Efficient Optimal Transport Computation with Medical Applications

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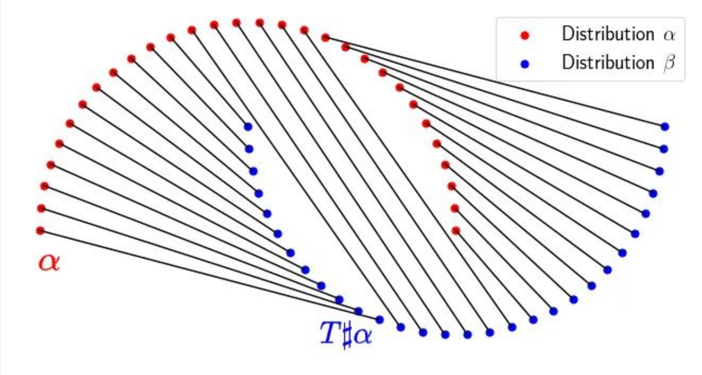
Optimal Transport

Given two distributions, optimal transport (OT) seeks to move mass of distribution $\boldsymbol{\alpha}$ to distribution $\boldsymbol{\beta}$ in a way that minimizes work (or cost).



More formally, in the case of 2-Wasserstein distance, we find a map $T : \mathbb{R}^n \to \mathbb{R}^n$ pushing $\boldsymbol{\alpha}$ to $\boldsymbol{\beta}$ such that $T_\sharp \alpha = \beta$ minimizes work.

$$W_2(\alpha, \beta)^2 := \min_T \int \|T(x) - x\|^2 \, d\alpha$$

Exact OT: Linear Program

$$\min_{\gamma \in \Pi(a,b)} \langle \gamma, \mathbf{C} \rangle_F$$

$$\text{s.t.} \quad \gamma \mathbf{1} = \mathbf{a}, \quad \gamma^T \mathbf{1} = \mathbf{b}, \quad \gamma \geq 0$$

a : Source
b: Target
C: Cost Matrix

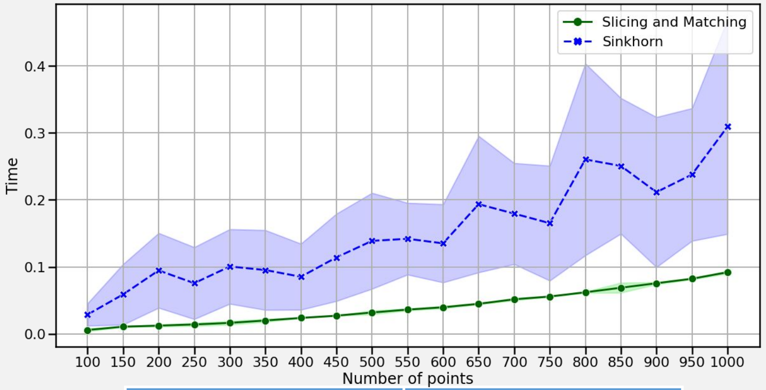
Solving this LP is costly! $O(n^3 log(n))$

Stochastic Slicing and Matching

Algorithm 1 Slicing and Matching

procedure PITIE_AVG(Source $X \in \mathbb{R}^{n \times d}$, Target $Y \in \mathbb{R}^{n \times d}$, K)
  for $k = 1$ to K **do**
    $t(k) \leftarrow \frac{k + log(k)}{k}$
    Sample random orthogonal matrix P ∼ Haar distribution
    $P \leftarrow [\vec{\theta_1}, \vec{\theta_2}, \ldots, \vec{\theta_d}]$
    Initialize C such that $C \in \mathbb{R}^{n \times d}$
    for $p = 1$ to d **do**
      $X\_proj \leftarrow X \cdot \vec{\theta_p}$
      $Y\_proj \leftarrow Y \cdot \vec{\theta_p}$
      Solve Optimal Transport in 1D between X_proj and Y_proj
      Find $\sigma = \sigma_{Y\_proj} \circ \sigma_{X\_proj^{-1}}$ (mapping from X_proj to Y_proj)
      $C_p \leftarrow [(1 - t(k)) \cdot X\_proj] + [(t(k)) \cdot Y\_proj \sharp \sigma]$
    end for
    Update $X \leftarrow P \cdot C$
  end for
end procedure

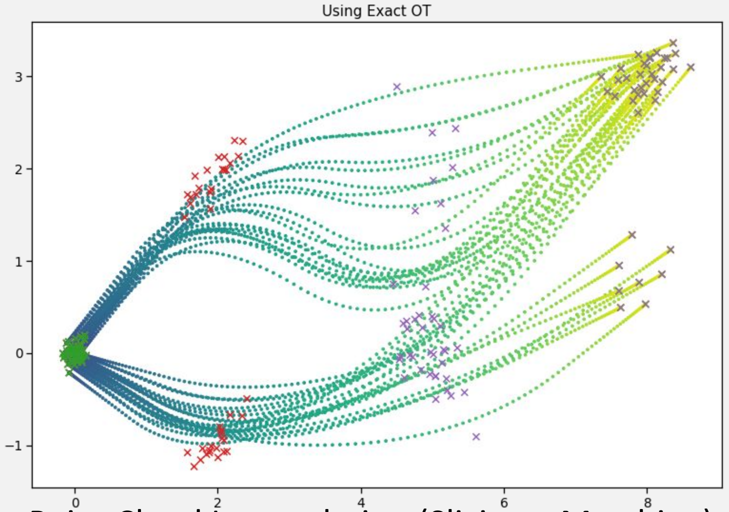
Runtime Comparisons



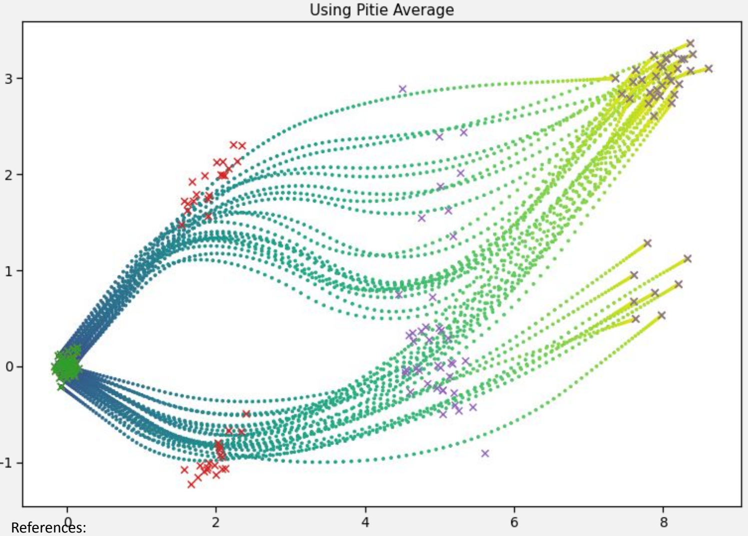
Method	Avg. Time (seconds)
Exact OT (LP)	16.427 ± 1.012
Sinkhorn + Ent. Reg.	0.1515 ± 0.077
Slicing + Matching	0.0407 ± 0.002

Preliminary Results and Future Work

Point Cloud Interpolation (Exact OT)



Point Cloud Interpolation (Slicing + Matching)



References:
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