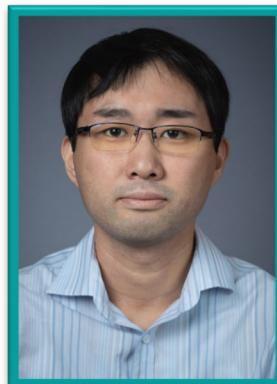
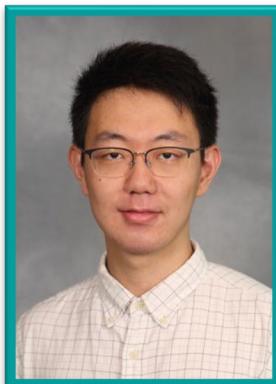
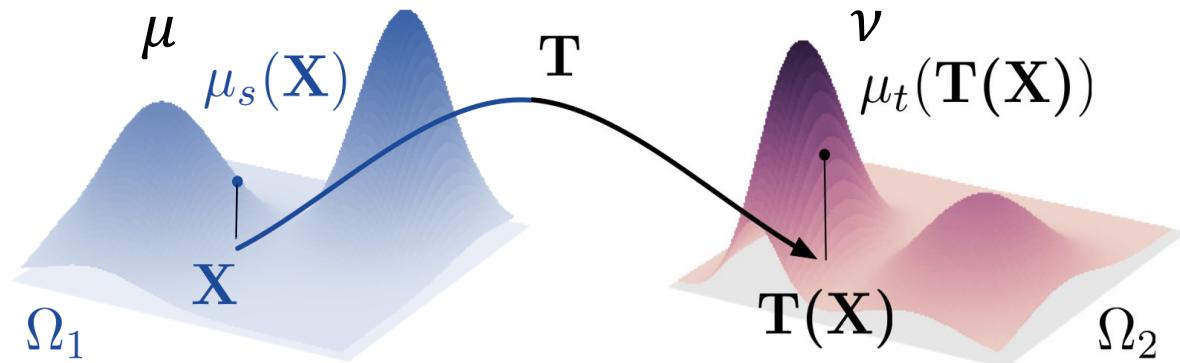


# Gromov-Wasserstein Alignment: Statistical & Computational Advancements via Duality

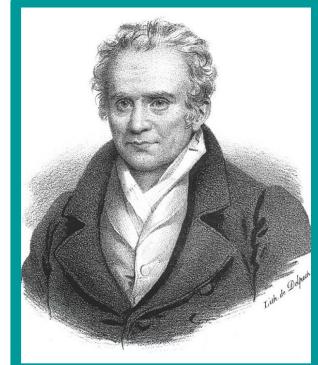
Ziv Goldfeld  
Cornell University



# Optimal Transport



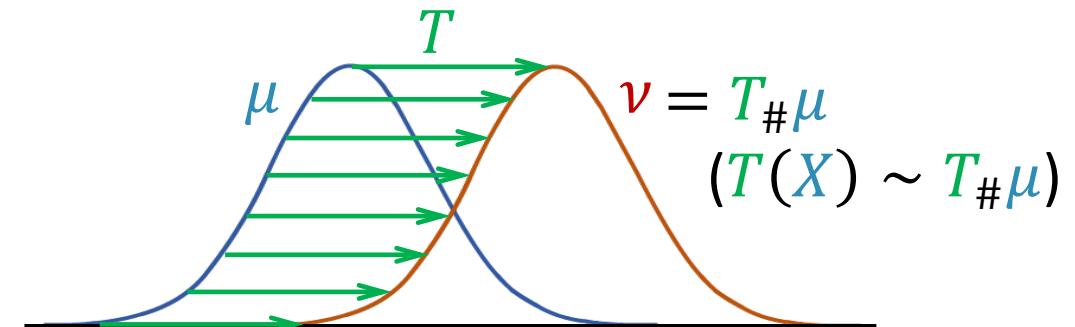
# Optimal Transport



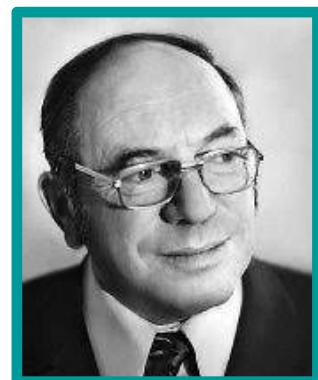
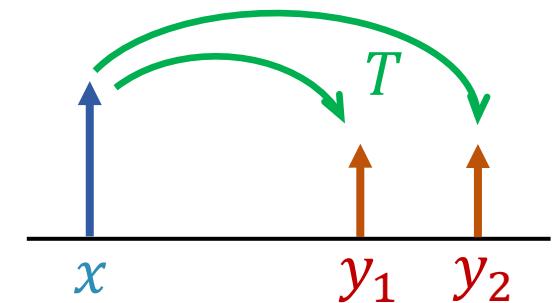
Monge (1781)

$$M_c(\mu, \nu) := \inf_{\substack{T: \mathcal{X} \rightarrow \mathcal{Y} \\ T_{\#}\mu = \nu}} \int c(x, T(x)) d\mu(x)$$

Transport map



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



Kantorovich (1942)

## Kantorovich Optimal Transport

$$\text{OT}_c(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \iint c d\pi = \sup_{\substack{(\varphi, \psi) \in L^1(\mu) \times L^1(\nu): \\ \varphi(x) + \psi(y) \leq c(x, y)}} \int \varphi d\mu + \int \psi d\nu$$

