Computational Optimal Transport

Stochastic Wasserstein Barycenters

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MATHÉMATIQUES
VISION
APPRENTISSAGE

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Overview

Problem statement

Article : Claici, Chien, and Solomon 2018, *Stochastic Wasserstein Barycenters*

- Compute the Wasserstein barycenter ν of a set of any probability measures $\{\mu_j\}_{j=1}^J$ defined of a metric space $(\mathcal{X}, d)$ with $\mathcal{X} \subset \mathcal{R}^D$
- Primal problem

$$\min_{\nu} \frac{1}{J} \sum_{j=1}^{J} W_2^2(\mu_j, \nu) \tag{1}$$

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- Compute the Wasserstein barycenter ν of a set of any probability measures $\{\mu_j\}_{j=1}^J$ defined of a metric space $(\mathcal{X}, d)$ with $\mathcal{X} \subset \mathcal{R}^D$
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$$\min_\nu \frac{1}{J} \sum_{j=1}^{J} W_2^2(\mu_j, \nu) \tag{1}$$

- Approximation of the barycenter

$$\hat{\nu} = \frac{1}{M} \sum_{i=1}^{M} \delta_{x_i}$$

with optimized support $\Sigma = \{x_i\}_{i=1}^M$

- **Problem.** Find a minimizer of (1) with $\Sigma \subset \mathcal{X}$ and $|\Sigma| = M$

Related Work and Applications ?

Overview

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   - Snap step
   - Theoretical and Empirical Convergence

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Proposed method

- Dual problem

$$F\left(\{\phi_j\}_{j=1}^{J}, \{x_i\}_{i=1}^{M}\right) = \frac{1}{J}\sum_{j=1}^{J} F_{dual}\left(\phi_j, \{x_i\}_{i=1}^{M}\right)$$

$$\begin{aligned} F_{dual}\left(\phi_j, \{x_i\}_{i=1}^{M}\right) &= \int_{\mathcal{X}} \phi_j(x)d\nu(x) + \int_{\mathcal{X}} \overline{\phi}_j(y)d\mu_j(y) \\ &= \frac{1}{M}\sum_{i=1}^{M} \phi_j(x_i) + \int_{\mathcal{X}} \overline{\phi}_j(y)d\mu_j(y) \end{aligned}$$

- **Stochastic Gradient Ascent** to optimize the potentials $\{\phi_j\}_{j=1}^{J}$ (*ascent step*)
- **Fixed point iteration** to optimize the positions $\{x_i\}_{i=1}^{M}$ (*snap step*)

Ascent step

Gradient $\frac{\partial F}{\partial \phi_j}$ depend on the terms

$$a_j^i = \int_{V_{\phi_j}^i} d\mu_j(y) = \mathbb{E}_{y\sim\mu_j}\left[\mathbf{1}_{y\in V_{\phi_j}^i}\right] \qquad b_j^i = \int_{V_{\phi_j}^i} y\, d\mu_j(y) = \mathbb{E}_{y\sim\mu_j}\left[y.\mathbf{1}_{y\in V_{\phi_j^i}}\right]$$

where $\mathbf{1}$ is the indicator function and the *power cell* $V_{\phi_j}^i$ of point x_i is

$$V_\phi^i = \{x \in \mathcal{X}, d(x, x_i)^2 - \phi_i \leq d(x, x_{i'})^2 - \phi_{i'}, \forall i'\}$$

where $d(x, y)^2 = \|x - y\|_2^2$.

Ascent step

Algorithm Ascent step

for $j = 1, \dots, J$ **do**
  $z^{(0)} \leftarrow 0$
  while $\left\| \frac{\widehat{\partial F}}{\partial \phi_j} \right\|_2^2 > \epsilon_{ascent}$ **do**
    Compute $\hat{a}_j^i$ by Monte Carlo approximation
    $z^{l+1} \leftarrow \beta z^{(l)} + \widehat{\partial_{\phi_j} F}(\phi_j)$ {Nesterov acceleration}
    $\phi_j^{(l+1)} \leftarrow \phi_j^{(l)} + \alpha z^{(l+1)}$
  end while
end for

