Stochastic Approximation versus Sample Average Approximation for population Wasserstein barycenters

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\textbf{ABSTRACT}

In machine learning and optimization community there are two main approaches for convex risk minimization problem, namely, the Stochastic Approximation (SA) and the Sample Average Approximation (SAA). In terms of oracle complexity (required number of stochastic gradient evaluations), both approaches are considered equivalent on average (up to a logarithmic factor). The total complexity depends on the specific problem, however, starting from work \cite{50} it was generally accepted that the SA is better than the SAA. Nevertheless, in case of large-scale problems SA may run out of memory as storing all data on one machine and organizing online access to it can be impossible without communications with other machines. SAA in contradistinction to SA allows parallel/distributed calculations. In this paper, we shed new light on the comparison of SA and SAA for particular problem of calculating the population (regularized) Wasserstein barycenter of discrete measures. The conclusion is valid even for non-parallel (non-decentralized) setup.

\textbf{KEYWORDS}

empirical risk minimization, stochastic approximation, sample average approximation, Wasserstein barycenter, Fréchet mean, stochastic gradient descent, mirror descent.

\section{1. Introduction}

In this work, we consider the problem of calculating the population \textit{mean} (barycenter) of probability measures with discrete support (e.g., images). We define the notion of the population barycenter by using Fréchet mean that is an extension of the Euclidean barycenter to non-linear spaces with non-Euclidean metrics. Fréchet mean of distribution \( \mathbb{P} \) on a metric space \( (\mathcal{M}, W_2) \) is the solution of the following optimization problem

\begin{equation}
    p^* = \arg\min_{p \in \mathcal{M}} \int W_2^2(p, q) d\mathbb{P}(q) = \arg\min_{p \in \mathcal{M}} \mathbb{E}_q W_2^2(p, q), \quad q \sim \mathbb{P},
\end{equation}

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where $W_2$ is the 2-Wasserstein distance defined by optimal transport (OT) problem. A nice survey of OT and Wasserstein barycenters is presented in books [56, 65]. In this paper, we refer to $p^*$ from (1) as the population Wasserstein barycenter. The optimization problem (1) is the risk minimization problem (the objective function is given in a form of the expectation) for which there are two classical approaches based on Monte Carlo sampling techniques: the Stochastic Approximation (SA) and the Sample Average Approximation (SAA). The SAA approach approximates the true problem (1) by the sample average (empirical barycenter)

$$\hat{p}^m = \arg\min_{p \in \mathcal{M}} \frac{1}{m} \sum_{k=1}^{m} W_2^2(p, q^k),$$

(2)

where $q^1, q^2, \ldots, q^m$ are realizations of random variable $q$ according to distribution $P$. The number of realizations $m$ is adjusted by the desired precision for the approximation of problem (1) by problem (2). An approximation of a probability measures by a measure with finite support were studied in [28, 49, 55, 66]. We notice that both SA and SAA methods are not algorithms as corresponding problems (1) and (2) require the use of appropriate numerical algorithms. The main difference of problem (1) from the standard risk minimization problems is the high computational complexity of calculating the objective under the expectation itself (Wasserstein distance) solving corresponding OT problem between two measures that requires $\tilde{O}(n^3)$ arithmetic iterations ($n$ is the size of the support of the measures) [11, 16, 24, 56, 64]. Entropic regularization of OT [13] improves statistical properties of Wasserstein distance [7, 43] and reduces the computational complexity to $n^2 \min\{\tilde{O}(\frac{1}{\varepsilon}), \tilde{O}(\sqrt{n})\}$ [11]. This regularization shows good results in generative models [29], multi-label learning [23], dictionary learning [60], image processing [14, 58], neural imaging [32].

The aim of this paper is to compare two approaches, which are SA and SAA, for two settings of the Wasserstein barycenter problem: when the barycenter is defined as the minimizer of the expectation of OT and as the minimizer of the expectation of entropy-regularized OT. Motivated by enormous applications of the Wasserstein distance and Wasserstein barycenters to discrete objects, such as images, videos and texts, we limit ourselves by considering only discrete probability measures. Indeed, a continuous measure can be approximated by its empirical counterpart and the convergence of these measures with respect to (w.r.t.) entropy-regularized OT cost was studied in [7, 49].