Coupling (transport plan)

# The Wasserstein Distance

**Construction:** Kantorovich OT with distance cost (or power)  $c(x, y) = \|x - y\|^p$ ,  $p \in [1, \infty)$

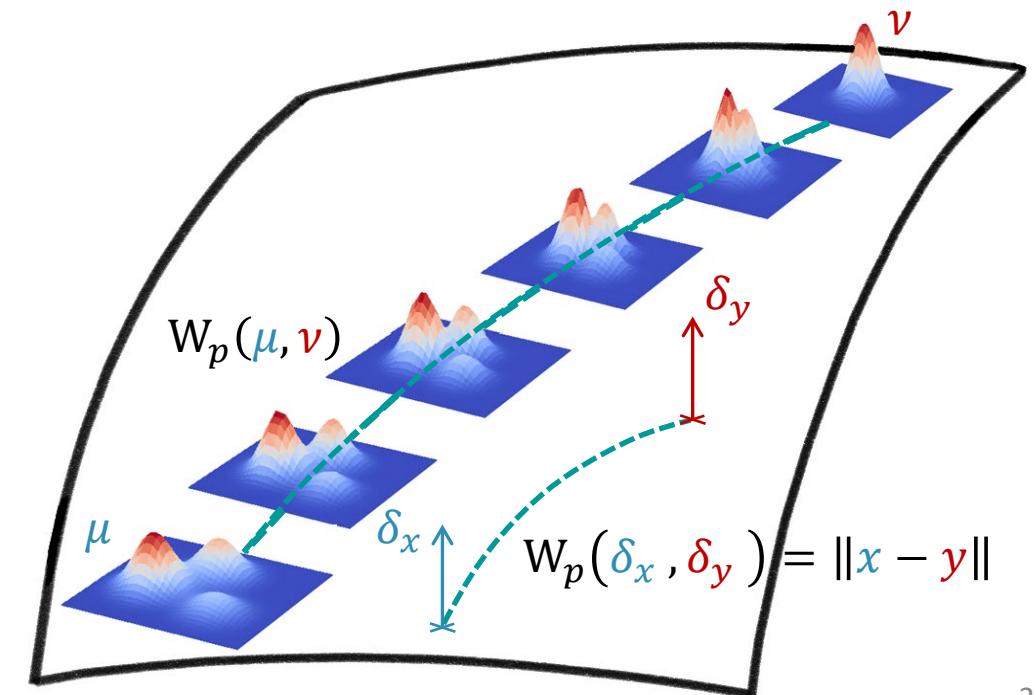
## $p$ -Wasserstein Distance

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

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

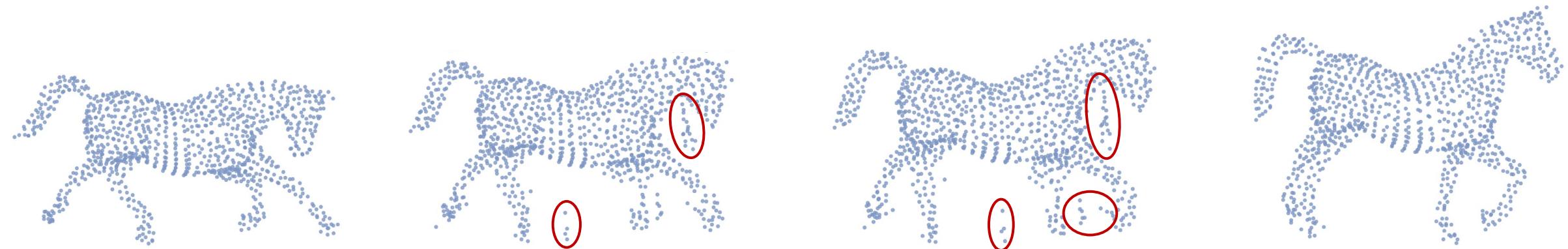
## Wasserstein geometry:

- Euclidean geometry
- Geodesic curves
- Barycenters
- Gradient flows

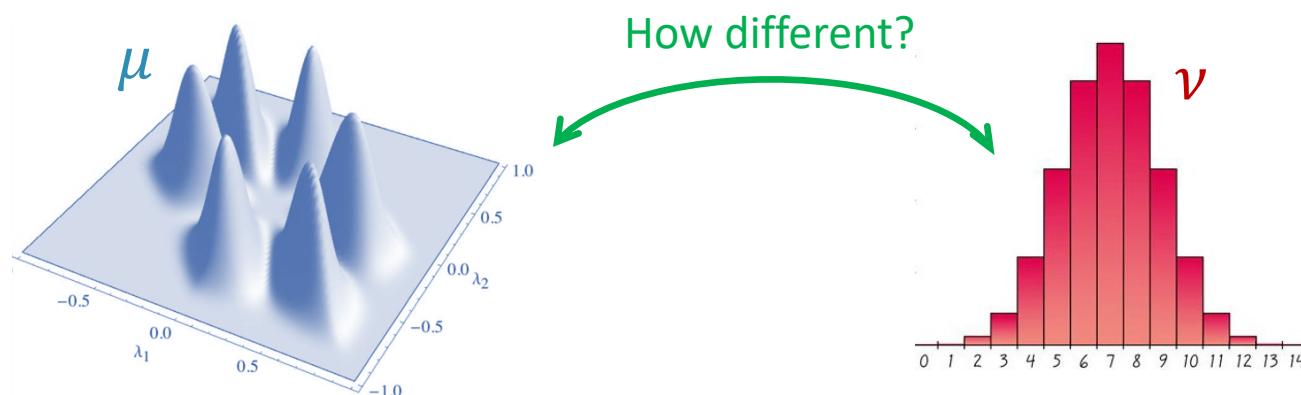


# Beyond OT and Wasserstein Distances

Structure Preserving Interpolation:



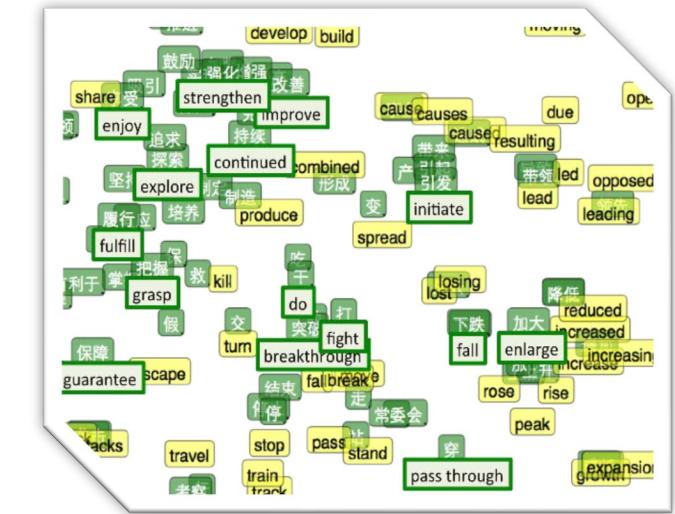
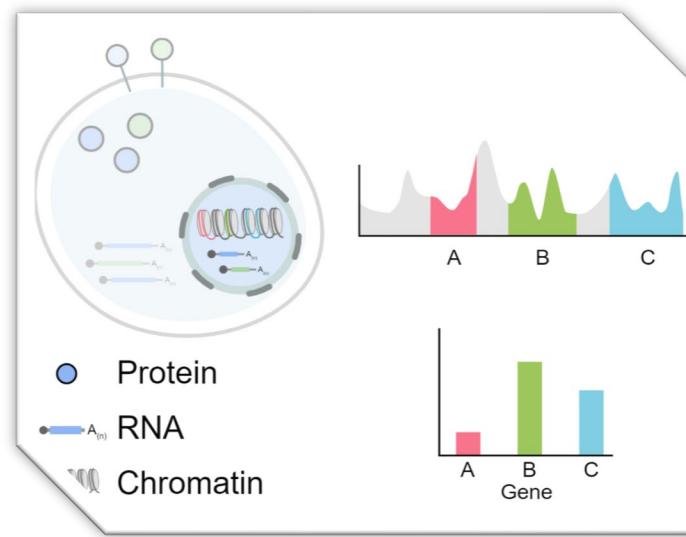
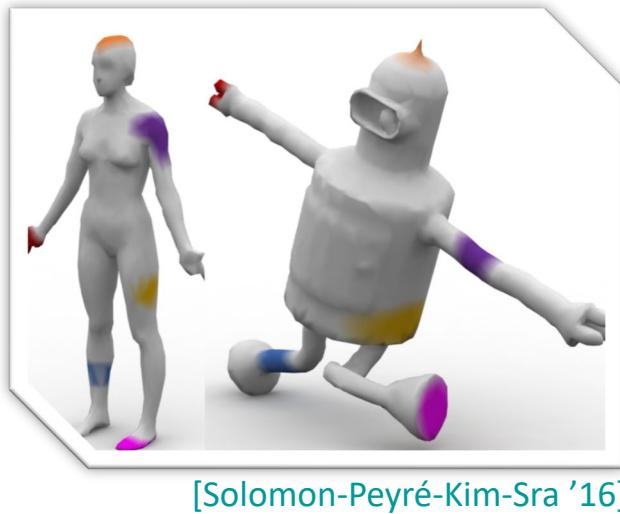
Discrepancy quantification btw incompatible spaces:



# Gromov-Wasserstein Alignment

# Heterogeneous & Structured Data

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



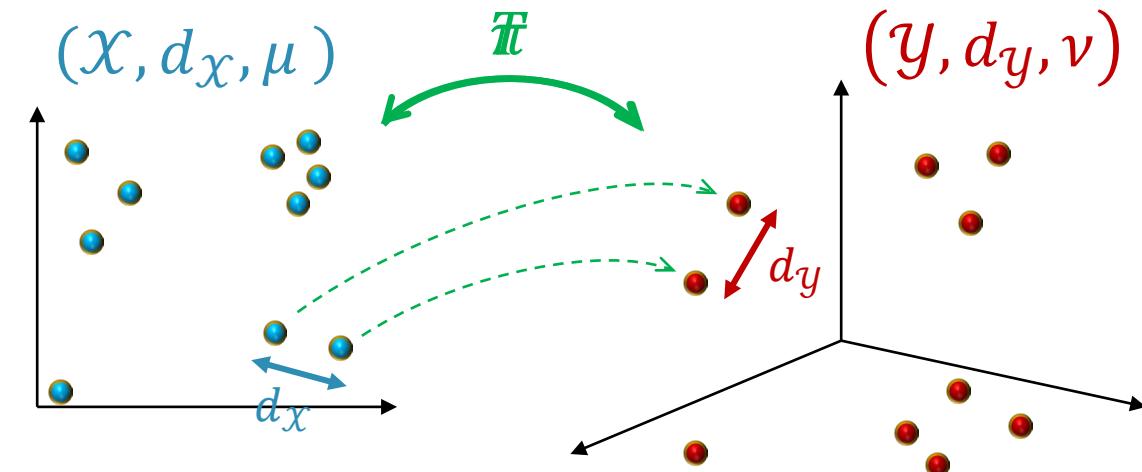
- Goals:**
1. Compare how similar/different two datasets are
  2. Obtain matching/alignment

