Efficient Algorithm in Computing Wasserstein Barycenter

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Abstract

The Wasserstein barycenter is a fundamental concept for analyzing and visualizing high-dimensional data in many applications. Computing the Wasserstein barycenter involves two stages: computing the Wasserstein distance (Using Optimal transport), and computing the mean of a set of point sets under the Wasserstein distance metric. Optimal transport problems can be considered a special form of linear programming problem. In here, we propose an effective approach for computing the Optimal Transport using the interior point method. Also, extend this idea to detect the Wasserstein barycenter of a given set of probability distributions. Our proposed method is computationally efficient, as demonstrated by numerical results.

Research Background

- Optimal transport(OT) theory is recognized as a powerful tool in many applications, including computer vision, Image processing, Economy, Medical science, and Machine learning. The Wasserstein barycenter is an extremely useful extension of OT, providing a broad range of opportunities to use OT in real-world applications.
  - ✓ In image processing - Useful in image denoising and super-resolution [1].
  - ✓ Machine learning - Useful in unsupervised learning and clustering[2].
  - ✓ Medical Science - Brain Tumor Segmentation [3].
- During the last decade the Matrix Balancing idea is starting to use to solve OT problems. In [5] the author uses the Sinkhorn matrix balancing method to develop one algorithm for this problem.
- In Taiwan, Prof. Pengwen Chen[4] and Prof. Mei-Heng Yueh[3] are notable researchers who have made significant contributions to the theory and applications of optimal transport.

Contribution

By converting the original OT problem into a matrix balancing problem, we use Newton's method-based Matrix balancing method with the Interior point method to implement one fast algorithm to solve the OT problem and named it as SNNE algorithm. We have also created a sparse support version of SNNE for large-scale problems. Additionally, we have extended this idea to generate the Wasserstein barycenter of a set of data sets under the Wasserstein distance metric.

Problem Introduction

- Here we consider two unlabeled point-sets $\{p_i\}_{i=1}^m, \{q_i\}_{i=1}^n \in \mathbb{R}^l$.

The 2-Wasserstein Distance between p and q is defined by

$$\min_{X\in\Sigma_n}\langle C, X\rangle \quad ; \quad C_{i,j} = ||p_i - q_j||_2^2$$

where $\Sigma_n = \{X \in \mathbb{R}^{m\times n} : Xe_n = b_1, X^\top e_m = b_2| \quad b_1 \in \mathbb{R}^m, b_2 \in \mathbb{R}^n\}$
$e_{\{.\}} \in \mathbb{R}^{\{.\}}$ is a vector with all elements are equal to one.

- Then for a given point sets $q^{(t)}; t = 1, \cdots, d, d \in \mathbb{Z}_+,$ the 2-Wasserstein

Barycenter is defined as : $\min_p \sum_{i=1}^{d} \lambda_i (W_2(p, q^{(t)}))^2$

where $\lambda_i > 0$ represent the weights with satisfying $\sum_{i=1}^{d} \lambda_i = 1.$

The value of p describe the Barycenter point set with m points.
Here $W_2^2(p, q^{(t)})$ describe the Wasserstein Distance from the barycenter point set to each of the other point sets for each t.

Method and Algorithm

- Using the negative entropy function, the regularized problem with t>0,

$$\min_{X\in\Sigma_n}\{\langle C, X\rangle + t^{-1}\langle 1, X\odot \log X - X\rangle\}$$

- Introducing $Mx = b$ constraint to represent the $X \in \Sigma_n$ condition and generate Lagrangian function with multiplier ν:

$$\min_x\{\langle c, x\rangle + t^{-1}\langle 1, x\odot \log x - x\rangle\} - \langle \nu, Mx - b\rangle\} \text{ where } \quad x = Vec(X) \quad \& \quad c = Vec(C)$$

- After the gradient computation,

$$x = \exp(-t(c - M^\top \nu))$$

- The multiplier vector $\nu = [\nu_1; \nu_2]$ can be computed in matrix balancing of $\exp(-tC)$.

Algorithm ➡ SNNE

- ➢ Initialize $t = t_0$ and $\nu = \nu_0$, Repeat the process until $t = t_{max}$,
- ➢ Use Newton method based Matrix balancing to solve $\exp(-t(c - M^T\nu))$,
- ➢ Update multiplier vector ν,
- ➢ Update $t \to \mu t$; $\mu \in \mathbb{R}$.

Algorithm ➡ WB - SNNE

Input: Point-sets $\{q_i^{(t)}\}_{i=1}^{n_t}; t = 1, \cdots, d,$
Initial Barycenter point set p_0 with m points.
weight order λ_t.
for $k = 1 : iter$ **do**
  for $t = 1 : d$ **do**
    Step 01: Get one point set from $(q^{(t)})$
    Step 02: Form cost matrix $C(p, q^{(t)})$
    Step 03: Perform SNNE to solve $W_2^2(p, q^{(t)})$
  end for
  Step 06: Update Barycenter p using

$$p_i := \frac{\sum_{t=1}^d \lambda_t X_{i,:}^{(t)} q^{(t)}}{\sum_{t=1}^d \lambda_t X_{i,:}^{(t)} e_{n_t}} \quad \forall \quad i = 1, \cdots, n$$

