On the Complexity of Approximating Wasserstein Barycenter

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Abstract

We study the complexity of approximating Wassertein barycenter of m discrete measures, or histograms of size n by contrasting two alternative approaches, both using entropic regularization. The first approach is based on the Iterative Bregman Projections (IBP) algorithm for which our novel analysis gives a complexity bound proportional to $\frac{mn^2}{\varepsilon^2}$ to approximate the original non-regularized barycenter. Using an alternative accelerated-gradient-descent-based approach, we obtain a complexity proportional to $\frac{mn^{2.5}}{\varepsilon}$. As a byproduct, we show that the regularization parameter in both approaches has to be proportional to ε, which causes instability of both algorithms when the desired accuracy is high. To overcome this issue, we propose a novel proximal-IBP algorithm, which can be seen as a proximal gradient method, which uses IBP on each iteration to make a proximal step. We also consider the question of scalability of these algorithms using approaches from distributed optimization and show that the first algorithm can be implemented in a centralized distributed setting (master/slave), while the second one is amenable to a more general decentralized distributed setting with an arbitrary network topology.

Keywords: Optimal transport, Wasserstein barycenter, Sinkhorn's algorithm, Accelerated Gradient Descent, distributed optimization
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Introduction

Optimal transport (OT) Monge [1781], Kantorovich [1942] is currently generating an increasing attraction in statistics, machine learning and optimization communities. Statistical procedures based on optimal transport are available Bigot et al. [2012], Del Barrio et al. [2015], Ebert et al. [2017], Le Gouic and Loubes [2017] as well as many applications in different areas of machine learning including unsupervised learning Arjovsky et al. [2017], Bigot et al. [2017], semi-supervised learning Solomon et al. [2014], clustering Ho et al. [2017], text classification Kusner et al. [2015]. Optimal transport distances lead to the concept of Wasserstein barycenter, which allows to define a mean of a set of complex objects, e.g. images, preserving their geometric structure Cuturi and Doucet [2014]. In this paper we focus on the computational aspects of optimal transport, namely on approximating Wasserstein barycenter of a set of histograms.

Starting with Altschuler et al. [2017], several groups of authors addressed the question of Wasserstein distance approximation complexity Chakrabarty and Khanna [2018], Dvurechensky et al. [2018b], Blanchet et al. [2018], Lin et al. [2019]. Implementable schemes are based on Sinkhorn's algorithm, which was first applied to OT in Cuturi [2013], and accelerated gradient descent proposed as an alternative in Dvurechensky et al. [2018b]. Much less is known about the complexity of approximating Wasserstein *barycenter*. The works Staib et al. [2017], Uribe et al. [2018], Dvurechensky et al. [2018a], are in some sense close, but do not provide an explicit answer. Following Genevay et al. [2016], Staib et al. [2017] use stochastic gradient descent and estimate the convergence rate of their algorithm. From their rate, one can obtain the iteration complexity $\frac{\kappa R^2}{\varepsilon^2}$ to achieve accuracy ε in approximation of the barycenter, where κ is some constant depending on the problem data, i.e. transportation cost matrices, R is some distance characterizing the solution of the dual problem. Dvurechensky et al. [2018a] consider regularized barycenter, but do not show, how to choose the regularization parameter to achieve ε-accuracy.

Following Dvurechensky et al. [2018b], we study two alternative approaches for approximating Wasserstein barycenter based on entropic regularization Cuturi [2013]. The first approach is based on Iterative Bregman Projection (IBP) algorithm Benamou et al. [2015], which can be considered as a general alternating projections algorithm and also as a generalization of the Sinkhorn's algorithm Sinkhorn [1974]. The second approach is based on constructing a dual problem and solving it by primal-dual accelerated gradient descent. For both approaches, we show, how the regularization parameter should be chosen in order to approximate the original, non-regularized barycenter. A kind of mixed approach, namely an accelerated Iterative Bregman Projection algorithm was proposed in Guminov et al. [2019].

We also address the question of scalability of computations in the Big Data regime, i.e. the size of histograms n and the number of histograms m are large. In this case the dataset of n histograms can be distributedly produced or stored in a network of agents/sensors/computers with the network structure given by an arbitrary connected graph. In a special case of centralized architecture, i.e. if there is a central "master" node surrounded by "slave" nodes, parallel algorithms such as Staib et al. [2017] can be applied. In a more general setup of arbitrary networks it makes sense to use decentralized distributed algorithms in the spirit of

distributed optimization algorithms Nedić et al. [2017], Scaman et al. [2017].

Related Work

It is very hard to cover all the increasing stream of works on OT and we mention these books Villani [2008], Santambrogio [2015], Peyré and Cuturi [2018] as a starting point and the references therein. Approximation of Wasserstein barycenter was considered in Cuturi and Doucet [2014], Bonneel et al. [2015], Benamou et al. [2015], Staib et al. [2017], Puccetti et al. [2018], Claici et al. [2018], Uribe et al. [2018], Dvurechensky et al. [2018a] using different techniques as Sinkhorn-type algorithm, first-order methods, Newton-type methods. Considering the primal-dual approach based on accelerated gradient descent, our paper shares some similarities with Cuturi and Peyré [2016] with the main difference that we are focused on complexity and scalability of computations and explicitly analyze the algorithm applied to the dual problem.

There is a vast amount of literature on accelerated gradient descent with the canonical reference being Nesterov [1983]. Primal-dual extensions can be found in Lan et al. [2011], Tran-Dinh et al. [2018], Yurtsever et al. [2015], Chernov et al. [2016], Dvurechensky et al. [2016, 2017], Anikin et al. [2017], Nesterov et al. [2018], Lin et al. [2019]. We are focused on the extensions amenable to the decentralized distributed optimization, so that these algorithms can be scaled for large problems.

Distributed optimization algorithms were considered by many authors with the classical reference being Bertsekas and Tsitsiklis [1989]. Initial algorithms, such as Distributed Gradient Descent Nedic and Ozdaglar [2009], were relatively slow compared with their centralized counterparts. However, recent work has made significant advances towards a better understanding of the optimal rates of such algorithms and their explicit dependencies to the function and network parameters Lan et al. [2017], Scaman et al. [2017], Uribe et al. [2018]. These approaches has been extended to other scenarios such as time-varying graphs Rogozin et al. [2018], Maros and Jaldén [2018], Wu and Lu [2017]. The distributed setup is particularly interesting for machine learning applications on the big data regime, where the number of data points and the dimensionality is large, due to its flexibility to handle intrinsically distributed storage and limited communication, as well as privacy constraints He et al. [2018], Wai et al. [2018].

Our contributions

- We consider γ-regularized Wasserstein barycenter problem and obtain complexity bounds for finding an approximation to the regularized barycenter by two algorithms. The first one is Iterative Bregman Projections algorithm Benamou et al. [2015], for which we prove complexity proportional to $\frac{1}{\gamma\varepsilon}$ to achieve accuracy ε. The second one is based on accelerated gradient descent (AGD) and has complexity proportional to $\sqrt{\frac{n}{\gamma\varepsilon}}$. The benefit of the second algorithm is that it is better scalable and can be implemented in the decentralized distributed optimization setting over an arbitrary network.

- We show, how to choose the regularization parameter in order to find an ε-approximation for the non-regularized Wasserstein barycenter and find the resulting complexity for IBP to be proportional to $\frac{mn^2}{\varepsilon^2}$ and for AGD to be proportional to $\frac{mn^{2.5}}{\varepsilon}$.
- As we can see from the complexity bounds for IBP and AGD, they depend on the regularization parameter γ quite badly regarding that this parameter has to be small. To overcome this drawback we propose a proximal-IBP method, which can be considered as a proximal method using IBP on each iteration to find the next iterate.

1 Problem Statement and Preliminaries

1.1 Notation

We define the probability simplex as $S_n(1) = \{q \in \mathbb{R}^n_+ \mid \sum_{i=1}^n q_i = 1\}$. Given two discrete measures p and q from $S_n(1)$ we introduce the set of their coupling measures as

$$\Pi(p,q) = \{\pi \in \mathbb{R}^{n\times n}_+ : \pi\mathbb{1} = p, \pi^T\mathbb{1} = q\}.$$

For coupling measure $\pi \in \mathbb{R}^{n\times n}_+$ we denote the negative entropy (up to an additive constant) as

$$H(\pi) := \sum_{i,j=1}^{n} \pi_{ij}\left(\ln \pi_{ij} - 1\right) = \langle \pi, \ln \pi - \mathbb{1}\mathbb{1}^T\rangle.$$

Here and further by $\ln(A)$ $(\exp(A))$ we denote the element-wise logarithm (exponent) of matrix or vector A, and $\langle A, B\rangle := \sum_{i,j=1}^n A_{ij}B_{ij}$ for any $A, B \in \mathbb{R}^{n\times n}$. For two matrices A B we also define element-wise multiplication and element-wise division as $A \odot B$ and $\frac{A}{B}$ respectively. Kullback-Leibler divergence for measures $\pi, \pi' \in \mathbb{R}^{n\times n}_+$ is defined as the Bregman divergence associated with $H(\cdot)$:

$$KL(\pi|\pi') := \sum_{i,j=1}^{n} \left(\pi_{ij}\ln\left(\frac{\pi_{ij}}{\pi'_{ij}}\right) - \pi_{ij} + \pi'_{ij}\right) = \langle \pi, \ln\pi - \ln\pi'\rangle + \langle \pi' - \pi, \mathbb{1}\mathbb{1}^T\rangle.$$

We also define a symmetric cost matrix $C \in \mathbb{R}^{n\times n}_+$, which element c_{ij} corresponds to the cost of moving bin i to bin j. $\|C\|_\infty$ denotes the maximal element of this matrix.

We refer to $\lambda_{\max}(W)$ as the maximum eigenvalue of a symmetric matrix W, and $\lambda^+_{\min}(W)$ as the minimal non-zero eigenvalue, and define the condition number of matrix W as $\chi(W)$. We use symbol $\mathbb{1}$ as a column of ones.

1.2 Wasserstein barycenters and entropic regularization

Given two probability measures $p, q \in S_n(1)$ and a cost matrix $C \in \mathbb{R}^{n\times n}$ we define optimal transportation distance between them as

$$\mathcal{W}(p,q) := \min_{\pi\in\Pi(p,q)} \langle \pi, C\rangle. \tag{1}$$

For a given set of probability measures $\{p_1, \ldots, p_m\}$ and cost matrices $C_1, \ldots, C_m \in \mathbb{R}_+^{n \times n}$ we define their weighted barycenter with weights $w \in S_n(1)$ as a solution of the following convex optimization problem:

$$\min_{q \in S_n(1)} \sum_{l=1}^{m} w_l \mathcal{W}(p_l, q), \tag{2}$$

where $w_l \geq 0$, $l = 1, ..., m$ and

$$\sum_{l=1}^{m} w_l = 1.$$

We use c to denote $\max_{l=1,\ldots,m} \|C_l\|_\infty$. Using entropic regularization proposed in Cuturi [2013] we define regularized OT-distance for $\gamma \geq 0$:

$$\mathcal{W}_\gamma(p, q) := \min_{\pi \in \Pi(p,q)} \{\langle \pi, C \rangle + \gamma H(\pi)\}. \tag{3}$$

Respectively, one can consider regularized barycenter that is a solution of the following problem:

$$\min_{q \in S_n(1)} \sum_{l=1}^{m} w_l \mathcal{W}_\gamma(p_l, q). \tag{4}$$

2 Complexity of WB by Iterative Bregman Projections

In this section we provide theoretical analysis of the Iterative Bregman Projections algorithm Benamou et al. [2015] for regularized Wasserstein barycenter and obtain iteration complexity $O\left(\frac{c}{\gamma\varepsilon}\right)$ with $c := \max_{l=1,\ldots,m} \|C_l\|_\infty$. Then we estimate the bias itroduced by regularization and estimate the value of γ to obtain an ε-approximation for the non-regularized barycenter. Combining this result with the iteration complexity of IBP, we obtain complexity $\widetilde{O}\left(\frac{c^2 m n^2}{\varepsilon^2}\right)$ for approximating non-regularized barycenter by the IBP algorithm. This algorithm can be implemented in a centralized distributed manner such that each node performs $\widetilde{O}\left(\frac{c^2 n^2}{\varepsilon^2}\right)$ arithmetic operations and the number of communication rounds is $\widetilde{O}\left(\frac{c^2}{\varepsilon^2}\right)$.

