Globally solving the Gromov-Wasserstein problem for point clouds in low dimensional Euclidean spaces

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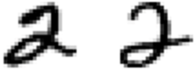
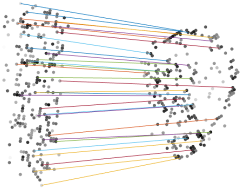
Motivation





Highlights

1. An algorithm that accurately compute Gromov-Wasserstein discrepancy for objects in embedded in low dimensional spaces
2. We prove that the proposed algorithm converges to a global optimal solution.
3. We show that the algorithm produces an optimality certificate in each iteration, in the form of upper- and lower bounds, which informs us of the potential suboptimality if the algorithm is terminated early.

The discrete Gromov-Wasserstein[1] distance ($p = 2$)

$$\min_{\Gamma \in P} \frac{1}{2} \sum_{i,i',j,j'=1}^{n} (d_{\mathcal{X}}(x_i, x_{i'}) - d_{\mathcal{Y}}(y_j, y_{j'}))^2 \Gamma_{i,j} \Gamma_{i',j'}$$

P the set of permutation matrices

$$\min_{\Gamma \in P} \quad -\langle C_x \Gamma, \Gamma C_y \rangle + \frac{1}{2}(\langle C_x, C_x \rangle + \langle C_y, C_y \rangle)$$

$$C_x = [d_{\mathcal{X}}(x_i, x_{i'})]_{i,i'=1}^{n}, C_y = [d_{\mathcal{Y}}(y_j, y_{j'})]_{j,j'=1}^{n}$$

[1] Mémoli, Facundu. "Gromov–Wasserstein Distances and the Metric Approach to Object Matching." Found Comput Math (2011) 11:417–487

Low rank Gromov-Wasserstein discrepancy and QAP

Discrepancy as squared Euclidean distance

$$x_i \in \mathbb{R}^{\ell_x}, y_j \in \mathbb{R}^{\ell_y}, X = \begin{pmatrix} x_1 & x_2 & \dots & x_n \end{pmatrix}, Y = \begin{pmatrix} y_1 & y_2 & \dots & y_n \end{pmatrix}$$
$$C_x = (\|x_i - x_j\|_2^2)_{i,j=1}^n = \mathbf{1} m_x^T - 2X^T X + m_x \mathbf{1}^T,$$
$$C_y = (\|y_i - y_j\|_2^2)_{i,j=1}^n = \mathbf{1} m_y^T - 2Y^T Y + m_y \mathbf{1}^T$$

where $m_x = (\|x_1\|^2, \|x_2\|^2, \dots, \|x_n\|^2)^T$, $m_y = (\|y_1\|^2, \|y_2\|^2, \dots, \|y_n\|^2)^T$ then

$$\langle C_x \Gamma, \Gamma C_y \rangle = \langle 2X\Gamma Y^T, 2X\Gamma Y^T \rangle + \langle L, \Gamma \rangle + 2\mathbf{1}^T m_y \mathbf{1}^T m_x,$$

where $L = 2n m_x m_y^T - 4 m_x \mathbf{1}^T Y^T Y - 4 X^T X \mathbf{1} m_y^T$.

$$\min_{\Gamma \in P} \quad -\|2X\Gamma Y^T\|_F^2 - \langle L, \Gamma \rangle + c_0 \tag{1}$$

Relaxation in two steps

Compact set of doubly stochastic matrices

$$\min_{\Gamma \in \overline{P}} \quad -\|2X\Gamma Y^T\|_F^2 - \langle L, \Gamma \rangle + c_0, \tag{2}$$

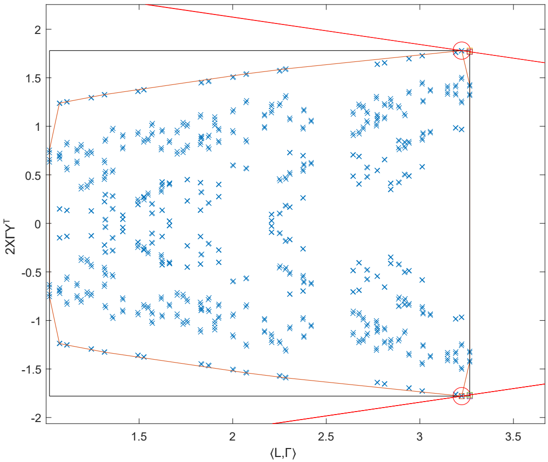
$\overline{P}$ the set of doubly stochastic matrices