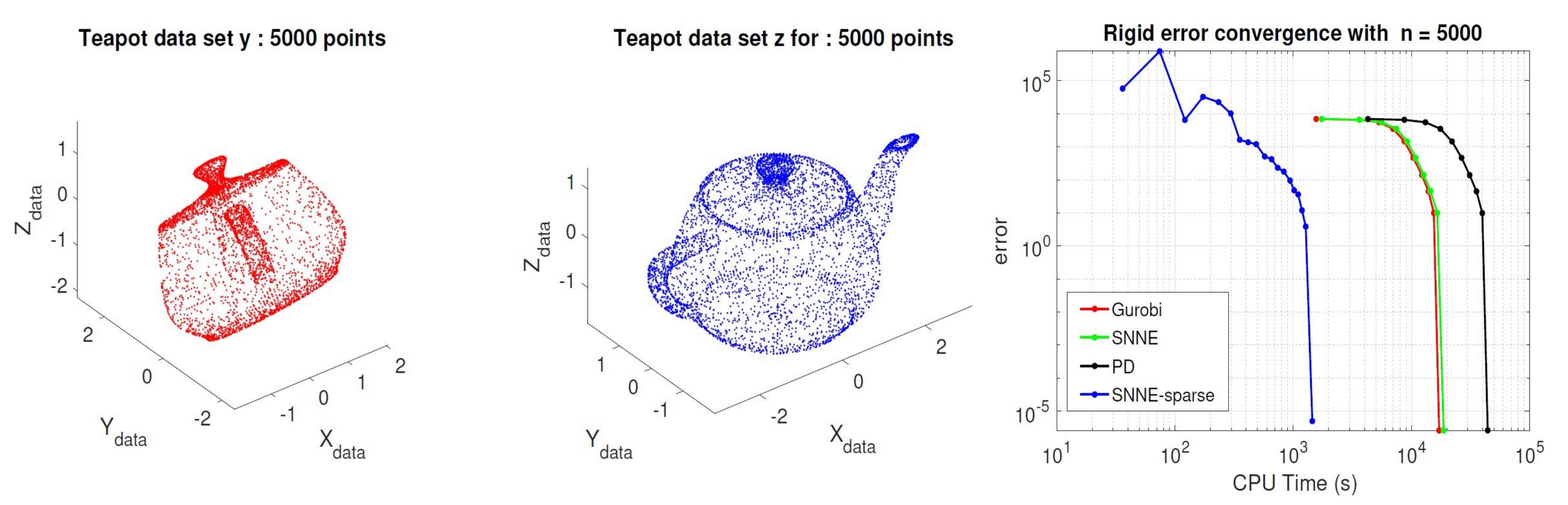
end for

Results and Discussion

➢ Rigid rotation reconstruct

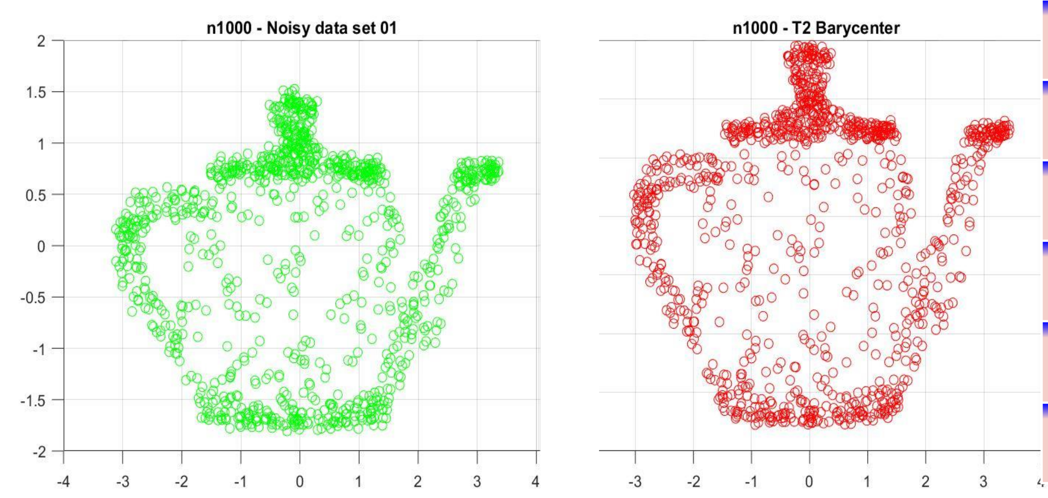
Consider a 3D teapot point set consisting of 5000 points(say y). Get one orthogonal matrix Q s.t. $z = Qy$. Then solve the following objective function to reconstruct the rotation.

$$\min_Q \min_x \{F(Q, x) = \langle c(Q), x\rangle + \eta||Q - I_3||_F^2\}$$



➢ Denoised experiment using Wasserstein barycenter.

Consider a five-teapot point set with the Gaussian noise. The target is to use the Wasserstein barycenter concept to obtain a denoised clear teapot.



Wasserstein Distance	
Teapots Data	Original Teapot
Noisy set 01	6.5536
Noisy set 02	6.4596
Noisy set 03	6.4595
Noisy set 04	6.3021
Noisy set 05	6.5841
Barycenter	1.8677

Conclusion

- We introduce the algorithm to compute the Wasserstein distance between two point sets and named SNNE.
- Then extend it to consider the problem of computing a Wasserstein barycenter for a set of 3D point sets.
- The numerical results illustrated the efficiency of our method.

References

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