2.1 Convergence of IBP for regularized barycenter

In this subsection we analyze Iterative Bregman Projection Algorithm [Benamou et al., 2015, Section 3.2] and analyze its complexity for solving problem (4). We slightly reformulate this

problem as

$$\min_{q\in S_n(1)} \sum_{l=1}^{m} w_l \mathcal{W}_\gamma(p_l, q) = \min_{\substack{q\in S_n(1),\\ \pi_l\in\Pi(p_l,q),\\ l=1,\dots,m}} \sum_{l=1}^{m} w_l \big\{ \langle \pi_l, C_l\rangle + \gamma H(\pi_l)\big\}$$

$$= \min_{\substack{\pi_l\in\mathbb{R}_+^{n\times n}\\ \pi_l\mathbb{1}=p_l,\, \pi_l^T\mathbb{1}=\pi_{l+1}^T\mathbb{1},\\ l=1,\dots,m}} \sum_{l=1}^{m} w_l \big\{ \langle \pi_l, C_l\rangle + \gamma H(\pi_l)\big\} \tag{5}$$

and construct its dual (see the details below). To solve the dual problem we reformulate the IBP algorithm as Algorithm 1[1]. Notably, our reformulation of the IBP algorithm allows to solve simultaneously the primal and dual problem and has an adaptive stopping criterion (see line 7), which does not require to calculate any objective values.

Algorithm 1 Dual Iterative Bregman Projection

Input: $C_1, \dots, C_m$, $p_1, \dots, p_m$, $\gamma > 0$, $\varepsilon' > 0$

1: $u_l^0 := 0$, $v_l^0 := 0$, $K_l := \exp\left(-\frac{C_l}{\gamma}\right)$, $l = 1, \dots, m$
2: **repeat**
3: $\quad v_l^{t+1} := \sum_{k=1}^m w_k \ln K_k^T e^{u_k^t} - \ln K_l^T e^{u_l^t}, \quad \mathtt{u}^{t+1} := \mathtt{u}^t$
4: $\quad t := t + 1$
5: $\quad u_l^{t+1} := \ln p_l - \ln K_l e^{v_l^t}, \quad \mathtt{v}^{t+1} := \mathtt{v}^t$
6: $\quad t := t + 1$
7: **until** $\sum_{l=1}^m w_l \left\| B_l^T(u_l^t, v_l^t)\mathbb{1} - \bar{q}^t \right\|_1 \le \varepsilon'$, where $B_l(u_l, v_l) = \operatorname{diag}(e^{u_l}) K_l \operatorname{diag}(e^{v_l})$, $\bar{q}^t := \sum_{l=1}^m w_l B_l^T(u_l^t, v_l^t)\mathbb{1}$

Output: $B_1(u_1^t, v_1^t), \dots, B_m(u_m^t, v_m^t)$

Before we move to the analysis of the algorithm let us discuss the scalability of this algorithm by using centralized distributed computations framework. This framework includes a master and slave nodes. Each l-th slave node stores data p_l, C_l, K_l and variables u_l^t, v_l^t. On each iteration t, it calculates $K_l^T e^{u_l^t}$ and sends it to the master node, which aggregates these products to the sum $\sum_{k=1}^m w_k \ln K_k^T e^{u_k^t}$ and sends this sum back to the slave nodes. Based on this information, slave nodes update v_l^t and u_l^t. So, the main computational cost of multiplying a matrix by a vector, can be distributed on m slave nodes and the total working time will be smaller. It is not clear, how this algorithm can be implemented on a general network, for example when the data is produced by a distributed network of sensors without one master

[1] In the original paper Benamou et al. [2015] there were misprints in description of IBP. Correct author's variant can be found in `https://github.com/gpeyre/2014-SISC-BregmanOT`. In Algorithm 1 we use different denotations. First of all, our u corresponds to $\ln v$ from Benamou et al. [2015] and our v corresponds to $\ln u$ from Benamou et al. [2015]. Secondly, our transport plan matrix equals to transpose transport plan matrix from Benamou et al. [2015]. Thirdly, we build a little bit different dual problem, by introducing additional constraint $\sum_{l=1}^m w_l v_l = 0$, see Lemma 1. This allows us to simplify calculations in line 3 of Algorithm 1.

node. In contrast, as we illustrate in Section 3, the alternative accelerated-gradient-based approach can be implemented on an arbitrary network.

Theorem 1. *For given ε' Algorithm 1 stops in number of iterations N satisfying*

$$N \leq 4 + \frac{44R_v}{\varepsilon'} = O\left(\frac{\max_l \|C_l\|_\infty}{\gamma\varepsilon'}\right).$$

It returns $B_1, \ldots, B_m$ s.t.

$$\sum_{l=1}^{m} w_l \|B_l\mathbb{1} - \bar{q}\|_1 \leq \varepsilon', \quad \bar{q} = \sum_{l=1}^{m} w_l B_l \mathbb{1},$$

and

$$\sum_{l=1}^{m} w_l \left(\langle C_l, B_l\rangle + \gamma H(B_l)\right) - \sum_{l=1}^{m} w_l \left(\left\langle C_l, \pi^*_{\gamma,l}\right\rangle + \gamma H(\pi^*_{\gamma,l})\right) \leq \max_l \|C_l\|_\infty \varepsilon', \tag{6}$$

where $\boldsymbol{\pi}^*_\gamma = [\pi^*_{\gamma,1}, \ldots, \pi^*_{\gamma,m}]$ is a solution of problem (5).

Our first step is to recall the IBP algorithm from Benamou et al. [2015], formulate the dual problem for (5) and show that our Algorithm 1 solves this dual problem and is equivalent to the IBP algorithm.

Following the approach from Benamou et al. [2015] we present the problem (5) in a Kullback–Leibler projection form.

$$\min_{\boldsymbol{\pi} \in \mathcal{C}_1 \cap \mathcal{C}_2} \sum_{l=1}^{m} w_l KL\left(\pi_l | \theta_l\right), \tag{7}$$

for $\theta_l = \exp\left(-\frac{C_l}{\gamma}\right)$ and the following affine convex sets $\mathcal{C}_1$ and $\mathcal{C}_2$

$$\begin{aligned} \mathcal{C}_1 &= \left\{\boldsymbol{\pi} = [\pi_1, \ldots, \pi_m] : \forall l \ \pi_l \mathbb{1} = p_l\right\}, \\ \mathcal{C}_2 &= \left\{\boldsymbol{\pi} = [\pi_1, \ldots, \pi_m] : \exists q \in S_n(1) \ \forall l \ \pi_l^T \mathbb{1} = q\right\}. \end{aligned} \tag{8}$$

Algorithm 2 introduced in Benamou et al. [2015] consists in alternating projections to sets $\mathcal{C}_1$ and $\mathcal{C}_2$ w.r.t. Kullback–Leibler divergence, and is a generalization of Sinkhorn's algorithm and a particular case of Dykstra's projection algorithm.

Algorithm 2 Iterative Bregman Projections, see Benamou et al. [2015]

Input: Cost matrices $C_1, \dots, C_m$, probability measures $p_1, \dots, p_m$, $\gamma > 0$, starting transport plans $\{\pi_l^0\}_{l=1}^m : \pi_l^0 := \exp\left(-\frac{C_l}{\gamma}\right)$, $l = 1, \dots, m$

1: **repeat**
2: **if** $t \bmod 2 = 0$ **then**
3: $\boldsymbol{\pi}^{t+1} := \underset{\boldsymbol{\pi} \in \mathcal{C}_1}{\operatorname{argmin}} \sum_{l=1}^m w_l KL\left(\pi_l | \pi_l^t\right)$
4: **else**
5: $\boldsymbol{\pi}^{t+1} := \underset{\boldsymbol{\pi} \in \mathcal{C}_2}{\operatorname{argmin}} \sum_{l=1}^m w_l KL\left(\pi_l | \pi_l^t\right)$
6: **end if**
7: $t := t + 1$
8: **until** Converge

Output: $\boldsymbol{\pi}^t$

As we will show below, this algorithm is equivalent to alternating minimization in dual problem of (5) presented in the next lemma.

Lemma 1. *The dual problem of* (5) *is (up to a multiplicative constant)*

$$\min_{\substack{\mathtt{u},\mathtt{v} \\ \sum_l w_l v_l = 0}} f(\mathtt{u}, \mathtt{v}) \quad \textit{where} \quad f(\mathtt{u}, \mathtt{v}) := \sum_{l=1}^m w_l \big\{ \langle \mathbb{1}, B_l(u_l, v_l)\mathbb{1} \rangle - \langle u_l, p_l \rangle \big\}, \tag{9}$$

$\mathtt{u} = [u_1, \dots, u_m]$, $\mathtt{v} = [v_1, \dots, v_m]$, $u_l, v_l \in \mathbb{R}^n$, *and*

$$B_l(u_l, v_l) := \operatorname{diag}\left(e^{u_l}\right) K_l \operatorname{diag}\left(e^{v_l}\right), \quad K_l := \exp\left(-\frac{C_l}{\gamma}\right). \tag{10}$$

Moreover, solution $\boldsymbol{\pi}_\gamma^*$ *to* (5) *is given by the formula*

$$[\boldsymbol{\pi}_\gamma^*]_l = B_l(u_l^*, v_l^*), \tag{11}$$

where $(\mathtt{u}^*, \mathtt{v}^*)$ *is a solution to the problem* (9).