1.1. Contribution and Related Work

SA and SAA approaches. This paper is inspired by the work [50], where it is stated that SA approach outperforms SAA approach for certain class of convex stochastic problems. Our aim is to show that for population Wasserstein barycenter problem this superiority is inverted. We provide detailed comparison with stating the complexity bounds of implementations of the SA and the SAA approaches for population Wasserstein barycenter problem and population Wasserstein barycenter problem defined w.r.t. regularized OT. As a byproduct, we also construct the confidence interval for barycenter $p^*$ defined w.r.t. $\mu$-regularized OT in the 2-norm.

1 The estimate $n^2 \min\{\tilde{O}(\frac{1}{\varepsilon}), \tilde{O}(\sqrt{n})\}$ is the best theoretically known estimate for solving OT problem [10, 37, 45, 57]. The best known practical estimates are $\sqrt{n}$ times worse (see [34] and references therein).
Consistency and rates of convergence. Consistency of empirical barycenter as an estimator of population barycenter w.r.t. Wasserstein distance as the number of measures tends to infinity was studied in many papers, e.g., \cite{9, 46, 47, 55, 59}, under some conditions on the process generated the measures. Moreover, the authors of \cite{11} provide the rate of this convergence but under restrictive assumption on the process (it must be from admissible family of deformations, i.e., it is a gradient of a convex function). Without any assumptions on generating process, the rate of convergence was obtained in \cite{8}, however, only for measures with one-dimensional support. For some specific types of metrics and measures, the rates of convergence were also provided in works \cite{12, 31, 44}.

**Penalization of barycenter problem.** Population Wasserstein barycenter can be defined by two ways: as the minimizer of the expectation of OT distance or entropy-regularized (also called smoothed) OT distance. The first problem can be led to the second problem if one wants to reduce the computational complexity of solving OT problem and get more stable optimization problem. Alternative regularization of the problem is introducing a strongly convex penalty function in the population Wasserstein problem itself. The advantages of convex penalization, which are the existence, uniqueness and stability of penalized barycenter, and the convergence of penalized barycenter to the population barycenter are studied in \cite{6}. For a general convex (but not strongly convex) optimization problem, empirical minimization may fail in offline approach despite the guaranteed success of an online approach if no regularization was introduced \cite{61}. The limitations of the SAA approach for non-strongly convex case are also discussed in \cite{33, 62}. Our contribution includes introducing new regularization for population Wasserstein barycenter problem that improves the complexity bounds for standard penalty (squared norm penalty) \cite{61}. This regularization relies on the Bregman divergence from \cite{3}.

1.2. Paper organization

The structure of the paper is the following. Section 2 recalls OT problem, entropy-regularized OT problem and its properties. Section 3 presents the comparison of SA and SAA approaches for the problem of population Wasserstein barycenter defined w.r.t. regularized OT. In Section 4, we refuse the entropic regularization of OT and compare SA and SAA for the population Wasserstein barycenter problem. Section 5 presents new regularization for population Wasserstein problem. Finally, in Section 6, we present numerical experiments to support our theoretical results.

2. Entropy-regularized OT

2.1. General setup and definitions

Here, we briefly recall some key definitions used throughout the paper. For any finite-dimensional real vector space $X$, we denote its dual space by $X^\ast$. Let $\| \cdot \|$ be some norm on $X$, then the dual norm $\| \cdot \|_\ast$ is the norm on $X^\ast$ that is defined as follows

$$\| \lambda \|_\ast = \max \{ \langle \lambda, x \rangle : \| x \| \leq 1 \}.$$ 

**Definition 2.1.** A function $f : \mathcal{X} \to \mathbb{R}$ is $M$-Lipschitz continuous w.r.t. norm $\| \cdot \|$ if
it satisfies
\[ \| f(x) - f(y) \|_* \leq M \| x - y \|, \quad \forall x, y \in \mathcal{X}. \]