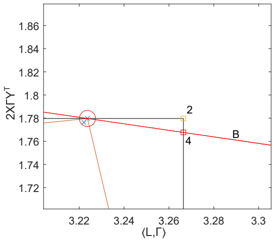
Approximation using a set linear constraints

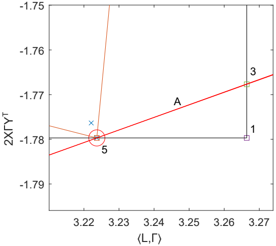
$$\min_{W \in \mathbb{R}^{\ell_x \times \ell_y}, w \in \mathbb{R}} \quad -\|W\|_F^2 - w + c_0 \tag{3a}$$

$$\text{subject to} \quad \langle Z_r, W \rangle + \alpha_r w \leq \beta_r, \quad \text{for} \quad r = 1, \dots, N. \tag{3b}$$

Procedure





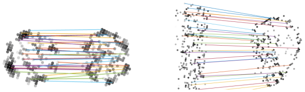


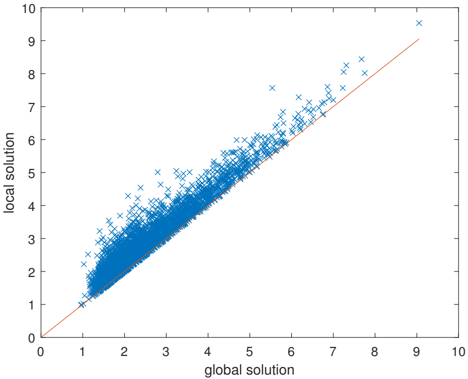
Numerical results

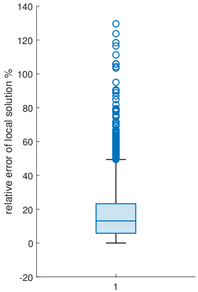
Type	n	ℓ_x, ℓ_y	Rel. error	Proposed [s] Extreme point / B&B	MILP1 [s] [2]	(2) B&B [s]
$\mathcal{U}$	10	2,2	10^{-8}	0.14 (0.07-0.3) / 21 (6-47)	39 (11-58)	0.15 (0.14-0.16)
$\mathcal{U}$	100	2,2	10^{-8}	0.48 (0.3-0.7) / 86 (52-107)	-	25 (19-39)
$\mathcal{U}$	500	2,2	10^{-8}	11 (9-16) / 408 (269-511)	-	-
$\mathcal{U}$	1000	2,2	10^{-8}	69 (54-85) / 576 (389-1059)	-	-
$\mathcal{U}$	2000	2,2	10^{-8}	460 (313-653) / -	-	-
$\mathcal{U}$	10	2,3	10^{-8}	1.8 (1.2-2.4) / 133 (45-296)	105 (49-147)	2.4(1.8-3.4)
$\mathcal{U}$	100	2,3	10^{-8}	278 (99-813) / -	-	172 (133-221)
$\mathcal{U}$	500	2,3	10^{-8}	9568 / -	-	-
$\mathcal{N}_1$	10	2,3	10^{-8}	0.51 (0.39-0.65) / 708 (233-1184)	146 (66-227)	3 (2.6-4.0)
$\mathcal{N}_1$	100	2,3	10^{-8}	86 (20-275) / -	-	95 (73-116)
$\mathcal{N}_1$	500	2,3	10^{-5}	5310!/ -	-	-
$\mathcal{N}_2$	10	3,3	10^{-2}	1.8 (0.7-3.2) / 142 (73-210)	117 (71-163)	0.2(0.1-0.3)
$\mathcal{N}_2$	100	3,3	10^{-2}	36 (22-55)/ -	-	45(36-65)
$\mathcal{N}_2$	500	3,3	10^{-2}	436 (228-862) / -	-	-
$\mathcal{N}_3$	10	3,3	10^{-2}	1.2 (0.5-2.3) / 22 (11-43)	72 (43-94)	0.2(0.1-0.3)
$\mathcal{N}_3$	100	3,3	10^{-2}	7 (5-8)/ 91 (76-111)	-	10 (9-12)
$\mathcal{N}_3$	2000	3,3	10^{-2}	93 (91-100) / 578 (429-691)	-	-

[2] Wang, Yang, et al. "The Rank-One Quadratic Assignment Problem." INFORMS Journal on Computing 33.3 (2021): 979-996.

Comparison with local search[3]







[3] Peyré, Gabriel, Marco Cuturi, and Justin Solomon. "Gromov-wasserstein averaging of kernel and distance matrices." International conference on machine learning. PMLR, 2016.

Thanks!