Proof. The Lagrangian for (5) is equal to

$$\begin{aligned} L(\boldsymbol{\pi}; \boldsymbol{\lambda}, \boldsymbol{\mu}) &= \sum_{l=1}^m w_l \big\{ \langle \pi_l, C_l \rangle + \gamma H(\pi_l) \big\} + \sum_{l=1}^m \langle \lambda_l, \pi_l \mathbb{1} - p_l \rangle + \sum_{l=1}^m \langle \mu_l, \pi_{l+1}^T \mathbb{1} - \pi_l^T \mathbb{1} \rangle \\ &= \sum_{l=1}^m \left[w_l \big\{ \langle \pi_l, C_l \rangle + \gamma \langle \pi_l, \ln \pi_l - \mathbb{1}\mathbb{1}^T \rangle \big\} + \langle \lambda_l, \pi_l \mathbb{1} - p_l \rangle + \langle \mu_{l-1} - \mu_l, \pi_l^T \mathbb{1} \rangle \right], \end{aligned}$$

where $\boldsymbol{\lambda} = [\lambda_1, \dots, \lambda_m]$, $\boldsymbol{\mu} = [\mu_1, \dots, \mu_m]$, $\lambda_l, \mu_l \in \mathbb{R}^n$ with convention $\mu_0 \equiv \mu_m \equiv 0$. Using the change of variables $u_l := -\lambda_l / (w_l \gamma)$ and $v_l := (\mu_l - \mu_{l-1}) / (w_l \gamma)$ we obtain

$$L(\boldsymbol{\pi}; \mathtt{u}, \mathtt{v}) = \gamma \sum_{l=1}^m w_l \left\{ \left\langle \pi_l, \frac{C_l}{\gamma} + \ln \pi_l - \mathbb{1}\mathbb{1}^T - u_l \mathbb{1}^T - \mathbb{1} v_l^T \right\rangle + \langle u_l, p_l \rangle \right\}. \tag{12}$$

Notice that $\sum_{l=1}^m w_l v_l = 0$ and this condition allows uniquely reconstruct $\mu_1, \ldots, \mu_m$. Then by min-max theorem

$$\begin{aligned}
&\min_{\substack{\boldsymbol{\pi}:\pi_l\in\mathbb{R}_+^{n\times n}\\ \pi_l\mathbb{1}=p_l,\ \pi_l^T\mathbb{1}=\pi_{l+1}^T\mathbb{1}}} \sum_{l=1}^m w_l\big\{\langle \pi_l, C_l\rangle + \gamma H(\pi_l)\big\} \\
&\qquad = \min_{\boldsymbol{\pi}:\pi_l\in\mathbb{R}_+^{n\times n}} \max_{\substack{\mathtt{u},\mathtt{v}\\ \sum_l w_l v_l = 0}} L(\boldsymbol{\pi};\mathtt{u},\mathtt{v}) = \max_{\substack{\mathtt{u},\mathtt{v}\\ \sum_l w_l v_l = 0}} \min_{\boldsymbol{\pi}:\pi_l\in\mathbb{R}_+^{n\times n}} L(\boldsymbol{\pi};\mathtt{u},\mathtt{v}) \\
&\qquad = \max_{\substack{\mathtt{u},\mathtt{v}\\ \sum_l w_l v_l = 0}} \gamma\sum_{l=1}^m w_l \left\{ \min_{\pi_l\in\mathbb{R}_+^{n\times n}} \left\langle \pi_l, \frac{C_l}{\gamma} + \ln\pi_l - \mathbb{1}\mathbb{1}^T - u_l\mathbb{1}^T - \mathbb{1}v_l^T \right\rangle + \langle u_l, p_l\rangle \right\}.
\end{aligned}$$

By straightforward computations and the definition (10) of $B_l(u_l, v_l)$ we obtain

$$\begin{aligned}
&\min_{\pi_l\in\mathbb{R}_+^{n\times n}} \left\langle \pi_l, \frac{C_l}{\gamma} + \ln\pi_l - \mathbb{1}\mathbb{1}^T - u_l\mathbb{1}^T - \mathbb{1}v_l^T \right\rangle \\
&\qquad\qquad = -\left\langle \mathbb{1}, \exp\left(u_l\mathbb{1}^T - \frac{C_l}{\gamma} + \mathbb{1}v_l^T\right)\mathbb{1}\right\rangle = -\left\langle \mathbb{1}, B_l(u_l,v_l)\mathbb{1}\right\rangle,
\end{aligned}$$

and the minimum is attained at point $\pi_l = B_l(u_l, v_l)$. Thus we have

$$\begin{aligned}
\min_{\substack{\boldsymbol{\pi}:\pi_l\in\mathbb{R}_+^{n\times n}\\ \pi_l\mathbb{1}=p_l,\ \pi_l^T\mathbb{1}=\pi_{l+1}^T\mathbb{1}}} \sum_{l=1}^m w_l\big\{\langle \pi_l, C_l\rangle + \gamma H(\pi_l)\big\} &= \max_{\substack{\mathtt{u},\mathtt{v}\\ \sum_l w_l v_l = 0}} \gamma\sum_{l=1}^m w_l\left\{-\langle \mathbb{1}, B_l(u_l,v_l)\mathbb{1}\rangle + \langle u_l, p_l\rangle + 1\right\} \\
&= -\gamma \min_{\substack{\mathtt{u},\mathtt{v}\\ \sum_l w_l v_l = 0}} \sum_{l=1}^m w_l\left\{\langle \mathbb{1}, B_l(u_l,v_l)\mathbb{1}\rangle - \langle u_l, p_l\rangle\right\}.
\end{aligned}$$

Consequently, the dual problem to (5) is equivalent to (9), and solution to (5) has the form $[\boldsymbol{\pi}_\gamma^*]_l = B_l(u_l^*, v_l^*)$. □

The following lemma shows that Algorithms 2 is equivalent to alternating minimization in dual problem (9) (what is a general fact for Dykstra's algorithm).

Lemma 2. *Sequence $\{\boldsymbol{\pi}^t\}_{t\geq 0}$ generated by Algorithm 2 has a form $\pi_l^t = B_l(u_l^t, v_l^t)$, where $B_l(\cdot,\cdot)$ is defined in* (10) *and*

$$\begin{aligned}
&\mathtt{u}^0 = \mathtt{v}^0 = 0, \\
&\mathtt{u}^{t+1} := \operatorname*{argmin}_{\mathtt{u}} f(\mathtt{u}, \mathtt{v}^t), \qquad && \mathtt{v}^{t+1} := \mathtt{v}^t \qquad && t \bmod 2 = 0, \qquad (13)\\
&\mathtt{v}^{t+1} := \operatorname*{argmin}_{\mathtt{v}:\sum_{l=1}^m w_l v_l = 0} f(\mathtt{u}^t, \mathtt{v}), \qquad && \mathtt{u}^{t+1} := \mathtt{u}^t \qquad && t \bmod 2 = 1. \qquad (14)
\end{aligned}$$

Proof. Let us prove it by induction. For $t = 0$ it is obviously true. Assume it holds for some $t \geq 0$. Then

$$KL\left(\pi_l|\pi_l^t\right) = H(\pi_l) - \langle \pi_l, \ln\pi_l^t\rangle + \langle \pi_l^t, \mathbb{1}\mathbb{1}^T\rangle = H(\pi_l) + \left\langle \pi_l, \frac{C_l}{\gamma} - u_l^t\mathbb{1}^t - \mathbb{1}(v_l^t)^T\right\rangle + \langle \pi_l^t, \mathbb{1}\mathbb{1}^T\rangle.$$

Therefore,

$$\sum_{l=1}^{m} w_l KL\left(\pi_l | \pi_l^t\right) \to \min_{\boldsymbol{\pi} \in \mathcal{C}}$$

$$\Longleftrightarrow \sum_{l=1}^{m} w_l \left(\langle C_l, \pi_l \rangle - \gamma \langle \pi_l \mathbb{1} - p_l, u_l^t \rangle - \gamma \langle \pi_l^T \mathbb{1}, v_l^t \rangle\right) = L(\boldsymbol{\pi}; \mathtt{u}^t, \mathtt{v}^t) \to \min_{\boldsymbol{\pi} \in \mathcal{C}},$$

where L comes from (12).

Thus for even t

$$\boldsymbol{\pi}^{t+1} = \operatorname*{argmin}_{\boldsymbol{\pi} \in \mathcal{C}_1} L(\boldsymbol{\pi}; \mathtt{u}^t, \mathtt{v}^t),$$

Lagrangian for this problem has form $L(\boldsymbol{\pi}, \mathtt{u}, \mathtt{v}^t)$, hence the dual problem is

$$\gamma f(\mathtt{u}, \mathtt{v}^t) \to \min_{\mathtt{v}}.$$

and as $\mathtt{u}^{t+1} = \operatorname{argmin}_{\mathtt{u}} f(\mathtt{u}, \mathtt{v}^t)$,

$$\pi_l^{t+1} = B_l(u_l^{t+1}, v_l^t).$$

Similarly, for odd t

$$\boldsymbol{\pi}^{t+1} = \operatorname*{argmin}_{\boldsymbol{\pi} \in \mathcal{C}_2} L(\boldsymbol{\pi}; \mathtt{u}^t, \mathtt{v}^t),$$

with Lagrangian $L(\boldsymbol{\pi}, \mathtt{u}^t, \mathtt{v})$ and dual problem

$$\gamma f(\mathtt{u}^t, \mathtt{v}) \to \min_{\mathtt{v}: \sum_{l=1}^m w_l v_l = 0}.$$

Consequently,

$$\pi_l^{t+1} = B_l(u_l^{t+1}, v_l^t).$$

□

The next lemma gives us explicit recurrent expressions for $\mathtt{u}^t$ and $\mathtt{v}^t$ defined in the previous lemma. Equation (15) immediately follows from [Benamou et al., 2015, Proposition 1], and equation (16) is a reformulation of [Benamou et al., 2015, Proposition 2].

Lemma 3. *Equation* (13) *for even t is equivalent to*

$$u_l^{t+1} = u_l^t + \ln p_l - \ln\left(B_l\left(\mathtt{u}^t, \mathtt{v}^t\right)\mathbb{1}\right) = \ln p_l - \ln K_l e^{v_l^t}, \tag{15}$$

and equation (14) *for odd t is equivalent to*

$$v_l^{t+1} = v_l^t + \ln q^{t+1} - \ln q_l^t = \sum_{k=1}^{m} w_k \ln K_k^T e^{u_k^t} - \ln K_l^T e^{u_l^t}, \tag{16}$$

where $q_l^t := B_l^T(u_l^t, v_l^t)\mathbb{1}$, $q^{t+1} := \exp\left(\sum_{l=1}^m w_l \ln q_l^t\right)$.

Now we turn to the proof of Theorem 1. Next lemmas are preliminaries to the proof of correctness and complexity bound for Algorithm 1.

Lemma 4. *For any $t \geq 0$, $l = \overline{1,m}$ it holds*

$$\max_j [v_l^t]_j - \min_j [v_l^t]_j \leq R_v, \qquad \max_j [v_l^*]_j - \min_j [v_l^*]_j \leq R_v,$$

where

$$R_v := \max_l \frac{\|C_l\|_\infty}{\gamma} + \sum_{k=1}^m w_k \frac{\|C_k\|_\infty}{\gamma}. \tag{17}$$

Proof. Bound can be derived in almost the same way as in Dvurechensky et al. [2018b]. For $t = 0$ it obviously holds. Let us denote by ν_l the minimal entry of K_l:

$$\nu_l := \min_{i,j} [K_l]_{ij} = e^{-\|C_l\|_\infty/\gamma}.$$

As $[K_l]_{ij} \leq 1$, we obtain for all $j = \overline{1,n}$

$$\ln \nu_l + \ln\langle \mathbb{1}, e^{u_l} \rangle \leq [\ln K_l^T e^{u_l}]_j \leq \ln\langle \mathbb{1}, e^{u_l} \rangle,$$

therefore

$$\max_j [\ln K_l^T e^{u_l}]_j - \min_j [\ln K_l^T e^{u_l}]_j \leq -\ln \nu_l = \frac{\|C_l\|_\infty}{\gamma}.$$

Hence at any update of $\mathtt{v}^t$ it holds

$$\max_j [v_l^t]_j - \min_j [v_l^t]_j \leq \frac{\|C_l\|_\infty}{\gamma} + \sum_{k=1}^m w_k \frac{\|C_k\|_\infty}{\gamma} \leq R_v.$$

For solution to the problem $(\mathtt{u}^*, \mathtt{v}^*)$ condition (16) also holds, and consequently the solution also meets derived bounds. □

Let us define an excess function

$$\tilde{f}(\mathtt{u}, \mathtt{v}) := f(\mathtt{u}, \mathtt{v}) - f(\mathtt{u}^*, \mathtt{v}^*)$$

for further complexity analysis of Algorithm 1.