**Definition 2.2.** A function \( f : \mathcal{X} \to \mathbb{R} \) is \( \mu \)-strongly convex w.r.t. norm \( \| \cdot \| \) if it is continuously differentiable and it satisfies
\[ f(x) - f(y) - \langle \nabla f(y), x - y \rangle \geq \mu \| x - y \|^2, \quad \forall x, y \in \mathcal{X}. \]

**Definition 2.3.** The Fenchel–Legendre conjugate for a function \( f : \mathcal{X} \to \mathbb{R} \) is
\[ f^*(y) \triangleq \sup_{x \in \mathcal{X}} \{ \langle x, y \rangle - f(x) \}. \]

We also use denotation \( \tilde{O}(\cdot) \) when we want to indicate the complexity hiding constants and logarithms.

### 2.2. Entropy-regularized OT, Dual Formulation and Properties

Let \( S_n(1) = \{ a \in \mathbb{R}_+^n \mid \sum_{i=1}^n a_i = 1 \} \) be the probability simplex and \( \delta_x \) be the Dirac measure at point \( x \), then measure \( p \) with finite support of size \( n \) can be presented in the form \( p = \sum_{i=1}^n p_i \delta_{x_i} \), where \( p \in S_n(1) \) is the histogram. For two histograms \( p, q \in S_n(1) \) we define optimal transport (OT) as the following optimization problem
\[ W(p, q) = \min_{\pi \in \Pi(p, q)} (C, \pi), \]
where \( \pi \) is a transport plan with marginals \( p \) and \( q \) from transportation polytype \( \Pi(p, q) = \{ \pi \in \mathbb{R}_+^{n \times n} : \pi 1 = p, \pi^T 1 = q \} \), \( C \) is the (ground) cost matrix (\( C_{ij} \) is the cost to move a unit mass from support point \( x_i \) of measure \( p \) to support point \( x_j \) of measure \( q \)). When \( C_{ij} = d(x_i, x_j)^2 \), where \( d(x_i, x_j) \) is the distance on support points \( x_i, x_j \), then \( W(p, q)^{1/2} \) is known as the 2-Wasserstein distance on \( S_n(1) \). In what follows we rewrite the population Wasserstein barycenter \( 1 \)

\[ p^* = \arg \min_{p \in S_n(1)} \int W(p, q) d\mathbb{P}(q) = \arg \min_{p \in S_n(1)} \mathbb{E}_q W(p, q). \]

and its empirical counter part \( 2 \)

\[ \hat{p}^m = \arg \min_{p \in S_n(1)} \frac{1}{m} \sum_{k=1}^m W(p, q^k). \]

in our introduced notations. We define entropy-regularized OT as the following optimization problem penalized by the negative entropy with \( \mu \geq 0 \)
\[ W_\mu(p, q) = \min_{\pi \in \Pi(p, q)} \left\{ (C, \pi) + \mu \langle \pi, \ln \pi \rangle \right\}. \]

\(^2\text{We omit the sub-index 2 for simplicity.}\)
One of the advantages of entropic regularization of OT is existing a closed-form representation for its dual (Fenchel–Legendre) function that leads to the following results.

**Proposition 2.4.** Given two histograms $p, q \in S_n(1)$, dual formulation of entropy-regularized OT is

$$W_\mu(p, q) = \max_{\lambda \in \mathbb{R}^n} \left\{ \langle \lambda, p \rangle - \mu \sum_{j=1}^n q_j \ln \left( \frac{1}{q_j} \sum_{i=1}^n e^{-\frac{C_{ij} + \lambda_i}{\mu}} \right) \right\},$$  \hspace{1cm} (3)