# Gromov-Wasserstein Distance

- Datasets as metric measure spaces  
⇒  $(\mathcal{X}, d_{\mathcal{X}}, \mu)$  &  $(\mathcal{Y}, d_{\mathcal{Y}}, \nu)$
- Find matching (transport map)  $T: \mathcal{X} \rightarrow \mathcal{Y}$   
⇒  $\nu = T_{\#}\mu$  (if  $X \sim \mu$  then  $T(X) \sim T_{\#}\mu$ )

- Preserve distances (minimize distance distortion)

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



**$(p, q)$ -Gromov-Wasserstein Distance (Memoli '11)**

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

# Gromov-Wasserstein Distance

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

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

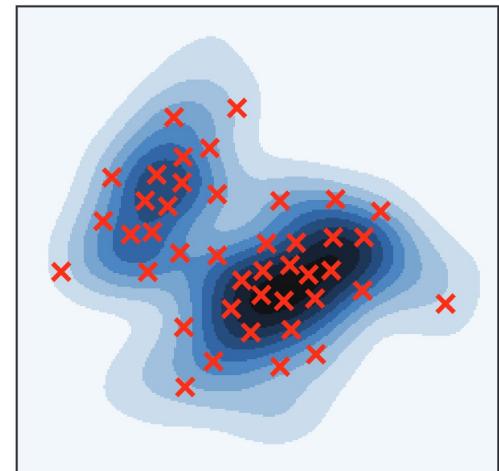
- **Finiteness:**  $D_{p,q}(\mu, \nu) < \infty \forall \mu, \nu$  with  $\mathbb{E}_{(X,X') \sim \mu \otimes \mu} [d_X(X, X')^{pq}] < \infty$  & resp. for  $\nu$
- **Identification:**  $D_{p,q}(\mu, \nu) = 0 \iff \exists$  isometry  $T: \mathcal{X} \rightarrow \mathcal{Y}$  with  $T_\# \mu = \nu$  (invariances)
- **Metric:** Metrizes space of equivalence classes of mm spaces with finite size

# Estimation from Data

**Question:**  $\mu, \nu$  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  $\hat{\nu}_n := \frac{1}{n} \sum_{i=1}^n \delta_{Y_i}$

→ Can we approximate  $D_{p,q}(\mu, \nu) \approx D_{p,q}(\hat{\mu}_n, \hat{\nu}_n)$ ?



**Asymptotic Ans:** Yes! For  $\mu, \nu$  w/ finite  $pq$ -size,  $D_{p,q}(\hat{\mu}_n, \hat{\nu}_n) \rightarrow D_{p,q}(\mu, \nu)$  a.s. [Mémoli '11]

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

🚫 **Open question:** Statistical (sample complex.) & computational (time complex.) implications

# Duality for Quadratic GW Distance

**Setting:** (2,2)-GW btw  $(\mathbb{R}^{d_x}, \|\cdot\|, \mu)$  and  $(\mathbb{R}^{d_y}, \|\cdot\|, \nu)$  with  $M_4(\mu) := \int \|x\|^4 d\mu(x), M_4(\nu) < \infty$

$$D(\mu, \nu)^2 = \inf_{\pi \in \Pi(\mu, \nu)} \iint \left| \|x - x'\|^2 - \|y - y'\|^2 \right|^2 d\pi \otimes \pi$$

**Decomposition:** Assume w.l.o.g. that  $\mu, \nu$  are centered (invariance to translation); then

$$D(\mu, \nu)^2 = S_1(\mu, \nu) + S_2(\mu, \nu)$$

where  $S_1(\mu, \nu) = \int \|x - x'\|^4 d\mu \otimes \mu + \int \|y - y'\|^4 d\nu \otimes \nu - 4 \int \|x\|^2 \|y\|^2 d\mu \otimes \nu$

$$S_2(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int -4\|x\|^2 \|y\|^2 d\pi - 8 \sum_{\substack{1 \leq i \leq d_x \\ 1 \leq j \leq d_y}} \left( \int x_i y_j d\pi \right)^2$$

Derive a dual form for  $S_2(\mu, \nu)!$



# Duality for the GW Distance

**Approach:** Linearize quadratic term using auxiliary variables

$$\begin{aligned}
 S_2(\mu, \nu) &= \inf_{\pi \in \Pi(\mu, \nu)} \int -4\|x\|^2\|y\|^2 d\pi - 8 \sum_{\substack{1 \leq i \leq d_x \\ 1 \leq j \leq d_y}} \left( \int x_i y_j d\pi \right)^2 \\
 &= \inf_{\pi \in \Pi(\mu, \nu)} \int -4\|x\|^2\|y\|^2 d\pi + 32 \sum_{\substack{1 \leq i \leq d_x \\ 1 \leq j \leq d_y}} \inf_{-\frac{M_{\mu, \nu}}{2} \leq a_{ij} \leq \frac{M_{\mu, \nu}}{2}} \left( a_{ij}^2 - \int a_{ij} x_i y_j d\pi \right) \\
 &= \inf_{\mathbf{A} \in \mathcal{D}_{M_{\mu, \nu}}} 32 \|\mathbf{A}\|_F^2 + \underbrace{\inf_{\pi \in \Pi(\mu, \nu)} \int \left( -4\|x\|^2\|y\|^2 - 32 \mathbf{x}^T \mathbf{A} \mathbf{y} \right) d\pi}_{=: c_{\mathbf{A}}(x, y)} = \text{OT}_{c_{\mathbf{A}}}(\mu, \nu)
 \end{aligned}$$