Lemma 5. *Let $\{\mathtt{u}^t, \mathtt{v}^t\}_{t \geq 0}$ be generated by Algorithm 1. Then for any even $t \geq 2$ we have*

$$\tilde{f}(\mathtt{u}^t, \mathtt{v}^t) \leq R_v \sum_{l=1}^m w_l \left\| q_l^t - \bar{q}^t \right\|_1. \tag{18}$$

Proof. Gradient inequality of any convex function g at point x^* reads as

$$g(x^*) \geq g(x) + \langle \nabla g(x), x^* - x \rangle, \quad \forall x \in \mathrm{dom}(g).$$

Applying the latter inequality to function f at point $(\mathtt{u}^*, \mathtt{v}^*)$ we obtain

$$\tilde{f}(\mathtt{u}^t, \mathtt{v}^t) = f(\mathtt{u}^t, \mathtt{v}^t) - f(\mathtt{u}^*, \mathtt{v}^*) \leq \sum_{l=1}^m w_l \langle u_l^t - u_l^*, B_l(u_l^t, v_l^t)\mathbb{1} - p_l \rangle + \sum_{l=1}^m w_l \langle v_l^t - v_l^*, q_l^t \rangle.$$

If $t \geq 2$ is even, then the first term in r.h.s. vanishes. Notice that $\langle q_l^t, \mathbb{1} \rangle = \langle \mathbb{1}, B_l(u_l^t, v_l^t)\mathbb{1} \rangle = \langle \mathbb{1}, p_l \rangle = 1$, thus

$$\begin{aligned}
\tilde{f}(\mathtt{u}^t, \mathtt{v}^t) &= \sum_{l=1}^m w_l \langle v_l^t - v_l^*, q_l^t \rangle = \sum_{l=1}^m w_l \langle v_l^t - v_l^*, q_l^t - \bar{q}^t \rangle \\
&= \sum_{l=1}^m w_l \langle (v_l^t - b_l^t \mathbb{1}) - (v_l^* - b_l^* \mathbb{1}), q_l^t - \bar{q}^t \rangle \\
&\leq \sum_{l=1}^m w_l \left(\left\| v_l^t - b_l^t \mathbb{1} \right\|_\infty + \left\| v_l^* - b_l^* \mathbb{1} \right\|_\infty \right) \left\| q_l^t - \bar{q}^t \right\|_1,
\end{aligned}$$

where

$$b_l^t := \frac{\min_i [v_l^t]_i + \max_i [v_l^t]_i}{2}, \quad b_l^* := \frac{\min_i [v_l^*]_i + \max_i [v_l^*]_i}{2}.$$

By Lemma 4 $\left\| v_l^t - b_l^t \mathbb{1} \right\|_\infty \leq R_v/2$ and $\left\| v_l^* - b_l^* \mathbb{1} \right\|_\infty \leq R_v/2$, therefore

$$\tilde{f}(\mathtt{u}^t, \mathtt{v}^t) \leq R_v \sum_{l=1}^m w_l \left\| q_l^t - \bar{q}^t \right\|_1.$$

□

Lemma 6. *For any odd $t \geq 1$ the following bound on the change of objective function $f(\cdot, \cdot)$ holds:*

$$f(\mathtt{u}^t, \mathtt{v}^t) - f(\mathtt{u}^{t+1}, \mathtt{v}^{t+1}) \geq \frac{1}{11} \sum_{l=1}^m w_l \left\| q_l^t - \bar{q}^t \right\|_1^2,$$

where $\bar{q}^t := \sum_{l=1}^m w_l q_l^t$.

Proof. If t is odd, then $\mathtt{v}^{t+1}$ satisfies (16) and $\mathtt{u}^t = \mathtt{u}^{t+1}$. Therefore,

$$\begin{aligned} f(\mathtt{u}^t, \mathtt{v}^t) - f(\mathtt{u}^{t+1}, \mathtt{v}^{t+1}) &= \sum_{l=1}^m w_l \big\{ \langle q_l^t, \mathbb{1}\rangle - \langle q_l^{t+1}, \mathbb{1}\rangle \big\} = \big\langle \bar{q}^t - q^{t+1}, \mathbb{1} \big\rangle \\ &= \left\langle \bar{q}^t - \exp\left(\sum_{l=1}^m w_l q_l^t \right), \mathbb{1} \right\rangle \geq \frac{4}{11} \sum_{j=1}^n \frac{1}{[\bar{q}^t]_j} \sum_{l=1}^m w_l \big([q_l^t - \bar{q}^t]_j^- \big)^2 \\ &= \frac{4}{11} \sum_{l=1}^m w_l \sum_{j=1}^n \frac{\big([q_l^t - \bar{q}^t]_j^- \big)^2}{[\bar{q}^t]_j} \geq \frac{4}{11} \sum_{l=1}^m w_l \frac{\Big(\sum_j [q_l^t - \bar{q}^t]_j^- \Big)^2}{\sum_{j=1}^n [\bar{q}^t]_j} \\ &= \frac{1}{11} \sum_{l=1}^m w_l \left\| q_l^t - \bar{q}^t \right\|_1^2 . \end{aligned}$$

Here we used equations $\langle q_l^t, \mathbb{1}\rangle = \langle \mathbb{1}, p_l\rangle = 1$, i.e. $q_l^t \in S_n(1)$ and thus $\bar{q}^t \in S_n(1)$, and the following fact: if $x \in \mathbb{R}_+^m$, $\bar{x} := \sum_{l=1}^m w_l x_l$, then

$$\bar{x} - \prod_{l=1}^m x_l^{w_l} \geq \frac{4}{11} \sum_{l=1}^m w_l \frac{\big[(x_l - \bar{x})^- \big]^2}{\bar{x}}.$$

Indeed, let $\Delta_l := x_l - \bar{x}$, then

$$\bar{x} - \prod_{l=1}^m x_l^{w_l} = \bar{x} - \exp\left\{ \sum_{l=1}^m w_l \ln(\bar{x} + \Delta_l) \right\} = \bar{x} \left(1 - \exp\left\{ \sum_{l=1}^m w_l \ln\left(1 + \frac{\Delta_l}{\bar{x}} \right) \right\} \right),$$

$$\sum_{l=1}^m w_l \ln\left(1 + \frac{\Delta_l}{\bar{x}} \right) \leq \sum_{l=1}^m w_l \left(\frac{\Delta_l}{\bar{x}} - \frac{(\Delta_l^-)^2}{2\bar{x}^2} \right) = - \sum_{l=1}^m w_l \frac{(\Delta_l^-)^2}{2\bar{x}^2}.$$

Notice that $\Delta_l^- := \max\{-\Delta_l, 0\} = \max\{\bar{x} - x_l, 0\} \leq \bar{x}$, thus $\sum_{l=1}^m w_l \frac{(\Delta_l^-)^2}{\bar{x}^2} \leq 1$ and

$$\exp\left\{ -\frac{1}{2} \sum_{l=1}^m w_l \frac{(\Delta_l^-)^2}{\bar{x}^2} \right\} \leq 1 - \big(1 - e^{-1/2} \big) \sum_{l=1}^m w_l \frac{(\Delta_l^-)^2}{\bar{x}^2} \leq 1 - \frac{4}{11} \sum_{l=1}^m w_l \frac{(\Delta_l^-)^2}{\bar{x}^2}.$$

Consequently,

$$\bar{x} - \prod_{l=1}^m x_l^{w_l} \geq \frac{4}{11} \sum_{l=1}^m w_l \frac{(\Delta_l^-)^2}{\bar{x}}.$$

□

Proof of Theorem 1. First, notice that

$$H\big(B_l(u_l, v_l) \big) = \langle u_l, B_l(u_l, v_l)\mathbb{1}\rangle + \langle v_l, B_l^T(u_l, v_l)\mathbb{1}\rangle - \langle \mathbb{1}, B_l(u_l, v_l)\mathbb{1}\rangle - \frac{1}{\gamma} \langle C_l, B_l(u_l, v_l)\rangle.$$

Since N is even, $B_l\mathbb{1} = p_l$ and therefore it holds

$$\begin{aligned}\sum_{l=1}^{m} w_l \left(\langle C_l, B_l\rangle + \gamma H(B_l)\right) &= \gamma \sum_{l=1}^{m} w_l \left(\langle u_l^N, B_l\mathbb{1}\rangle + \langle v_l^N, B_l^T\mathbb{1}\rangle - \langle \mathbb{1}, B_l\mathbb{1}\rangle\right) \\ &= -\gamma \sum_{l=1}^{m} w_l \left(\langle \mathbb{1}, B_l\mathbb{1}\rangle - \langle u_l^N, p_l\rangle\right) + \gamma \sum_{l=1}^{m} w_l \langle v_l^N, q_l^N\rangle \\ &= -\gamma f(\mathtt{u}^N, \mathtt{v}^N) + \gamma \sum_{l=1}^{m} w_l \langle v_l^N, q_l^N - \bar{q}^N\rangle.\end{aligned}$$

Now Lemmas 1, 4, 5, and stopping criterion yield

$$\begin{aligned}&\sum_{l=1}^{m} w_l \left(\langle C_l, B_l\rangle + \gamma H(B_l)\right) - \sum_{l=1}^{m} w_l \left(\langle C_l, \pi_l^*\rangle + \gamma H(\pi_{\gamma,l}^*)\right) \\ &\qquad = \gamma\big(f(\mathtt{u}^*, \mathtt{v}^*) - f(\mathtt{u}^N, \mathtt{v}^N)\big) + \gamma \sum_{l=1}^{m} w_l \langle v_l^N, q_l^N - \bar{q}^N\rangle \\ &\qquad \le \gamma \sum_{l=1}^{m} w_l \frac{R_v}{2} \left\|q_l^N - \bar{q}^N\right\|_1 \le \frac{\gamma R_v}{2}\varepsilon' \le \max_l \|C_l\|_\infty \varepsilon'.\end{aligned}$$

Now let us prove the complexity bound. We will do it in two steps.

1. If $t \ge 2$ is even, then by Lemma 5

$$\tilde{f}(\mathtt{u}^t, \mathtt{v}^t) \le R_v \sum_{l=1}^{m} w_l \left\|q_l^t - \bar{q}^t\right\|_1$$

and since stopping criterion is not fulfilled,

$$\sum_{l=1}^{m} w_l \left\|q_l^t - \bar{q}^t\right\|_1 > \varepsilon'.$$

Inequality $\sum_{l=1}^{m} w_l \|q_l^t - \bar{q}^t\|_1^2 \ge \left(\sum_{l=1}^{m} w_l \|q_l^t - \bar{q}^t\|_1\right)^2$ together with Lemma 6 give us the following bound:

$$\begin{aligned}\tilde{f}(\mathtt{u}^t, \mathtt{v}^t) - \tilde{f}(\mathtt{u}^{t+1}, \mathtt{v}^{t+1}) &= f(\mathtt{u}^t, \mathtt{v}^t) - f(\mathtt{u}^{t+1}, \mathtt{v}^{t+1}) \\ &\ge \frac{1}{11} \max\left\{(\varepsilon')^2, \left(\frac{\tilde{f}(\mathtt{u}^t, \mathtt{v}^t)}{R_v}\right)^2\right\} = \max\left\{\frac{(\varepsilon')^2}{11}, \frac{1}{11R_v^2}\tilde{f}^2(\mathtt{u}^t, \mathtt{v}^t)\right\}.\end{aligned}$$

If t is odd then we have at least $\tilde{f}(\mathtt{u}^{t+1}, \mathtt{v}^{t+1}) \le \tilde{f}(\mathtt{u}^t, \mathtt{v}^t)$. To simplify derivation we define

$$\delta_t := \tilde{f}(\mathtt{u}^t, \mathtt{v}^t). \tag{19}$$

Now we have two possibilities to estimate number of iteration. The first one is based on inequalities

$$\frac{1}{\delta_{t+1}} \geq \begin{cases} \frac{1}{\delta_t} + \frac{1}{11R_v^2}\frac{\delta_t}{\delta_{t+1}} \geq \frac{1}{\delta_t} + \frac{1}{11R_v^2}, & t \bmod 2 = 0, \\ \frac{1}{\delta_t}, & t \bmod 2 = 1. \end{cases}$$

Summation of these inequalities gives

$$\frac{1}{\delta_t} \geq \frac{1}{\delta_1} + \frac{t-2}{22R_v^2}$$

and hence

$$t \leq 2 + 22R_v^2\left(\frac{1}{\delta_t} - \frac{1}{\delta_1}\right). \tag{20}$$