Moreover, the gradient of $W_\mu(p, q)$ w.r.t. $p$ is the solution $\lambda^*$ of this optimization problem \([3]\) such that $\langle \lambda^*, 1 \rangle = 0$ \([26, 56]\)

$$\nabla_p W_\mu(p, q) = \lambda^*. \hspace{1cm} (4)$$

The (Fenchel–Legendre) dual function for $W_\mu(p, q)$ has the following closed-form representation

$$D_q(\lambda) = \mu \sum_{j=1}^n q_j \ln \left( \frac{1}{q_j} \sum_{i=1}^n e^{-\frac{C_{ij} + \lambda_i}{\mu}} \right), \quad \forall \lambda \in \mathbb{R}^n. \hspace{1cm} (5)$$

**Proof.** We add the constraints $\pi^T 1 = p$ and $\pi^T 1 = q$ into the objective in regularized OT with corresponding Lagrangian dual variables $\lambda$ and $\nu$, and solve the problem w.r.t. $\nu$ analytically

$$W_\mu(p, q) = \min_{\pi \in \Pi(p, q)} \sum_{i,j=1}^n (C_{ij} \pi_{i,j} + \mu \pi_{i,j} \ln \pi_{i,j})$$

$$= \max_{\lambda, \nu \in \mathbb{R}^n} \left\{ \langle \lambda, p \rangle + \langle \nu, q \rangle - \mu \sum_{i,j=1}^n \exp \left( -\frac{C_{ij} + \lambda_i + \nu_j}{\mu} \right) - 1 \right\}$$

$$= \max_{\lambda \in \mathbb{R}^n} \left\{ \langle \lambda, p \rangle - \mu \sum_{j=1}^n q_j \ln \left( \frac{1}{q_j} \sum_{i=1}^n \exp \left( -\frac{C_{ij} + \lambda_i}{\mu} \right) \right) \right\}. $$

The next two statements of the proposition directly follows from this representation. \hfill \Box

The proposition below describes the properties of entropy-regularized OT.

**Proposition 2.5** (Properties of $W_\mu(p, q)$). Given two histograms $p$ and $q$ from the entry of $S_n(1)$, entropy-regularized OT $W_\mu(p, q)$ is

- $\mu$-strongly convex in $p$ w.r.t. the 2-norm

$$W_\mu(p, q) \geq W_\mu(p', q) + \langle \nabla W_\mu(p', q), p - p' \rangle + \frac{\mu}{2} ||p - p'||^2_2,$$

for any $p, p'$ from the interior of $S_n(1)$
• $M_\infty$-Lipschitz continuous in $p$ w.r.t the 1-norm.

$$|W_\mu(p, q) - W_\mu(p', q)| \leq M_\infty\|p - p'\|_1,$$

for any $p, p'$ from the interior of $S_n(1)$. Hence, $W_\mu(p, q)$ is also $M$-Lipschitz in $p$ w.r.t the 2-norm. Hereby, $M \leq \sqrt{n}M_\infty$, $M_\infty = O(\|C\|_\infty)$.

**Proof.** The gradient of function $D_q(\lambda)$ in (5) is $\frac{1}{\mu}$-Lipschitz continuous in the 2-norm [19, Lemma 1]. From this and dual formulation of regularized OT [3] we conclude that $W_\mu(p, q)$ is $\mu$-strongly convex w.r.t $p$ in the 2-norm [11, Theorema 6], [51]. We also used here that the dual norm for the 2-norm is again the 2-norm.

The second statement follows from the fact that the $\infty$-norm of the solution $\lambda^*$ of (3) is upper bounded (10, Lemma 10) for the $\infty$-norm and (34, Lemma 7) for the 2 norm. From this and (4) we get that the gradient of $W_\mu(p, q)$ in $p$ is upper bounded that means Lipschitz continuity of $W_\mu(p, q)$. From (11) assuming that the measures are separated from zero, we roughly take $M_\infty = O(\|C\|_\infty)$ . This separation can be achieved by simple preprocessing of measures, moreover, the most of transport algorithms require this preprocessing.

In what follows, we use Preposition 2.5 for any $p, q \in S_n(1)$ keeping in mind that $p, q$ are from the interior of $S_n(1)$ as we can easily get this condition by adding some noise and normalize the measures. We also notice that if some measures are from the interior of $S_n(1)$ then their barycenter will be also from the interior of $S_n(1)$.