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

$\mathcal{D}_{M_{\mu, \nu}}$  = entry-wise bdd  $d_x \times d_y$ -sized matrices

**Theorem (Zhang-G.-Mroueh-Sriperumbudur '22)**

$$S_2(\mu, \nu) = \inf_{\mathbf{A} \in \mathcal{D}_{M_{\mu, \nu}}} 32 \|\mathbf{A}\|_F^2 + \text{OT}_{c_{\mathbf{A}}}(\mu, \nu)$$

# Sample Complexity of GW: Upper Bound

## Theorem (Zhang-G.-Mroueh-Sriperumbudur '22)

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

$$\mathbb{E}[|D(\mu, \nu)^2 - D(\hat{\mu}_n, \hat{\nu}_n)^2|] \lesssim_{d_x, d_y, R} \underbrace{R^4 n^{-\frac{1}{2}}}_{S_1 \text{ rate} + \text{centering bias}} + \underbrace{(1 + R^4)n^{-\frac{2}{(d_x \wedge d_y)\vee 4}} (\log n)^{\mathbb{1}_{\{d_x \wedge d_y = 4\}}}}_{S_2 \text{ rate}}$$

## Comments:

- **Optimality:** These rates are sharp!
- **Data dimension:** Rate depends on smaller dimension (but curse of dimensionality occurs)
- **Comparison to OT:** Rate matches best known for OT
- **One-sample:** When only  $\mu$  is estimated

# Sample Complexity of GW: Proof Outline

**Decomposition:** Split  $D^2$  into  $S_1 + S_2$  by centering empirical measures

$$\mathbb{E}[|D(\mu, \nu)^2 - D(\hat{\mu}_n, \hat{\nu}_n)^2|] \leq \mathbb{E}[|S_1(\mu, \nu) - S_1(\hat{\mu}_n, \hat{\nu}_n)|] + \mathbb{E}[|S_2(\mu, \nu) - S_2(\hat{\mu}_n, \hat{\nu}_n)|] + \frac{R^4}{\sqrt{n}}$$

**$S_1$  Analysis:** Involves only estimation of moments  $\implies$  Rate is parametric  $\asymp \frac{1}{\sqrt{n}}$

**$S_2$  Analysis:** Hinges on dual form + regularity analysis of optimal potentials

# Sample Complexity of GW: Proof Outline

**$S_2$  Analysis:** Invoke duality with radius  $M = R^2$

1. **OT reduction:**  $\mathbb{E}[|S_2(\mu, \nu) - S_2(\hat{\mu}_n, \hat{\nu}_n)|] \leq \mathbb{E} \left[ \sup_{\mathbf{A} \in \mathcal{D}_M} |\text{OT}_{c_{\mathbf{A}}}(\mu, \nu) - \text{OT}_{c_{\mathbf{A}}}(\hat{\mu}_n, \hat{\nu}_n)| \right]$
2. **Dual potentials:**  $\forall \mathbf{A} \in \mathcal{D}_M, \quad \varphi_{\mathbf{A}}$  is concave and  $\|\varphi_{\mathbf{A}}\|_{\text{Lip}} \vee \|\varphi_{\mathbf{A}}\|_{\infty} \lesssim R^4 \sqrt{d_x d_y}$  (resp.  $\psi_{\mathbf{A}}$ )
3. **Empirical processes:**  $\mathcal{F}_R := \{\varphi: \mathbb{R}^{d_x} \rightarrow \mathbb{R}: \text{concave}, \|\varphi\|_{\text{Lip}} \vee \|\varphi\|_{\infty} \lesssim R^4 \sqrt{d_x d_y}\}$  &  $\mathcal{G}_R$

$$(*) \leq \mathbb{E} \left[ \sup_{\varphi \in \cup_{\mathbf{A}} \mathcal{F}_{\mathbf{A}}} |(\mu - \hat{\mu}_n)\varphi| \right] + \mathbb{E} \left[ \sup_{\psi \in \cup_{\mathbf{A}} \mathcal{G}_{\mathbf{A}}} |(\nu - \hat{\nu}_n)\psi| \right]$$

OT duality  $\leq \mathbb{E} \left[ \sup_{\varphi \in \mathcal{F}_R} |(\mu - \hat{\mu}_n)\varphi| \right] + \mathbb{E} \left[ \sup_{\psi \in \mathcal{G}_R} |(\nu - \hat{\nu}_n)\psi| \right] \lesssim_{R, d_x, d_y} n^{-\frac{2}{d_x}} + n^{-\frac{2}{d_y}} \leq n^{-\frac{2}{d_x \vee d_y}}$

Regularity

Covering bound:  $\log N(\epsilon, \mathcal{F}_R, \|\cdot\|_{\infty}) \lesssim_d \epsilon^{-d_x/2}$

