y}} \int_{\mathcal{X}\times\mathcal{Y}} \left| d_{\mathcal{X}}(x, x')^q - d_{\mathcal{Y}}(y, y')^q \right|^p d\pi \otimes \pi(x, y, x', y') \right)^{1/p}$$

The Gromov-Wasserstein Distance

Gromov-Wasserstein Distance (Memoli '11)

$$\mathrm{D}_{p,q}(\mu,\nu) := \inf_{\pi\in\Pi(\mu,\nu)} \left(\int_{\mathcal{X}\times\mathcal{Y}} \int_{\mathcal{X}\times\mathcal{Y}} \left| d_{\mathcal{X}}(x,x')^q - d_{\mathcal{Y}}(y,y')^q \right|^p d\pi \otimes \pi(x,y,x',y') \right)^{1/p}$$

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:** $\mathrm{D}_{p,q}(\mu,\nu) = 0 \iff \exists$ isomorphism $T: \mathcal{X} \to \mathcal{Y}$ with $T_{\#}\mu = \nu$ (invariance)
- **Metric:** Metrizes space of isomorphism (equivalence) classes of mm spaces with finite size
- **Computation:** $\mathrm{D}_{p,q}\left(\frac{1}{n}\sum_{i=1}^n \delta_{x_i}, \frac{1}{n}\sum_{i=1}^n \delta_{y_i}\right)^p = \frac{1}{n^2} \min_{\sigma\in S_n} \sum_{i,j=1}^n \left| d_{\mathcal{X}}(x_i,x_j)^q - d_{\mathcal{Y}}(y_{\sigma(i)},y_{\sigma(j)})^q \right|^p$

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

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

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

⊛ 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]

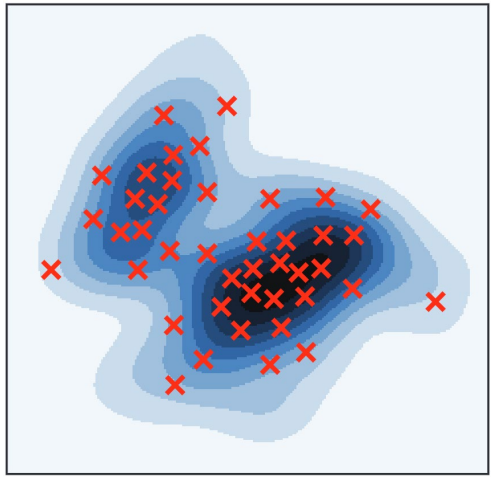
A Statistical Question

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

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



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 $\mathrm{S}^{\epsilon}_{p,q}$

↳ **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 $\Phi_c := \{(\varphi,\psi) \in C_b(\mathbb{R}^d) \times C_b(\mathbb{R}^d) \colon \varphi(x) + \psi(y) \le c(x,y) \ \ \forall x, y\}$

Empirical Convergence Analysis: Follow these steps

1. **Potentials:** Find regular classes $\mathcal{F}_c, \mathcal{G}_c$ containing optimal potentials $\Longrightarrow \Phi_c \subseteq \mathcal{F}_c \times \mathcal{G}_c$
2. **Suprema of emp. process:** Decompose

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

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:** $\left(\mathbb{R}^{d_x}, \|\cdot\|, \mu\right)$ and $\left(\mathbb{R}^{d_y}, \|\cdot\|, \nu\right)$ 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

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

$$= \inf_{\pi\in\Pi(\mu,\nu)} \int -4\|x\|^2\|y\|^2 d\pi + 32\sum_{\substack{1\le i\le d_x\\ 1\le j\le d_y}} \inf_{-\frac{M_{\mu,\nu}}{2}\le a_{ij}\le \frac{M_{\mu,\nu}}{2}} \left(a_{ij}^2 - \int a_{ij}x_i y_j d\pi\right) + \epsilon \mathrm{D}_{\mathrm{KL}}(\pi\|\mu\otimes\nu)$$