### 3. Population Wasserstein barycenter w.r.t regularized OT

In this section, we present the comparison of SA and SAA approaches for population Wasserstein barycenter defined w.r.t. regularized OT

$$p^*_\mu = \arg \min_{p \in S_n(1)} E_q W_\mu(p, q).$$

(6)

Throughout this section we use the following simplification for the objective

$$W_\mu(p) \triangleq E_q W_\mu(p, q).$$

**3.1. Stochastic Approximation (SA)**

We present an implementation of the SA approach for problem (6). To do so, we assume that we can sample measures $q^1, q^2, q^3, \ldots$ from distribution $\mathbb{P}$ ($q \sim \mathbb{P}$). We define stochastic subgradient w.r.t. $p$ by $\nabla_p W_\mu(p, q^k)$ ($k = 1, 2, 3, \ldots$). The classical SA algorithm with stochastic oracle is the following

$$p^{k+1} = \Pi_{S_n(1)} \left( p^k - \eta_k \nabla_p W_\mu(p^k, q^k) \right),$$

(7)
where \( \Pi_{S_n(1)}(p) \) is the projection onto \( S_n(1) \) and \( \nabla_p^\delta W_\mu(p^k, q^k) \) is \( \delta \)-approximation for the true gradient \( \nabla_p W_\mu(p^k, q^k) \)

\[
\|\nabla_p^\delta W_\mu(p, q) - \nabla_p W_\mu(p, q)\|_2 \leq \delta, \quad \forall q \in S_n(1). \tag{8}
\]

Using [61] we can compute the approximate gradient \( \nabla_p^\delta W_\mu(p, q) \) by Sinkhorn algorithm [20, 56]. Based on (7) we provide online algorithm (Alg. 1) that inputs online sequence of measures \( q^1, q^2, q^3, \ldots \) (realizations of \( q \)) and at each stochastic gradient descent iteration calls Sinkhorn algorithm to compute the approximation for the gradient of \( W_\mu(p^k, q^k) \) with precision \( \delta \). We take step size \( \eta \) according to [36].

**Algorithm 1 Online Stochastic Gradient Descent (SGD)**

**Input:** starting point \( p^1 \in S_n(1) \), realization \( q^1 \), precision of gradient calculation \( \delta, \mu \)

1. for \( k = 1, 2, 3, \ldots \) do
2. \( \eta_k = \frac{1}{\mu k} \)
3. \( p^{k+1} = \Pi_{S_n(1)} \left(p^k - \eta_k \nabla_p^\delta W_\mu(p^k, q^k)\right) \),
   where \( \nabla_p^\delta W_\mu(p^k, q^k) \) is calculated by Sinkhorn algorithm (\( \delta \) is defined by (8)), \( \Pi_{S_n(1)}(p) = \arg \min_{v \in S_n(1)} \|p - v\|_2 \) is the projection onto \( S_n(1) \) (\( \Pi_{S_n(1)}(p) \) is calculated by algorithm from [17])
4. Sample \( q^{k+1} \)

**Output:** \( p^1, p^2, p^3, \ldots \)

One of the benefits of online approach is no need to fix the number of measures that allows to regulate the precision of the estimate for the barycenter. Moreover, the problem of storing a large number of measures in a computing node is not present if we have an access to online oracle, e.g., some measuring device.

To approximate population barycenter \( p^*_\mu \) by the outputs of Algorithm 1 we use online-to-batch conversions [61] and define \( \tilde{p}^N \) as the average of online outputs \( p^1, \ldots, p^N \) from Algorithm 1: \( \tilde{p}^N = \frac{1}{N} \sum_{k=1}^N p^k \). The convergence properties of \( \tilde{p}^N \) to population barycenter \( p^*_\mu \) are presented in the following theorem.