# Sample Complexity of GW: Proof Outline

**S<sub>2</sub> Analysis:** Invoke duality with radius  $M = R^2$

Assume  $d_x < d_y$

1. OT reduction:  $\mathbb{E}[|S_2(\mu, \nu) - S_2(\hat{\mu}_n, \hat{\nu}_n)|] \leq \mathbb{E} \left[ \sup_{\mathbf{A} \in \mathcal{D}_M} |\text{OT}_{c_{\mathbf{A}}}(\mu, \nu) - \text{OT}_{c_{\mathbf{A}}}(\hat{\mu}_n, \hat{\nu}_n)| \right]$  \*
2. Dual potentials:  $\forall \mathbf{A} \in \mathcal{D}_M$ ,  $\varphi_{\mathbf{A}}$  is concave and  $\|\varphi_{\mathbf{A}}\|_{\text{Lip}} \vee \|\varphi_{\mathbf{A}}\|_{\infty} \lesssim R^4 \sqrt{d_x d_y}$  (resp.  $\psi_{\mathbf{A}}$ )

3. Empirical processes:  $\mathcal{F}_R := \{\varphi: \mathbb{R}^{d_x} \rightarrow \mathbb{R}: \text{concave}, \|\varphi\|_{\text{Lip}} \vee \|\varphi\|_{\infty} \lesssim R^4 \sqrt{d_x d_y}\}$  & ~~R~~

$$(*) \leq \mathbb{E} \left[ \sup_{\varphi \in \cup_{\mathbf{A}} \mathcal{F}_{\mathbf{A}}} |(\mu - \hat{\mu}_n)\varphi| \right] + \mathbb{E} \left[ \sup_{\psi \in \cup_{\mathbf{A}} \mathcal{F}_{\mathbf{A}}^c} |(\nu - \hat{\nu}_n)\psi| \right]$$

$(\varphi_{\mathbf{A}}, \varphi_{\mathbf{A}}^c)$  are optimal

$$\varphi^c(y) := \inf_x c_{\mathbf{A}}(x, y) - \varphi(x)$$

$$\leq \mathbb{E} \left[ \sup_{\varphi \in \mathcal{F}_R} |(\mu - \hat{\mu}_n)\varphi| \right] + \mathbb{E} \left[ \sup_{\psi \in \mathcal{F}_R^c} |(\nu - \hat{\nu}_n)\psi| \right] \lesssim_{R, d_x, d_y} n^{-\frac{2}{d_x}} + n^{-\frac{2}{d_x}} \leq n^{-\frac{2}{d_x \wedge d_y}}$$

LCA principle [Hundrieser et al. '22]:  $N(\epsilon, \mathcal{F}, \|\cdot\|_{\infty}) = N(\epsilon, \mathcal{F}^c, \|\cdot\|_{\infty}) \Rightarrow \log N(\epsilon, \mathcal{F}_R^c, \|\cdot\|_{\infty}) \lesssim_d \epsilon^{-d_x/2}$

# Sample Complexity of GW: Lower Bound

## Theorem (Zhang-G.-Mroueh-Sriperumbudur '23)

For  $\mathcal{X} \subseteq \mathbb{R}^{d_x}$  and  $\mathcal{Y} \subseteq \mathbb{R}^{d_y}$  with diameter at most  $R$  and any  $n$  sufficiently large, we have

$$\sup_{(\mu, \nu) \in \mathcal{P}(\mathcal{X}) \times \mathcal{P}(\mathcal{Y})} \mathbb{E}[|D(\mu, \nu)^2 - D(\hat{\mu}_n, \hat{\nu}_n)^2|] \gtrsim_{d_x, d_y, R} n^{-\frac{2}{(d_x \wedge d_y) \vee 4}}$$

## Proof Idea:

- **Wasserstein Procrustes Lemma:**  $D(\mu, \nu) \gtrsim_{\lambda_{\min}(\Sigma_\mu), \lambda_{\min}(\Sigma_\nu)} \inf_{\mathbf{U} \in O(d)} W_2(\mu, \mathbf{U}_\# \nu)$

- **Construction:**  $\mu = \text{Unif}(B_d(0,1))$  &  $\nu = \text{Unif}(B_d(0,2))$

[Dudley' 69]

- **Lower bound:**  $\mathbb{E} \left[ \inf_{\mathbf{U} \in O(d)} W_2(\hat{\mu}_n, \mathbf{U}_\# \mu) \right] \gtrsim \inf_{\mathbf{U} \in O(d)} \mathbb{E}[W_2(\hat{\mu}_n, \mathbf{U}_\# \mu)] \geq \mathbb{E}[W_1(\hat{\mu}_n, \mu)] \gtrsim_d n^{-\frac{1}{d}}$

# Computation via Entropic Gromov-Wasserstein

**GW is QAP:**  $D_{p,q} \left( \frac{1}{n} \sum_{i=1}^n \delta_{x_i}, \frac{1}{n} \sum_{i=1}^n \delta_{y_i} \right)^p = \frac{1}{n^2} \min_{\sigma \in S_n} \sum_{i,j=1}^n \left| d_X(x_i, x_j)^q - d_Y(y_{\sigma(i)}, y_{\sigma(j)})^q \right|^p$

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

## Entropic Gromov-Wasserstein Distance (Peyré-Cuturi-Solomon '16)

$$S_\epsilon(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \mathbb{E}_{\pi \otimes \pi} \left[ \left| \|X - X'\|^2 - \|Y - Y'\|^2 \right|^2 \right] + \epsilon D_{\text{KL}}(\pi \| \mu \otimes \nu)$$