The second estimate can be obtain from

$$\delta_{t+1} \leq \begin{cases} \delta_t - \frac{(\varepsilon')^2}{11}, & t \bmod 2 = 0, \\ \delta_t, & t \bmod 2 = 1. \end{cases}$$

Similarly, summation of these inequalities gives

$$\delta_t \geq \delta_t - \delta_{t+k} \geq \frac{k-1}{22}(\varepsilon')^2, \tag{21}$$

$$k \leq 1 + \frac{22\delta_t}{(\varepsilon')^2}. \tag{22}$$

2. To combine the two estimates (20) and (21), we consider a switching strategy parametrized by number $s \in (0, \delta_1)$. First t iterations we use (20), resulting in δ_t becomes below some s. Then, we use s as a starting point and estimate the remaining number of iteration by (21). The quantity s can be found from the minimization

$$N = t + k \leq 4 + \frac{2s}{(\varepsilon')^2} + 22R_v^2\left(\frac{1}{s} - \frac{1}{\delta_1}\right).$$

Minimizing the r.h.s. of the latter inequality in s leads to

$$N \leq \min_{0 \leq s \leq \delta_1}\left\{4 + \frac{22s}{(\varepsilon')^2} + 22R_v^2\left(\frac{1}{s} - \frac{1}{\delta_1}\right)\right\} \leq 4 + \frac{44R_v}{\varepsilon'}. \tag{23}$$

The last inequality is obtained by the substitution $s = R_v\varepsilon'$ that is the solution to the minimization problem. Of course, the switching strategy is impossible if $\delta_1 < s$. But in this case (21) gives

$$N \leq 2 + \frac{22\delta_1}{(\varepsilon')^2} < 4 + \frac{44R_v}{\varepsilon'}. \tag{24}$$

In both cases (23) and (24) we have

$$N \leq 4 + \frac{44R_v}{\varepsilon'} = O\left(\frac{\max_l \|C_l\|_\infty}{\gamma\varepsilon'}\right).$$

□

2.2 Approximating Non-regularized WB by IBP

To find an approximate solution to the initial problem (2) we apply Algorithm 1 with a suitable choice of γ and ε' and average marginals $q_1, \ldots, q_m$ with weights w_l, what leads to Algorithm 3.

Algorithm 3 Finding Wasserstein barycenter by IBP

Input: Accuracy ε; cost matrices $C_1, \ldots, C_m$; marginals $p_1, \ldots, p_m$

1: Set $\gamma := \frac{1}{4}\frac{\varepsilon}{\ln n}, \quad \varepsilon' := \frac{1}{4}\frac{\varepsilon}{\max_l \|C_l\|_\infty}$

2: Find $B_1 := B_1(u_1^t, v_1^t), \ldots, B_m := B_m(u_m^t, v_m^t)$ by Algorithm 1 with accuracy ε'

3: $q := \frac{1}{\sum_{l=1}^m w_l \langle \mathbb{1}, B_l \mathbb{1} \rangle} \sum_{l=1}^m w_l B_l^T \mathbb{1}$

Output: q

To present our final complexity bound for Algorithm 3, which calculates approximated non-regularized Wasserstein barycenter, we formulate the following auxiliary Algorithm 4 finding a projection to the feasible set. It is based on Algorithm 2 from Altschuler et al. [2017]. Notice that the bound (25) follows immediately from the proof of [Altschuler et al., 2017, Theorem 4], although it was not stated explicitly.

Algorithm 4 Round to feasible solution

Input: $B_1, \ldots, B_m \in \mathbb{R}_+^{n \times n}$, $p_1, \ldots, p_m \in S_n(1)$

1: $q := \frac{1}{\sum_{l=1}^m w_l \langle \mathbb{1}, B_l \mathbb{1} \rangle} \sum_{l=1}^m w_l B_l^T \mathbb{1}$

2: Calculate $\check{B}_1, \ldots, \check{B}_m$ by Algorithm 2 from Altschuler et al. [2017] s.t.

$$\check{B}_l \in \Pi(p_l, q), \quad \left\|\check{B}_l - B_l\right\|_1 \leq 2\left(\sum_i [B_l \mathbb{1} - p_l]_i^+ + \sum_j [B_l^T \mathbb{1} - q]_j^+\right) \tag{25}$$

Output: $\check{B}_1, \ldots, \check{B}_m$

Next theorem presents complexity bound for Algorithm 3.

Theorem 2. *For given ε Algorithm 3 returns $q \in S_n(1)$ s.t.*

$$\sum_{l=1}^m w_l \mathcal{W}(p_l, q) - \sum_{l=1}^m w_l \mathcal{W}(p_l, q^*) \leq \varepsilon,$$

where q^* is a solution to non-regularized problem (2). It requires

$$O\left(\left(\frac{\max_l \|C_l\|_\infty}{\varepsilon}\right)^2 M_{m,n} \ln n + mn\right)$$

arithmetic operations, where $M_{m,n}$ is a time complexity of one iteration of Algorithm 1.

Remark 1. As each iteration of Algorithm 1 requires m matrix-vector multiplications, the general bound is $M_{m,n} = O(mn^2)$. However, for some specific form of matrices C_l it's possible to achieve better complexity, e.g. $M_{m,n} = O(mn \log n)$ via FFT Peyré and Cuturi [2018].

Proof. Let $\boldsymbol{\pi}^*_\gamma = [\pi^*_{\gamma,1}, \ldots, \pi^*_{\gamma,m}]$ be a solution to (5) and $\boldsymbol{\pi}^* = [\pi^*_1, \ldots, \pi^*_m]$ be a solution to the non-regularized problem. Consider $\check{B}_1, \ldots, \check{B}_m$ obtained from $B_1(u_1^t, v_1^t), \ldots, B_m(u_m^t, v_m^t)$ via Algorithm 4, where t is the number of IBP iterations. Then we obtain

$$\sum_{l=1}^m w_l \langle C_l, \check{B}_l \rangle \leq \sum_{l=1}^m w_l \left(\langle C_l, B_l(u_l^t, v_l^t) \rangle + \|C_l\|_\infty \left\| B_l(u_l^t, v_l^t) - \check{B}_l \right\|_1 \right).$$

By Theorem 1 one obtains

$$\begin{aligned}
\sum_{l=1}^m w_l \langle C_l, B_l(u_l^t, v_l^t) \rangle &\leq \sum_{l=1}^m w_l \left(\langle C_l, \pi^*_{\gamma,l} \rangle + \gamma H(\pi^*_{\gamma,l}) - \gamma H(B_l(u_l^t, v_l^t)) \right) + \max_l \|C_l\|_\infty \varepsilon' \\
&\leq \sum_{l=1}^m w_l \left(\langle C_l, \pi^*_l \rangle + \gamma H(\pi^*_l) - \gamma H(B_l(u_l^t, v_l^t)) \right) + \max_l \|C_l\|_\infty \varepsilon' \\
&\leq \sum_{l=1}^m w_l \mathcal{W}(p_l, q^*) + 2\gamma \ln n + \max_l \|C_l\|_\infty \varepsilon'.
\end{aligned}$$

Here we used inequalities $-2 \ln n \leq H(\pi) + 1 \leq 0$ holding on $S_{n \times n}(1)$. As stopping time t is even, $B_l(u_l^t, v_l^t)\mathbb{1} = p_l$ and $\langle q_l^t, \mathbb{1} \rangle = 1$, therefore

$$\left\| B_l(u_l^t, v_l^t) - \check{B}_l \right\|_1 \leq 2 \sum_j [q_l^t - \bar{q}^t]_j^+ = \left\| q_l^t - \bar{q}^t \right\|_1,$$

and hence

$$\sum_{l=1}^m w_l \left\| B_l(u_l^t, v_l^t) - \check{B}_l \right\|_1 \leq \varepsilon'.$$

Notice that $\check{B}_l \in \Pi(p_l, q)$ for all $1 \leq l \leq m$, consequently

$$\begin{aligned}
\sum_{l=1}^m w_l \mathcal{W}(p_l, q) &\leq \sum_{l=1}^m w_l \langle C_l, \check{B}_l \rangle \\
&\leq \sum_{l=1}^m w_l \langle C_l, B_l(u_l^t, v_l^t) \rangle + \max_l \|C_l\|_\infty \sum_{l=1}^m w_l \left\| B_l(u_l^t, v_l^t) - \check{B}_l \right\|_1 \\
&\leq \sum_{l=1}^m w_l \mathcal{W}(p_l, q^*) + 2\gamma \ln n + 2 \max_l \|C_l\|_\infty \varepsilon' \leq \sum_{l=1}^m w_l \mathcal{W}(p_l, q^*) + \varepsilon.
\end{aligned}$$

Complexity bound for the algorithm is a simple corollary of Theorem 1. □

Remark 2. Notice that according to the proof of the above theorem, one can also reconstruct approximated optimal transportation plans $\check{B}_l$ between p_l and approximated barycenter q using Algorithm 4.

2.3 Proximal IBP for Wasserstein barycenter problem

As we see from Theorems 1 and 2, to obtain an ε-approximation of the non-regularized barycenter, the regularization parameter γ should be chosen proportional to small ε and the complexity of the IBP is inversely proportional to γ, which leads to large working time and instability issues. To overcome this obstacle we propose a novel proximal-IBP algorithm. It is inspired by proximal point algorithm with general Bregman divergence $V(x, y)$ Chen and Teboulle [1993]. The idea of this algorithm for minimization of a function $f(x)$ is to perform steps $x_{k+1} = \mathbf{prox}(x_k) = \arg\min_{x \in Q}\{f(x) + \gamma V(x, x_k)\}$. We use the KL-divergence as the Bregman divergence since in this case the proximal step leads to a similar problem to the entropic-regularized WB (4). Given the sets $\mathcal{C}_1, \mathcal{C}_2$ defined in (8), we define proximal operator $\mathbf{prox} : \mathcal{C}_1 \cap \mathcal{C}_2 \to \mathcal{C}_1 \cap \mathcal{C}_2$ for function $\sum_{l=1}^m w_l W_\gamma(p_l, q_l)$ as follows

$$
\begin{aligned}
\mathbf{prox}(\boldsymbol{\pi}^k) &= \arg\min_{\boldsymbol{\pi} \in \mathcal{C}_1 \cap \mathcal{C}_2} \sum_{l=1}^m w_l \left\{ \langle \mathcal{C}_l, \pi_l \rangle + \gamma KL(\boldsymbol{\pi} | \boldsymbol{\pi}^k) \right\} \\
&= \arg\min_{\boldsymbol{\pi} \in \mathcal{C}_1 \cap \mathcal{C}_2} \sum_{i,j=1}^n \sum_{l=1}^m w_l \left\{ [\mathcal{C}_l]_{ij} \cdot [\pi_l]_{ij} + \gamma \left([\pi_l]_{ij} \ln \left(\frac{[\pi_l]_{ij}}{[\pi_l^k]_{ij}} \right) - [\pi_l]_{ij} + [\pi_l^k]_{ij} \right) \right\} \\
&= \arg\min_{\boldsymbol{\pi} \in \mathcal{C}_1 \cap \mathcal{C}_2} \sum_{l=1}^m w_l KL \left(\pi_l | \pi_l^k \odot \exp\left(-\frac{C_l}{\gamma} \right) \right),
\end{aligned}
$$

The proximal gradient method has the following form

$$
\boldsymbol{\pi}^{k+1} = \mathbf{prox}(\boldsymbol{\pi}^k). \tag{26}
$$

Then we use Iterative Bregman Projection for finding the barycenter.