**Theorem 3.1.** Let \( \tilde{p}^N \) be the average of \( N \) online outputs of Algorithm 1. Then, with probability \( \geq 1 - \alpha \) we have

\[
\mathbb{E}_q \left[W_\mu(\tilde{p}^N, q) - W_\mu(p^*_\mu, q)\right] = O \left( \frac{M^2 \ln(N/\alpha)}{\mu N} + \delta D_2 \right) = O \left( \frac{M^2 \ln(N/\alpha)}{\mu N} + \delta \right),
\]

where \( D_2 = \max_{p', p'' \in S_n(1)} \|p' - p''\|_2 = \sqrt{2} \). Let Algorithm 1 run with \( \delta = O(\varepsilon) \) and \( N = \tilde{O} \left( \frac{M^2}{\mu^2} \right) \). Then, with probability \( \geq 1 - \alpha \) the following holds

\[
\mathbb{E}_q \left[W_\mu(\tilde{p}^N, q) - W_\mu(p^*_\mu, q)\right] \leq \varepsilon \quad \text{and} \quad \|\tilde{p}^N - p^*_\mu\|_2 \leq \sqrt{2\varepsilon/\mu}.
\]

The total complexity of Algorithm 1 is

\[
\tilde{O} \left( \frac{M^2}{\mu \varepsilon n^2} \min \left\{ \exp \left( \frac{\|C\|_\infty}{\mu} \right) \left( \frac{\|C\|_\infty}{\mu} + \ln \left( \frac{\|C\|_\infty}{\gamma \varepsilon^2} \right) \right), \sqrt{\frac{n}{\gamma \mu \varepsilon^2}} \right\} \right).
\]
where \( \gamma \triangleq \sigma_{\min}(\nabla^2 D_q(\lambda^*)) > 0 \), \( \sigma_{\min}(A) \) is the smallest positive eigenvalue of positive semi-definite matrix \( A \).

**Proof.** From \( \mu \)-strongly convexity of \( W_\mu(p, q^k) \) w.r.t. to \( p \), it follows

\[
W_\mu(p^*, q^k) \geq W_\mu(p^k, q^k) + \langle \nabla_p W_\mu(p^k, q^k), p^* - p^k \rangle + \frac{\mu}{2} ||p^* - p^k||_2.
\]

Adding and subtracting the term \( \langle \nabla_\delta p W_\mu(p^k, q^k), p^* - p^k \rangle \) we get using Cauchy–Schwarz inequality

\[
W_\mu(p^*, q^k) \geq W_\mu(p^k, q^k) + \langle \nabla_\delta p W_\mu(p^k, q^k), p^* - p^k \rangle + \frac{\mu}{2} ||p^* - p^k||_2 + \delta ||p^* - p^k||_2.
\]

(9)

From the update rule for \( p^{k+1} \) we have

\[
||p^{k+1} - p^*||_2 = ||\Pi_{S_1(n)}(p^k - \eta_k \nabla_\delta p W_\mu(p^k, q^k)) - p^*||_2 \leq ||p^k - \eta_k \nabla_\delta p W_\mu(p^k, q^k) - p^*||_2 \leq ||p^k - p^*||_2^2 + \eta_k^2 ||\nabla_\delta p W_\mu(p^k, q^k)||_2^2 - 2\eta_k \langle \nabla_\delta p W_\mu(p^k, q^k), p^k - p^* \rangle.
\]

From this it follows

\[
\langle \nabla_\delta p W_\mu(p^k, q^k), p^k - p^* \rangle \leq \frac{1}{2\eta_k} (||p^k - p^*||_2^2 - ||p^{k+1} - p^*||_2^2) + \eta_k^2 ||\nabla_\delta p W_\mu(p^k, q^k)||_2^2.
\]

Together with (9) we get

\[
W_\mu(p^k, q^k) - W_\mu(p^*, q^k) \leq \frac{1}{2\eta_k} (||p^k - p^*||_2^2 - ||p^{k+1} - p^*||_2^2) - \left( \frac{\mu}{2} + \delta \right) ||p^* - p^k||_2 + \frac{\eta_k^2}{2} ||\nabla_\delta p W_\mu(p^k, q^k)||_2^2.
\]