- Algorithms:** Heuristic methods [Peyré-Cuturi-Solomon '16], [Solomon-Peyré-Kim-Sra '16]
- Approximation:**  $|D(\mu, \nu)^2 - S_\epsilon(\mu, \nu)| \lesssim_{d_x, d_y} \epsilon \log(1/\epsilon)$  [Zhang-G.-Mroueh-Sriperumbudur '23]
- Estimation:**  $\mathbb{E}[|S_\epsilon(\mu, \nu) - S_\epsilon(\hat{\mu}_n, \hat{\nu}_n)|] \asymp_{d_x, d_y, \epsilon} n^{-1/2}$  [\_\_\_\_\_]

# From Stability Analysis to Convexity

$$S_\epsilon(\mu, \nu) = S_1(\mu, \nu) + \min_{\mathbf{A} \in \mathcal{D}_M} \left\{ \underbrace{32\|\mathbf{A}\|_F^2}_{\text{EOT}_{\epsilon, c_A}(\mu, \nu)} \right\} =: \Phi(\mathbf{A})$$

## Analysis:

- Fréchet derivatives  $D\Phi_{[\mathbf{A}]}$  and  $D^2\Phi_{[\mathbf{A}]}$
- Bound  $\lambda_{\max}(D^2\Phi_{[\mathbf{A}]}) \leq 64$  &  $\lambda_{\min}(D^2\Phi_{[\mathbf{A}]}) \geq 64 - 32^2\epsilon^{-1}\sqrt{M_4(\mu)M_4(\nu)}$

## Theorem (RiouxB.-Kato '23)

1.  $\Phi$  is strictly convex whenever  $\epsilon > 16\sqrt{M_4(\mu)M_4(\nu)}$
2.  $\Phi$  is  $L$ -smooth on  $\mathcal{D}_M$  with  $L \leq 64 \vee (32^2\epsilon^{-1}\sqrt{M_4(\mu)M_4(\nu)} - 64)$

# Accelerated First-Order Inexact Oracle Methods

$$\min_{\mathbf{A} \in \mathcal{D}_M} 32\|\mathbf{A}\|_F^2 + \text{EOT}_{\epsilon, c_{\mathbf{A}}}(\mu, \nu)$$

**First-order methods:** Gradient of objective at  $\mathbf{A} \in \mathcal{D}_M$  depends on optimal EOT coupling  $\pi^{\mathbf{A}}$

$$D\Phi_{[\mathbf{A}]} = 64\mathbf{A} - 32\sum_{i,j=1}^n x_i y_j^T \pi_{i,j}^{\mathbf{A}}$$

**Inexact oracle (Sinkhorn):**  $\tilde{\pi}^{\mathbf{A}}$  s.t.  $\|\pi^{\mathbf{A}} - \tilde{\pi}^{\mathbf{A}}\|_{\infty} \leq \delta$

- Gradient approximation  $\tilde{D}\Phi_{[\mathbf{A}]}$  ( $\tilde{\pi}^{\mathbf{A}}$  instead of  $\pi^{\mathbf{A}}$ )
- First-order method under convexity [d'Aspremont '08]

⇒ Computes EGW cost and (approx.) coupling

**Algorithm 1** Fast gradient method with inexact oracle

```
Fix  $L = 64$  and let  $\alpha_k = \frac{k+1}{2}$ , and  $\tau_k = \frac{2}{k+3}$ 
1:  $k \leftarrow 0$ 
2:  $\mathbf{A}_0 \leftarrow \mathbf{0}$ 
3:  $\mathbf{G}_0 \leftarrow \tilde{D}\Phi_{[\mathbf{A}_0]}$ 
4:  $\mathbf{W}_0 \leftarrow \alpha_0 \mathbf{G}_0$ 
5: while stopping condition is not met do
6:    $\mathbf{B}_k \leftarrow \frac{M}{2} \text{sign}(\mathbf{A}_k - L^{-1} \mathbf{G}_k) \min\left(\frac{2}{M} |\mathbf{A}_k - L^{-1} \mathbf{G}_k|, 1\right)$ 
7:    $\mathbf{C}_k \leftarrow \frac{M}{2} \text{sign}(-L^{-1} \mathbf{W}_k) \min\left(\frac{2}{M} |L^{-1} \mathbf{W}_k|, 1\right)$ 
8:    $\mathbf{A}_{k+1} \leftarrow \tau_k \mathbf{C}_k + (1 - \tau_k) \mathbf{B}_k$ 
9:    $\mathbf{G}_{k+1} \leftarrow \tilde{D}\Phi_{[\mathbf{A}_{k+1}]}$ 
10:   $\mathbf{W}_{k+1} \leftarrow \mathbf{W}_k + \alpha_{k+1} \mathbf{G}_{k+1}$ 
11:   $k \leftarrow k + 1$ 
12: return  $\mathbf{B}_k$ 
```

# Global Convergence Guarantees (Convex)

$$\min_{\mathbf{A} \in \mathcal{D}_M} 32\|\mathbf{A}\|_F^2 + \text{EOT}_{\epsilon, c_{\mathbf{A}}}(\mu, \nu)$$