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

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

Theorem (Zhang-G.-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

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

Sample Complexity of Entropic GW

Theorem (Zhang-G.-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

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

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

$\Longrightarrow$ Rate is parametric $\asymp 1/\sqrt{n}$

$\mathrm{S}_{2,\epsilon}$ Analysis: Hinges on dual form + duality-based analysis

Sample Complexity of Entropic GW: Proof Outline

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 $\mathbf{A} \in \mathcal{D}_M$: $|\varphi_{\boldsymbol{A}}(x)| \leq C_{d_x,d_y}(1+\tilde{\sigma}^5)(1+\|x\|^4)$

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

$\Longrightarrow$ $\forall \mathbf{A} \in \mathcal{D}_M \quad (\varphi_{\boldsymbol{A}},\psi_{\boldsymbol{A}}) \in \mathcal{F}_s \times \mathcal{G}_s$ for Hölder classes of arbitrary smoothness

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

- Partition $\mathbb{R}^{d_x} = \bigcup_{i\in\mathbb{N}_0} B_i$ (compact sets) **&** each $\mathcal{F}_s|_{B_i}$ has bounded $\mathcal{C}^s(B_i)$-Hölder norm
- Entropy bound for Hölder class $\log N\left(\epsilon,\mathcal{F}_s,L^2(\hat{\mu}_n)\right) \lesssim \epsilon^{-\frac{d_x}{s}}$

$\Longrightarrow$ $\mathbb{E}\left[\left|\mathrm{S}_{2,\epsilon}(\mu,\nu) - \mathrm{S}_{2,\epsilon}(\hat{\mu}_n,\hat{\nu}_n)\right|\right] \lesssim \frac{1}{\sqrt{n}}$

Standard GW: Duality & Sample Complexity

Theorem (Zhang-G.-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

$$\mathrm{S}_{2,0}(\mu,\nu) = \inf_{\mathbf{A}\in\mathcal{D}_M} 32\|\mathbf{A}\|_{\mathrm{F}}^2 + \sup_{\substack{(\varphi,\psi)\in C_b(\mathbb{R}^{d_x})\times C_b(\mathbb{R}^{d_x}) \\ \varphi(x)+\psi(y)\leq c_{\mathbf{A}}(x,y)}} \int \varphi d\mu + \int \psi d\nu$$

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

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

$$\mathrm{S}_{2,0}(\mu,\nu) = \cdots = \inf_{\mathbf{A}\in\mathcal{D}_{M_{\mu,\nu}}} 32\|\mathbf{A}\|_{\mathrm{F}}^2 + \boxed{\inf_{\pi\in\Pi(\mu,\nu)} \int \left(-4\|x\|^2\|y\|^2 - 32x^{\mathrm{T}}\mathbf{A}y\right)d\pi}$$

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

Standard GW: Duality & Sample Complexity

Theorem (Zhang-G.-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 via Lipschitzness **&** concavity of dual potentials (using 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 vs. Non-Entropic Gromov-Wasserstein

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

Theorem (Zhang-G.-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 $\mathrm{S}_\epsilon(\mu,\nu)$.

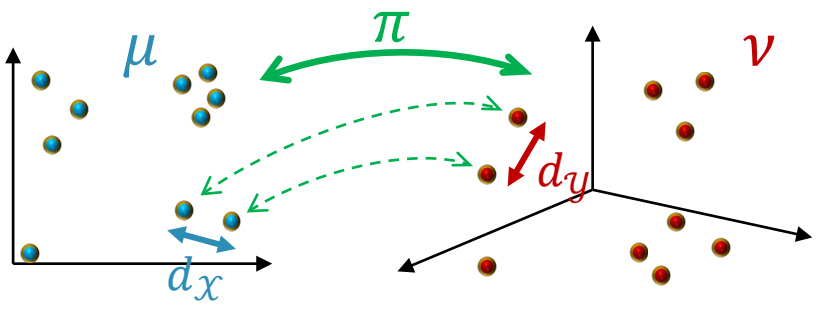
Comments: Stability of GW cost and coupling in regularization parameter

- **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 discrapency 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, uniqueness of $\boldsymbol{A}$

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!