3Due to the results of [22], we may expect \( \gamma \) to be \( n^{-\beta} \) with \( \beta \geq 0 \).
Summing this from 1 to \( N \), using \( \eta_k = \frac{1}{\mu k} \) and \( \| \nabla W_\mu(p, q) \|_2 \leq M \) we get

\[
\sum_{k=1}^{N} \left( W_\mu(p^k, q^k) - W_\mu(p^*, q^k) \right) \leq \frac{1}{2} \sum_{k=1}^{N} \left( \frac{1}{\eta_k} - \frac{1}{\eta_{k-1}} + \mu + \delta \right) \| p^* - p^k \|_2
\]

\[
+ \frac{1}{2} \sum_{k=1}^{N} \eta_k \| \nabla_\mu W_\mu(p^k, q^k) \|_2^2
\]

\[
\leq \frac{1}{2} \sum_{k=1}^{N} \delta \| p^* - p^k \|_2 + M^2 \sum_{k=1}^{N} \frac{1}{\mu k}
\]

\[
\leq \frac{1}{2} \delta D_2 N + \frac{M^2}{\mu} (1 + \ln N) = O \left( \frac{M^2 \ln N}{\mu} + \delta D_2 N \right),
\]

where \( D_2 = \max_{p', p'' \in S_n(1)} \| p' - p'' \|_2 = \sqrt{2} \). Here the last bound takes place due to the sum of harmonic series.

Next we estimate the codomain (image) of \( W(p, q) \)

\[
\max_{p, q \in S_n(1)} W_\mu(p, q) = \max_{p, q \in S_n(1)} \min_{\pi \in R^n \times n, \pi^T \pi = 1} \sum_{i,j=1}^{n} (C_{ij} \pi_{ij} + \mu \pi_{ij} \ln \pi_{ij})
\]

\[
\leq \max_{\pi \in R^n \times n, \sum_{i,j=1}^{n} \pi_{ij} = 1} \sum_{i,j=1}^{n} (C_{ij} \pi_{ij} + \mu \pi_{ij} \ln \pi_{ij}) \leq \| C \|_{\infty}.
\]

Therefore, \( W_\mu(p, q) : S_n(1) \times S_n(1) \rightarrow [-2\mu \ln n, \| C \|_{\infty}] \).

Then using this we refer to [42, Theorem 2] with the regret estimated by (10) and get with probability \( \geq 1 - \alpha \) the first statement of the theorem

\[
W_\mu(\tilde{p}^N) - W_\mu(p^*_\mu) = O \left( \frac{M^2 \ln(N/\alpha)}{\mu N} + \delta D_2 \right) = O \left( \frac{M^2 \ln(N/\alpha)}{\mu N} + \delta \right).
\]

Equating the right-hand side (r.h.s.) of this equality to epsilon we get the expressions for \( N \) and \( \delta \). The statement about the confidence region for the barycenter follows directly from strong convexity of \( W_\mu(p, q) \) and \( W_\mu(p) \).

The proof of algorithm complexity follows from the complexity of Sinkhorn algorithm. To state the complexity of Sinkhorn algorithm we firstly define \( \tilde{\delta} \) as the accuracy in function value of the inexact solution \( \lambda \) of max-problem in (3). Using this we formulate the number of iteration of Sinkhorn [45 [63]

\[
\tilde{O} \left( \exp \left( \frac{\| C \|_{\infty}}{\mu} \right) \left( \frac{\| C \|_{\infty}}{\mu} + \ln \left( \frac{\| C \|_{\infty}}{\delta} \right) \right) \right).
\]

The number of iteration for Accelerated Sinkhorn can be improved [34]

\[
\tilde{O} \left( \sqrt{\frac{n}{\mu \delta}} \right)
\]
Multiplying both of this estimates by the number of iterations $N$ (measures) and complexity of each iteration of Sinkhorn algorithm $O(n^2)$, taking the minimum we get the last statement of the theorem, where we used the transition from accuracy in function value $\tilde{\delta}$ to accuracy in argument $\delta$. From $\gamma \triangleq \sigma_{\text{min}}(\nabla^2 D_q(\lambda^*)) > 0$ we can conclude that $\tilde{\delta}$ is proportionally to $\frac{\gamma}{2}\delta^2$.