For convenience let's determine after Dual_IBP$(\mathtt{u}^0, \mathtt{v}^0, \{K_l\}, M)$ the following objects $\mathtt{u}^M$, $\mathtt{v}^M$; $\{B_l(u_l^M, v_l^M)\}$; $\bar{q}^M$ obtained after M iterations of Algorithm 1 applied with starting points $\mathtt{u}^0$, $\mathtt{v}^0$ and set of matrices $\{K_l\}$.

Algorithm 5 Finding Wasserstein barycenter by proximal IBP

Input: M, N — numbers of internal and external iterations respectively; $\mathtt{u}^{0,0} = 0$ $\mathtt{v}^{0,0} = 0$; starting transport plans $\{\pi_l^0\}_{l=1}^m : \pi_l^0 = \exp\left(-\frac{C_l}{\gamma}\right) \ \ \forall l = 1, \ldots, m$

1: For each agent $l \in V$:
2: **for** $k = 0, \ldots, N-1$ **do**
3: $K_l^k := \pi_l^k \odot \exp(-\frac{C_l}{\gamma})$
4: Run Algorithm 1 for M iterations with starting point $\mathtt{u}^{0,k}, \mathtt{v}^{0,k}$ and kernels $\{K_l^k\}$ instead of $\{K_l\}$.
5: Set $u_l^{0,k+1} = u_l^M$, $v_l^{0,k+1} = v_l^M$, where the sequence of dual variables (u_l^t, v_l^t) is generated by Algorithm 1.
6: Set $\pi_l^{k+1} = B_l(u_l^M, v_l^M)$.
7: **end for**

Output: $\bar{q}^M$, generated on the last inner iteration of Algorithm 1 on the last outer iteration.

We underline that in this setting, there is no need to choose γ to be small as it prescribed by Theorem 3. Algorithm 5 has two loops: external loop of proximal gradient step and internal loop of computing the next iterate $\boldsymbol{\pi}^k$ by IBP and as a byproduct an approximation q^k to the barycenter. The number of external iterations is proportional to $\frac{\gamma}{\varepsilon}$, see Chen and Teboulle [1993], and the complexity of internal loop is proportional to $\min\left\{\frac{\text{const}}{\gamma\tilde{\varepsilon}}, \exp\left(\frac{\text{const}}{\gamma}\right)\ln\left(\frac{1}{\tilde{\varepsilon}}\right)\right\}$, where $\tilde{\varepsilon} = O(\epsilon^2/(mn^3))$ is a required precision for inner problem Stonyakin et al. [2019]. The first estimate directly follows from IBP complexity (see Theorem 1) and the second estimate (analogous to Franklin and Lorenz [1989] for Sinkhorn's algorithm) can be obtained using strong convexity of $f(\mathtt{u}, \mathtt{v})$. Namely, one can show that (cf. Lemma 1 in Dvurechensky et al. [2018b])

$$\max_i [u_l^t]_i - \min_i [u_l^t]_i \leq \ln(\max_i [p_l]_i) - \ln(\min_i [p_l]_i) + \frac{\|C_l\|_\infty}{\gamma}$$

and thus for any l, t it holds

$$0 \leq -[\ln B_l(u_l^t, v_l^t)]_{ij} \leq 4\frac{\max_l \|C_l\|_\infty}{\gamma} + 2\ln n - \ln \min_i [p_l]_i \quad \forall i, j.$$

Moreover, this bound holds on the convex hull of $\{(\mathtt{u}^t, \mathtt{v}^t)\}_{t\geq 0}$. Therefore

$$\lambda^+_{min}(\nabla^2_{(u_l,v_l)} f(\mathtt{u}^t, \mathtt{v}^t)) \geq w_l \frac{\min_i [p_l]_i}{n^2} \exp\left(-4\frac{\max_l \|C_l\|_\infty}{\gamma}\right).$$

This estimate implies linear convergence and thus the following complexity bound for IBP:

$$O\left(\frac{n^2}{\min_{l,i}[p_l]_i} \exp\left(\frac{4\max_l \|C_l\|_\infty}{\gamma}\right)\ln\left(\frac{1}{\tilde{\varepsilon}}\right)\right) = O\left(\exp\left(\frac{\text{const}}{\gamma}\right)\ln\left(\frac{1}{\tilde{\varepsilon}}\right)\right).$$

Note that since in practice const is not too big, then setting $\gamma = \tilde{O}(\text{const})$ one can typically improve the complexity of IBP by KL-proximal envelope as is follows: $1/\varepsilon^2 \to 1/\varepsilon$. The last bound (based on the similar reasons as in Blanchet et al. [2018]) seems to be unimprovable for this problem (see also item 3). In practice one should try to find const by restart procedure on γ on the first external loop iteration. That is, we start with large enough γ and solve internal problem by IBP, then put $\gamma := \gamma/2$ and solve internal problem (with the same precision $\tilde{\epsilon}$) once again. We stop this repeating procedure at the moment when the complexity of internal problem growth significantly. This moment allows us to detect the moment of $\gamma = \widetilde{O}(\text{const})$. On the next external iterations one may use this γ.

Numerical experiments and more accurate theoretical analysis can be found in the follow-up paper Stonyakin et al. [2019].

Algorithm 5 can be implemented in centralized distributed setting in the same way as Algorithm 1, see Section 2.1.

3 Complexity by Primal-Dual Accelerated Gradient Descent

In this subsection we consider Primal-Dual Accelerated Gradient Descent for approximating Wasserstein barycenter. First, we consider regularized barycenter, construct a dual problem to (4) and apply primal-dual accelerated gradient descent to solve it and approximate the regularized berycenter. Our dual problem is constructed via a matrix W, which can be quite general. We explain how the choice of this matrix is connected to distributed optimization and allows to implement the algorithm in the decentralized distributed setting. Then, we show, how the regularization parameter should be chosen in order to obtain an ε-approximation for the non-regularized Wasserstein barycenter, and estimate the complexity of the resulting algorithm. The proposed algorithms can be implemented in a decentralized distributed manner such that each node fulfils $\widetilde{O}(n^{2.5}/\varepsilon)$ arithmetic operations and the number of communication rounds is $\widetilde{O}(\sqrt{n}/\varepsilon)$.

3.1 Consensus view on Wasserstein barycenter problem

We rewrite the problem (4) in an equivalent way as

$$\min_{\substack{q_1,\dots,q_m\in S_n(1)\\ q_1=\dots=q_m}} W_\gamma(\mathtt{p},\mathtt{q}) := \sum_{l=1}^m w_l \mathcal{W}_{\gamma(l)}(p_l,q_l), \tag{27}$$

where $\mathtt{p}=[p_1,\dots,p_m]^T$ and $\mathtt{q}=[q_1,\dots,q_m]^T$, we also use different regularizer $\gamma_l=\gamma(l)$ for l-th Wasserstein distance. Next we write a dual problem by dualizing equality constraints $q_1=\dots=q_m$. This can be done in many different ways and we do it by introducing a matrix $\bar{W}\in\mathbb{R}^{n\times n}$ which is a symmetric positive semi-definite matrix s.t. $\mathrm{Ker}(\bar{\mathrm{W}})=\mathrm{span}(\mathbb{1})$. Then, defining $W=\bar{W}\otimes I_n$ and using the fact $q_1=\dots=q_m \iff \sqrt{W}\mathtt{q}=0$, we equivalently rewrite problem (27) as

$$\max_{\substack{q_1,\dots,q_m\in S_n(1),\\ \sqrt{W}\mathtt{q}=0}} -\sum_{l=1}^m w_l \mathcal{W}_{\gamma(l)}(p_l,q_l), \tag{28}$$

Dualizing the linear constraint $\sqrt{W}\mathtt{q}=0$, we obtain the dual problem

$$\min_{\mathtt{u}\in\mathbb{R}^{mn}} \max_{\mathtt{q}\in\mathbb{R}^{nm}} \left\{\sum_{l=1}^m \langle u_l,[\sqrt{W}\mathtt{q}]_l\rangle - \sum_{l=1}^m w_l\mathcal{W}_{\gamma(l)}(p_l,q_l)\right\} = \min_{\mathtt{u}\in\mathbb{R}^{mn}} \sum_{l=1}^m w_l \mathcal{W}^*_{\gamma(l),p_l}([\sqrt{W}\mathtt{u}]_l/w_l) \tag{29}$$

where $\mathcal{W}^*_{\gamma(l),p_l}(\cdot)$ is the Fenchel–Legendre transform of $\mathcal{W}_{\gamma(l)}(p_l,\cdot)$, $[\sqrt{W}\mathtt{q}]_i$ and $[\sqrt{W}\mathtt{u}]_i$ represent the i-th n-dimensional block of vectors $\sqrt{W}\mathtt{q}$ and $\sqrt{W}\mathtt{u}$ respectively. We apply distributed primal-dual accelerated gradient descent Algorithm 6 to solve the constructed pair of primal and dual problems.

Before we move to the theoretical analysis of the algorithm, let us discuss the scalability of Algorithm 6. Assume that we have an arbitrary network of agents given by connected undirected graph $G = (V, E)$ without self-loops with the set V of n vertices and the set of edges $E = \{(i, j) : i, j \in V\}$. Then matrix $\bar{W}$ can be chosen as the Laplacian matrix for this graph, which is such that a) $[\bar{W}]_{ij} = -1$ if $(i, j) \in E$, b) $[\bar{W}]_{ij} = \deg(i)$ if $i = j$, c) $[\bar{W}]_{ij} = 0$ otherwise. Here $\deg(i)$ is the degree of the node i, i.e., the number of neighbors of the node. We assume that an agent i can communicate with an agent j if and only if the edge $(i, j) \in E$. In particular, the Laplacian matrix for star graph, which corresponds to the centralized distributed computations discussed in Section 2 is

$$\bar{W} : \{\forall i = 1, \ldots, m-1 \ \bar{W}_{ii} = 1, \ \bar{W}_{im} = \bar{W}_{mi} = -1, \ \bar{W}_{mm} = m-1\}. \tag{30}$$

Algorithm 6 allows to perform calculations in an arbitrary connected undirected network of agents. This is in contrast to the IBP algorithm as discussed in Section 2.

Algorithm 6 Accelerated Distributed Computation of Wasserstein barycenter

Input: Each agent $l \in V$ is assigned its measure p_l and an upper bound L for the Lipschitz constant of the gradient of the dual objective.

1: Each agent finds $\tilde{p}_l \in S_n(1)$ s.t. $\|\tilde{p}_l - p_l\|_1 \leq \varepsilon/4$ and $\min_i [\tilde{p}_l]_i \geq \varepsilon/(8n)$ and redefine $p_l := \tilde{p}_l$. E.g., $\tilde{p}_l = \left(1 - \frac{\varepsilon}{8}\right)\left(p_l + \frac{\varepsilon}{n(8-\varepsilon)}\mathbb{1}\right)$.

2: All agents $l \in V$ set $\gamma(l) = \frac{\varepsilon}{4mw_l \ln n}$, $\eta_l^0 = \zeta_l^0 = \lambda_l^0 = \hat{q}_l^0 = \mathbf{0} \in \mathbb{R}^n$, $A_0 = \alpha_0 = 0$ and N.

3: For each agent $l \in V$:

4: **for** $k = 0, \ldots, N-1$ **do**

5: Find α_{k+1} as the largest root of the equation $A_{k+1} := A_k + \alpha_{k+1} = 2L\alpha_{k+1}^2$.

6: $\lambda_l^{k+1} = (\alpha_{k+1}\zeta_l^k + A_k\eta_l^k)/A_{k+1}$.

7: Calculate $\nabla \mathcal{W}^*_{\gamma(l),p_l}(\lambda_l^{k+1})$:
$[\nabla \mathcal{W}^*_{\gamma(l),p_l}(u)]_i = \sum_{j=1}^n [p_l]_j \frac{\exp(([u]_i - [C_l]_{ij})/\gamma(l))}{\sum_{r=1}^n \exp(([u]_r - [C_l]_{rj})/\gamma(l))}$

8: Share $\nabla \mathcal{W}^*_{\gamma(l),p_l}(\lambda_l^{k+1})$ with $\{j \mid (i, j) \in E\}$.