## Theorem (Rioux-G.-Kato '23)

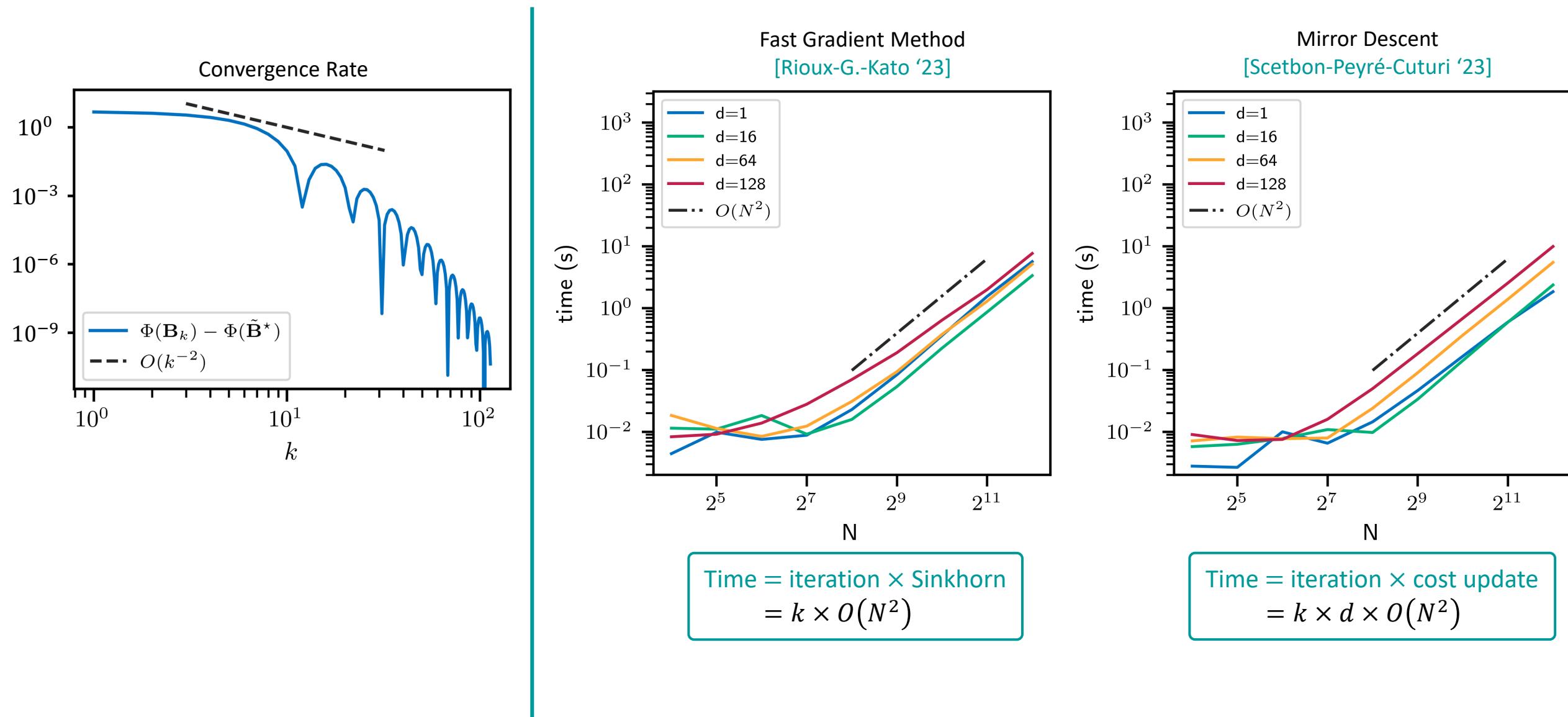
If  $\Phi$  is convex and  $L$ -smooth on  $\mathcal{D}_M$  with global min  $\mathbf{B}_*$ , then  $\mathbf{B}_k$  from Algorithm 1 satisfies

$$\Phi(\mathbf{B}_k) - \Phi(\mathbf{B}_*) \leq \frac{2L\|\mathbf{B}_*\|_F^2}{(k+1)(k+2)} + O(M\delta)$$

## Comments:

- **Optimality:** Optimal complexity of  $O(1/k^2)$  for smooth constrained opt. [Nesterov '03]
- **Non-convex regime:** Via smooth non-convex opt. with inexact oracle [Ghadimi-Lan '16]
  - ↳ Adapts to convexity of  $\Phi$  (yields improved rates if convex)

# Numerical Results



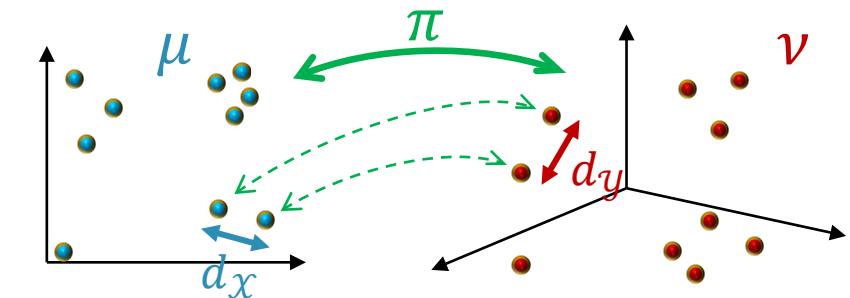
# Summary

**Gromov-Wasserstein Distance:** Quantifies discrepancy between mm spaces

- Alignment of heterogeneous datasets
- Foundational statistical & computational questions open

**Contributions:** Duality, empirical rates, and algorithms

- Dual form that connects to OT
- Sharp sample complexity for quadratic GW
- First algorithms w/ convergence rates for entropic GW
- Duality and empirical rates for EGW



**Thank you!**

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

[B] Rioux, Goldfeld, Kato, "Entropic Gromov-Wasserstein distances: stability, algorithms, and distributional limits", ArXiv:2306.00182