We will use $\epsilon_{ascent} = 10^{-4}$ and set a maximum number of iterations for the while loop to $T_{max} = 1500$

And fix $\alpha = 0.05$ and $\beta = 0.99$ like in (Claici, Chien, and Solomon 2018)

Snap step

The update of the point $\{x_i\}$ is given by

$$\frac{\partial F}{\partial x_i} = 0 \implies x_i = \frac{\sum_{j=1}^{J} b_j^i}{\sum_{j=1}^{J} a_j^i}$$

Intuition :

$$\frac{\partial F_{dual}}{\partial \phi_j^i} = \frac{1}{M} - \int_{V_{\phi_j}^i} d\mu_j(y) = 0$$

→ Each cell V_ϕ^i contains as much mass as its associated source point x_i

→ the fixed point iteration moves each point to the center of its power cell.

Ascent Snap algorithm

Algorithm Ascent and Snap algorithm for computing Stochastic Wasserstein Barycenters

```
for t = 1, ..., T do
    Update {φ_j} with algorithm {Ascent step}
    Compute b̂_j^i by Monte Carlo approximation
    for x_i ∈ Σ do
        x_i ← (Σ_{j=1}^J b̂_j^i) / (Σ_{j=1}^J â_j^i)   {Snap step}
    end for
end for
return Opitimized barycenter support Σ* = {x_i}_{i=1}^M
```

$$x_i \leftarrow \frac{\sum_{j=1}^{J} \hat{b}_j^i}{\sum_{j=1}^{J} \hat{a}_j^i}$$

Assumptions

- At least one of the input distribution μ_j is absolutely continuous with respect to the Lebesgue measure.
- The domain $\mathcal{X}$ is a compact subset of the Euclidean space $\mathbb{R}^d$.

Garantees

- The global minimizer of (1) efficiently approximate the true barycenter as $M \to \infty$
- No garantee of convergence toward ν_M^*
- The ascent snap algorithm converges to a local minimum
- Algorithm monotonically $\searrow F_{primal}$ (1)
- The support of the estimated barycenter is empirically demonstrated to be contained within the support of the true barycenter
- Empirical evidences $\implies$ convergence even in cases where these assumptions are not met

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Experiment 1

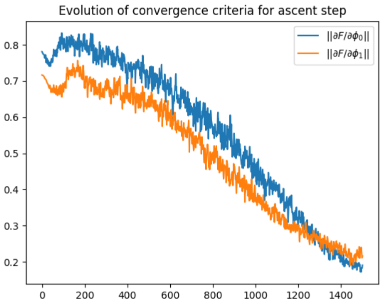
Experiment 2

Computation time

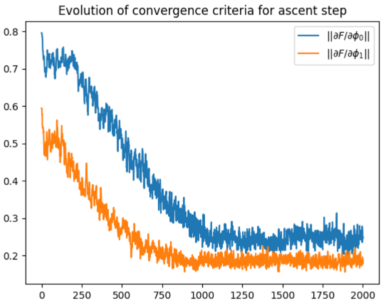
Experiment	McCann	Iterative Bregman	POT free support	Ascent Snap
1D skewnorm	0.02 ± 0.01	0.22 ± 0.02	0.74 ± 0.28	7814.27 ± 0.37
2D discrete	-	2.18 ± 0.34	0.38 ± 0.30	16351.66 ± 0.23

Table: Computation time (in seconds) for the different methods

Ascent step convergence



(a) Two 1D continuous distributions



(b) Two 2D discrete distributions

Figure: Evolution of $\left\| \frac{\partial F}{\partial \phi_j} \right\|$ during the ascent step for each experiment. In the x-axis, is the number of interations of the while loop.

Experiment	Ascent step	Snap step
1D skewnorm	8309.44 ± 0.33	5.28 ± 0.23
2D discrete	11938.70 ± 0.34	9.81 ± 0.34

Table: Computation time (in seconds) for each step of the Algorithm **??**. The experiences are repeated 3 times.

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References I

Claici, Sebastian, Edward Chien, and Justin Solomon (June 6, 2018). *Stochastic Wasserstein Barycenters*. arXiv: 1802.05757[cs,math,stat]. URL: http://arxiv.org/abs/1802.05757 (visited on 12/21/2023).