9: $\zeta_l^{k+1} = \zeta_l^k - \alpha_{k+1} \sum_{j=1}^m W_{lj} \nabla \mathcal{W}^*_{\gamma(l),p_j}(\lambda_j^{k+1})$.

10: $\eta_l^{k+1} = (\alpha_{k+1}\zeta_l^{k+1} + A_k\eta_l^{k+1})/A_{k+1}$.

11: $q_l^{k+1} = \frac{1}{A_{k+1}} \sum_{l=0}^{k+1} \alpha_i q_i(\lambda_l^{k+1}) = (\alpha_{k+1} q_i([\lambda_{k+1}]_l) + A_k q_l^k)/A_{k+1}$,
where $q_l(\cdot)$ is defined as $\nabla \mathcal{W}^*_{\gamma(l),p_l}(\cdot)$.

12: **end for**

Output: $\mathtt{q}^N = [q_1^T, \ldots, q_m^T]^T$.

For simplicity and comparison with the complexity of the IBP algorithm, we analyze the complexity of Algorithm 6 as if it is implemented on one machine, disregarding that it can be used for distributed setup.

Theorem 3. *Algorithm 6 after* $N = \frac{1}{\varepsilon}\sqrt{64\chi(\bar{W})mn\ln n\sum_{l=1}^m w_l^2\|C_l\|_\infty^2}$ *iterations generates an* ε*-solution of problem* (2)*, i.e. finds a vector* $\mathtt{q}^N = [q_1^T,\dots,q_m^T]^T$ *s.t.*

$$\sum_{l=1}^m w_l\mathcal{W}(p_l,q_l^N) - \sum_{l=1}^m w_l\mathcal{W}(p_l,q^*) \le \varepsilon, \quad \|\sqrt{W}\mathtt{q}^N\|_2 \le \varepsilon/2R, \tag{31}$$

where q^* *is an unregularized barycenter, i.e. is a solution to* (2)*, and* R *is a bound on the solution to the dual problem. Moreover, the number of arithmetic operations is* $O\left(N\cdot n(mn+\mathrm{nnz}(\bar{W}))/\varepsilon\right)$.

The proof is based on the complexity theorem of primal-dual accelerated gradient descent for a partivular pair of primal-dual problems (27)–(29).

Theorem 4 (see [Dvurechensky et al., 2017, Theorem 2])**.** *Let accelerated primal-dual gradient descent be applied to the pair of problems* (27)–(29)*. Then inequalities*

$$\sum_{l=1}^m w_l\mathcal{W}_{\gamma(l)}(p_l,q_l^N) - \sum_{l=1}^m w_l\mathcal{W}_{\gamma(l)}(p_l,q^*) \le \varepsilon/2, \quad \|\sqrt{W}\mathtt{q}^N\|_2 \le \varepsilon/2R \tag{32}$$

hold no later than after $N = \sqrt{\frac{32LR^2}{\varepsilon}}$ *iterations, where* L *is the Lipschitz constant of the gradient of the dual objective and* R *is such that* $\|\mathtt{u}^*\|_2 \le R$*,* $\mathtt{u}^*$ *being an optimal dual solution.*

Our next steps are to find the bounds for L in the next Lemma and R in Lemma 8.

Lemma 7. *Let in* (27) $\gamma(l) = \gamma/w_l$ *for some* $\gamma > 0$*, and* $\mathcal{W}_\gamma^*(\mathtt{u})$ *denote the dual objective in* (29)*. Then its gradient is* $L = \lambda_{\max}(W)/\gamma$*-Lipschitz continuous w.r.t.* 2*-norm.*

Proof. Making the change of variable $[\boldsymbol{\lambda}]_l = [\sqrt{W}\mathtt{u}]_l/w_l$, by the chain rule, the i-th n-dimensional block of $\nabla\mathcal{W}_\gamma^*(\mathtt{u})$ is

$$\left[\nabla\mathcal{W}_\gamma^*(\mathtt{u})\right]_i = \left[\nabla\sum_{l=1}^m w_l\mathcal{W}^*_{\gamma(l),p_l}([\sqrt{W}\mathtt{u}]_l/w_l)\right]_i = \sum_{l=1}^m\sqrt{W}_{il}\nabla\mathcal{W}^*_{\gamma(l),p_l}(\lambda_l),\ i=1,\dots,m. \tag{33}$$

Thus,

$$\begin{aligned}
\|\nabla \mathcal{W}^*_\gamma(\mathtt{u}_1) - \nabla \mathcal{W}^*_\gamma(\mathtt{u}_2)\|_2^2 &\overset{(33)}{=} \left\| \sqrt{W} \begin{pmatrix} \nabla \mathcal{W}^*_{\gamma(1),p_1}([\boldsymbol{\lambda}_1]_1) \\ \dots \\ \nabla \mathcal{W}^*_{\gamma(m),p_m}([\boldsymbol{\lambda}_1]_m) \end{pmatrix} - \sqrt{W} \begin{pmatrix} \nabla \mathcal{W}^*_{\gamma(1),p_1}([\boldsymbol{\lambda}_2]_1) \\ \dots \\ \nabla \mathcal{W}^*_{\gamma(m),p_m}([\boldsymbol{\lambda}_2]_m) \end{pmatrix} \right\|_2^2 \\
&\leq (\lambda_{\max}(\sqrt{W}))^2 \left\| \begin{matrix} \nabla \mathcal{W}^*_{\gamma(1),p_1}([\boldsymbol{\lambda}_1]_1) - \nabla \mathcal{W}^*_{\gamma(m),p_1}([\boldsymbol{\lambda}_2]_1) \\ \dots \\ \nabla \mathcal{W}^*_{\gamma(1),p_m}([\boldsymbol{\lambda}_1]_m) - \nabla \mathcal{W}^*_{\gamma(m),p_m}([\boldsymbol{\lambda}_2]_m) \end{matrix} \right\|_2^2 \\
&= (\lambda_{\max}(\sqrt{W}))^2 \sum_{i=1}^m \left\| \nabla \mathcal{W}^*_{\gamma(i),p_i}([\boldsymbol{\lambda}_1]_i) - \nabla \mathcal{W}^*_{\gamma(i),p_i}([\boldsymbol{\lambda}_2]_l) \right\|_2^2 \\
&\leq (\lambda_{\max}(\sqrt{W}))^2 \sum_{i=1}^m \frac{1}{\gamma^2(i)} \left\| [\boldsymbol{\lambda}_1]_l - [\boldsymbol{\lambda}_2]_l \right\|_2^2 \\
&= (\lambda_{\max}(\sqrt{W}))^2 \sum_{i=1}^m \frac{1}{\gamma^2(i)} \left\| [\sqrt{W}(\mathtt{u}_1 - \mathtt{u}_2)]_i / w_i \right\|_2^2,
\end{aligned}$$

where we used notation $[\boldsymbol{\lambda}]_i = [\sqrt{W}\mathtt{u}]_i / w_i$, the definition of matrix $\sqrt{W}$, $1/\gamma(i)$-Lipschitz continuity of $\nabla \mathcal{W}^*_{\gamma(i),p_i}(\cdot)$ for all $i = 1, \dots, m$ by [Cuturi and Peyré, 2016, Theorem 2.4]. Since $\gamma(i) = \gamma / w_i$, $i = 1, \dots, m$, we obtain

$$\|\nabla \mathcal{W}^*_\gamma(\mathtt{u}_1) - \nabla \mathcal{W}^*_\gamma(\mathtt{u}_2)\|_2^2 \leq \frac{(\lambda_{\max}(\sqrt{W}))^2}{\gamma^2} \left\| \sqrt{W}(\mathtt{u}_1 - \mathtt{u}_2) \right\|_2^2 \tag{34}$$

$$\leq \frac{(\lambda_{\max}(\sqrt{W}))^4}{\gamma^2} \|\mathtt{u}_1 - \mathtt{u}_2\|_2^2, \tag{35}$$

Since $(\lambda_{\max}(\sqrt{W}))^4 = (\lambda_{\max}(W))^2$, we get the statement of Lemma. □

The following Lemma is inspired by Lan et al. [2017].

Lemma 8. *Let $\mathtt{q}^*_\gamma$ be the optimal solution of problem (4) with minimal 2-norm, then there exists an optimal dual solution $\boldsymbol{\lambda}^* = [\lambda^*_1, \dots, \lambda^*_m]$ for problem (29) satisfying $\|\boldsymbol{\lambda}^*\|_2 \leq R$ with*

$$R^2 = \frac{2n \sum_{l=1}^m w_l^2 \|C_l\|_\infty^2}{\lambda^+_{min}(W)}. \tag{36}$$

Here $\lambda^+_{min}(W)$ is the minimal positive eigenvalue of the matrix W.

Proof. Recall that $\mathcal{W}_\gamma(\mathtt{p}, \cdot)$ denotes the objective value in the primal problem (27). Then

$$\begin{aligned}
-\mathcal{W}_\gamma(\mathtt{p}, \mathtt{q}^*_\gamma) &= \langle \boldsymbol{\lambda}^*, \sqrt{W}\mathtt{q}^*_\gamma \rangle - \mathcal{W}_\gamma(\mathtt{p}, \mathtt{q}^*_\gamma) = \mathcal{W}^*_{\gamma,\mathtt{p}}(\sqrt{W}\boldsymbol{\lambda}^*) = \max_{\substack{q_l \in S_n(1), \\ l=1,\dots,m}} \{\langle \boldsymbol{\lambda}^*_l, \sqrt{W}\mathtt{q}_l \rangle - \mathcal{W}_\gamma(\mathtt{p}, \mathtt{q})\} \\
&\geq \langle \boldsymbol{\lambda}^*, [\sqrt{W}\mathtt{q}]_l \rangle - \mathcal{W}_\gamma(\mathtt{p}, \mathtt{q}) = \langle \boldsymbol{\lambda}^*, \sqrt{W}\mathtt{q} - \sqrt{W}\mathtt{q}^*_\gamma \rangle - \mathcal{W}_\gamma(\mathtt{p}, \mathtt{q}) \\
&= \langle \sqrt{W}\boldsymbol{\lambda}^*, \mathtt{q}^*_\gamma - \mathtt{q} \rangle - \mathcal{W}_{\gamma,\mathtt{p}}(\mathtt{q}),
\end{aligned}$$

where we used $W^T = W$ and $\mathtt{q}^*_\gamma$ is the regularized barycenter.
From this inequality and using the convexity of $\mathcal{W}_\gamma(\mathtt{p}, \mathtt{q})$ we have $\nabla \mathcal{W}_\gamma(\mathtt{p}, \mathtt{q}^*) = -\sqrt{W}\boldsymbol{\lambda}^*$. Then we have

$$\|\nabla \mathcal{W}_\gamma(\mathtt{p}, \mathtt{q}^*)\|_2^2 = \left\|-\sqrt{W}\boldsymbol{\lambda}^*\right\|_2^2 = \langle \sqrt{W}\boldsymbol{\lambda}^*, \sqrt{W}\boldsymbol{\lambda}^*\rangle = \langle \boldsymbol{\lambda}^*, W\boldsymbol{\lambda}^*\rangle \geq \lambda^+_{min}(W)\,\|\boldsymbol{\lambda}^*\|_2^2, \quad (37)$$

where the last inequality holds due to $\boldsymbol{\lambda}^* \in \left(\mathrm{Ker}(\sqrt{\mathrm{W}})\right)^\perp$

Hence, we get

$$\|\boldsymbol{\lambda}^*\|_2^2 \leq R^2 = \frac{\left\|\nabla \mathcal{W}_\gamma(\mathtt{p}, \mathtt{q}^*_\gamma)\right\|_2^2}{\lambda^+_{min}(W)} = \frac{\sum_{l=1}^m w_l^2 \left\|\nabla \mathcal{W}_{\gamma(l)}(p_l, q^*_\gamma)\right\|_2^2}{\lambda^+_{min}(W)} \quad (38)$$

Let us now estimate $\left\|\nabla \mathcal{W}_{\gamma(l)}(p_l, q^*_\gamma)\right\|_2^2$. From (3), we can construct the dual problem to the regularized optimal transport problem

$$\mathcal{W}_{\gamma(l)}(p, q) = \min_{\pi \in \Pi(p,q)} \{\langle \pi, C\rangle + \gamma(l) H(\pi)\} = \max_{\mu,\nu} \left\{-\langle \mu, p\rangle - \langle \nu, q\rangle - \frac{\gamma(l)}{e} e^{-\frac{\mu}{\gamma(l)}} e^{-\frac{C}{\gamma(l)}} e^{-\frac{\nu}{\gamma(l)}}\right\}$$

By [Cuturi and Peyré, 2016, Proposition 2.3], $\nabla_q \mathcal{W}_{\gamma(l)}(p, q) = -\nu^*$, where ν^* is the solution to the dual problem satisfying $\langle \nu^*, \mathbb{1}\rangle = 0$. Hence, $\min_{i=1,\dots,n} \nu_i^* \leq 0 \leq \max_{i=1,\dots,n} \nu_i^*$. As it follows from [Dvurechensky et al., 2018b, Lemma 1]

$$\max_{i=1,\dots,n} \nu_i^* - \min_{i=1,\dots,n} \nu_i^* \leq \|C_l\|_\infty - \gamma(l) \ln\left(\min_i [p_l]_i\right) = \|C_l\|_\infty + \gamma(l) \ln\left(\frac{8n}{\varepsilon}\right),$$

where we used the fact that the p_l was redefined in Algorithm 6 in such a way that $\min_i [p_l]_i \geq \frac{\varepsilon}{8n}$ and also that our variable ν^* and their dual variable u^* satisfy $u^* = -\frac{\nu^*}{\gamma(l)} - \frac{1}{2}$. Making the same arguments as in the proof [Lin et al., 2019, Lemma 3.2.], we obtain from the above two facts that

$$\|\nu^*\|_2 \leq \|\nu^*\|_\infty \sqrt{n} \leq \|C_l\|_\infty \sqrt{n} + \frac{\gamma\sqrt{n}}{w_l} \ln\left(\frac{8n}{\varepsilon}\right),$$

where we used that $\gamma(l) = \gamma / w_l$. Thus,

$$\sum_{l=1}^m w_l^2 \left\|\nabla \mathcal{W}_{\gamma(l)}(p_l, q^*_\gamma)\right\|_2^2 \leq 2n \sum_{l=1}^m w_l^2 \|C_l\|_\infty^2 + 2n\gamma^2 \ln^2\left(\frac{8n}{\varepsilon}\right).$$

Since γ is chosen proportional to ε which is small, we can neglect the second term in comparison with the first one.

□

Proof of Theorem 3. By Theorem 4, we have

$$\sum_{l=1}^m w_l \mathcal{W}_{\gamma(l)}(p_l, q_l^N) - \sum_{l=1}^m w_l \mathcal{W}_{\gamma(l)}(p_l, q^*) \leq \varepsilon/2, \quad \|\sqrt{W}\mathtt{q}^N\|_2 \leq \varepsilon/2R \quad (39)$$

Since $KL(\pi|\theta) \geq 0$, we have

$$\sum_{l=1}^{m} w_l \mathcal{W}(p_l, q_l^N) - \sum_{l=1}^{m} w_l \mathcal{W}(p_l, q^*) \leq \sum_{l=1}^{m} w_l \mathcal{W}_{\gamma(l)}(p_l, q_l^N) - \sum_{l=1}^{m} w_l \mathcal{W}(p_l, q^*). \tag{40}$$

By definition of the objective $\mathcal{W}_\gamma(\mathtt{p}, \cdot)$ in (27),

$$\begin{aligned}
\sum_{l=1}^{m} w_l \mathcal{W}_{\gamma(l)}(p_l, q^*) = & \min_{\substack{q_1=\cdots=q_m \\ q_1,\ldots q_m \in S_n(1)}} \sum_{l=1}^{m} w_l \min_{\pi \in \Pi(p_l, q_l)} \left\{ \sum_{i,j=1}^{n} C_{ij}\pi_{ij} + \gamma KL(\pi|\theta) \right\} \\
\leq & \min_{\substack{q_1=\cdots=q_m \\ q_1,\ldots q_m \in S_1(n)}} \sum_{l=1}^{m} \left\{ \min_{\pi \in \Pi(p_l, q_l)} w_l \sum_{i,j=1}^{n} C_{ij}\pi_{ij} + w_l \max_{\pi \in \Pi(p_l, q_l)} \gamma KL(\pi|\theta) \right\} \\
\leq & \min_{\substack{q_1=\cdots=q_m \\ q_1,\ldots q_m \in S_n(1)}} \sum_{l=1}^{m} \left\{ \min_{\pi \in \Pi(p_l, q_l)} \sum_{i,j=1}^{n} C_{ij}\pi_{ij} + 2\sum_{l=1}^{m} w_l \gamma(l) \ln n \right\} \\
\leq & \min_{\substack{q_1=\cdots=q_m \\ q_1,\ldots q_m \in S_n(1)}} \sum_{l=1}^{m} \mathcal{W}(p_l, q_l) \ + 2\ln n \sum_{l=1}^{m} w_l \gamma(l) \\
= & \sum_{l=1}^{m} \mathcal{W}(p_l, q^*) + 2\ln n \sum_{l=1}^{m} w_l \gamma(l),
\end{aligned} \tag{41}$$

where we chose $\theta_{ij} = 1/n^2$ for all $i, j = 1, \ldots n$ so $KL(\pi|\theta) \in [0, 2\ln n]$.

Substituting (41) in (40) we get

$$\begin{aligned}
\sum_{l=1}^{m} w_l \mathcal{W}_{\gamma(l)}(p_l, q_l^N) - \sum_{l=1}^{m} w_l \mathcal{W}(p_l, q^*) \leq & \sum_{l=1}^{m} w_l \mathcal{W}_{\gamma(l)}(p_l, q_l^N) \\
& - \sum_{l=1}^{m} w_l \mathcal{W}_{\gamma(l)}(p_l, q^*) + 2\ln n \sum_{l=1}^{m} w_l \gamma(l)
\end{aligned} \tag{42}$$

Using this inequality and (39) we get

$$\sum_{l=1}^{m} w_l \mathcal{W}(p_l, q_l^N) - \sum_{l=1}^{m} w_l \mathcal{W}(p_l, q^*) \leq \varepsilon/2 + 2\ln n \sum_{l=1}^{m} w_l \gamma_l. \tag{43}$$

Since $\gamma(l) = \gamma/w_l$ with $\gamma = \varepsilon/(4m\ln n)$, we obtain thath the inequality (39) hold. Combining the values of γ, L from Lemma 7, R from Lemma 8 with the estimate for N in Theorem 4 and the fact that $\chi(W) = \chi(\bar{W})$, we obtain an estimate for the number of iterations of the algorithm. Let us estimate the complexity of the algorithm. For each l we need to calculate the gradient $\mathcal{W}^*_{\gamma(l),p_l}(\cdot)$, which requires $O(n^2)$ arithmetic operations. To calculate $\sum_{j=1}^{m} W_{lj} \nabla \mathcal{W}^*_{\gamma(l),p_l)}(\lambda_j^{k+1})$ one needs $O(n \cdot \mathrm{nnz}(\bar{W}_l))$ arithmetic operations, where $\mathrm{nnz}(\bar{W}_l)$ is the number of non-zero elements in matrix $\bar{W}$ in the l row. More precisely, the dimension

of $\nabla \mathcal{W}^*_{\gamma(l),p_l}(\cdot)$ is n and the matrix W_{lj} is diagonal for each $l, j = 1, \ldots, m$. Using definition of W we get that the complexity of calculating the gradient. Other operations require $O(n)$ operations. Hence, the complexity of one iteration is

$$O\left(mn^2 + \sum_{l=1}^{m} n \cdot \text{nnz}(\bar{W}_l)\right) = O\left(mn^2 + n \cdot \text{nnz}(\bar{W})\right) \tag{44}$$

and the total complexity follows from multiplying this value by N.

□

Let us make a couple of remarks. As for the choice of $\bar{W}$ one can show (by using graph sparsificators) that it can be chosen such that $\chi(W) = \chi(\bar{W}) = O(\text{Poly}(\ln(m)))$ and $\text{nnz}(\bar{W}) = O(m\text{Poly}(\ln(m)))$. For details on the graph sparsificators we refer to Vaidya [1990], Bern et al. [2006], Spielman and Teng [2014]. In the simple case of equal weights $w_l = \frac{1}{m}$, the complexity of approximating non-reguarized barycenter by accelerated gradient descent can be estimated as $\widetilde{O}(mn^{2.5}/\varepsilon)$. In the distributed setting, each of m nodes makes $\widetilde{O}(n^{2.5}/\varepsilon)$ arithmetic operations, while the number of communications rounds is $\widetilde{O}(\sqrt{n}/\varepsilon)$. The case of general weights is interesting with respect to bootstrap procedure allowing to construct confidence sets for barycenter Ebert et al. [2017].

There is an interesting connection of our work with Cuturi and Peyré [2016]. Consider a particular case of equal weights $w_1 = \cdots = w_m = 1$ and matrix $\bar{W}$ corresponding to the star graph topology. Then the dual problem (27) has the form

$$\min_{\lambda_1,\ldots,\lambda_m \in \mathbb{R}^n} \left\{ \sum_{l=1}^{m-1} \mathcal{W}^*_{\gamma,p_l}\left(\lambda_l - \frac{1}{m}\lambda_m\right) + \mathcal{W}^*_{\gamma,p_m}\left(\frac{m-1}{m}\lambda_m - \sum_{l=1}^{m-1}\lambda_l\right)\right\} \tag{45}$$

Changing the variable $\hat{\lambda}_l = \lambda_l - \frac{1}{m}\lambda_m$ we come to the following formulation.

$$\min_{\hat{\lambda}_1,\ldots,\hat{\lambda}_{m-1} \in \mathbb{R}^n} \sum_{l=1}^{m-1} \mathcal{W}^*_{\gamma,p_l}(\hat{\lambda}_l) + \mathcal{W}^*_{\gamma,p_m}\left(-\sum_{l=1}^{m-1}\hat{\lambda}_l\right) \tag{46}$$

Hence, the approach presented in Cuturi and Peyré [2016], in Theorem 3.1 is the particular case for the approach described above, corresponding to the the star graph.

Conclusion

In this paper we show that IBP algorithm from Benamou et al. [2015] for Wasserstein barycenter problem can be implemented in a centralized distributed manner such that each node fulfils $\widetilde{O}\left(n^2/\varepsilon^2\right)$ arithmetic operations and the number of communication rounds is $\widetilde{O}\left(1/\varepsilon^2\right)$. We note that proper proximal envelope of this algorithm can sometimes accelerate this bounds in terms of the dependence of ε. We also describe accelerated primal-dual gradient algorithm for the same problem. The proposed algorithm can be implemented in

a more general decentralized distributed setting such that, to find an ε-approximation for the non-regularized barycenter, each node performs $\widetilde{O}(n^{2.5}/\varepsilon)$ arithmetic operations and the number of communication rounds is $\widetilde{O}(\sqrt{n}/\varepsilon)$.

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