3.2. Sample Average Approximation (SAA)

Now we suppose that we sample measures $q^1, \ldots, q^m$ in advance (with proper chosen $m$). This offline setting can be relevant when we are interested in parallelization or decentralization. The SAA approach approximates the true problem (6) by the following empirical problem

$$\hat{p}_\mu^m = \arg \min_{p \in S_n(1)} \frac{1}{m} \sum_{k=1}^{m} W_\mu(p, q^k).$$

We refer to $\hat{p}_{\varepsilon'}$ as an approximation of empirical barycenter of $\hat{p}_\mu^m$ if it satisfies the following inequality for some precision $\varepsilon'$

$$\frac{1}{m} \sum_{k=1}^{m} W_\mu(\hat{p}_{\varepsilon'}, q^k) - \frac{1}{m} \sum_{k=1}^{m} W_\mu(\hat{p}_\mu^m, q^k) \leq \varepsilon'.$$

The convergence properties of $\hat{p}_{\varepsilon'}$ to population barycenter $p^*_\mu$ and the proper number of measures $m$ needed to approximate the problem (6) by the problem (11) are presented in the following theorem.

**Theorem 3.2.** Let $\hat{p}_{\varepsilon'}$ satisfies (12) with precision $\varepsilon'$, where $m$ is the number of measures in empirical average (11). Then, with probability $\geq 1 - \alpha$ we have

$$\mathbb{E}_q \left[ W_\mu(\hat{p}_{\varepsilon'}, q) - W_\mu(p^*_\mu, q) \right] \leq \sqrt{\frac{2M^2}{\mu} \varepsilon'} + 4M^2 \alpha \mu m.$$

Let $\varepsilon' = O \left( \frac{\mu \varepsilon^2}{M^2} \right)$ and $m = O \left( \frac{M^2}{\alpha \mu \varepsilon} \right)$. Then, with probability $\geq 1 - \alpha$ the following holds

$$\mathbb{E}_q \left[ W_\mu(\hat{p}_{\varepsilon'}, q) - W_\mu(p^*_\mu, q) \right] \leq \varepsilon \quad \text{and} \quad \|\hat{p}_{\varepsilon'} - p^*_\mu\|_2 \leq \sqrt{2\varepsilon}/\mu.$$

The total complexity of offline algorithm from (45) computing $\hat{p}_{\varepsilon'}$ that satisfies (12) is

$$O \left( mn^2 \sqrt{\frac{M^2}{\mu \varepsilon'}} \right) = O \left( mn^2 \frac{M^2}{\mu \varepsilon} \right).$$

If parallel or distributed architecture is available, then the total complexity per each node is the following

$$O \left( \kappa n^2 \frac{M^2}{\mu \varepsilon} \right).$$
where $\kappa$ is the parameter of the architecture:

$$
\kappa = \begin{cases} 
1 & \text{in fully parallel } m \text{ nodes architecture} \\
\sqrt{m} & \text{in parallel } \sqrt{m} \text{ nodes architecture} \\
m & \text{if we have only one node (machine)} \\
d & \text{in centralized } m \text{ nodes architecture (} d \text{ is the communication network diameter)} \\
\sqrt{\chi} & \text{in decentralized } m \text{ nodes architecture (} \sqrt{\chi} \text{ is the condition number for the network)} 
\end{cases}
$$

**Proof.** Consider for any $p \in S_n(1)$ the following difference

$$
W_\mu(p) - W_\mu(p^*_\mu) \leq W_\mu(\hat{p}_\mu^m) - W_\mu(p^*_\mu) + W_\mu(p) - W_\mu(\hat{p}_\mu^m).
$$

(14)

From [61, Theorem 6] with probability $\geq 1 - \alpha$ for the empirical minimizer $\hat{p}_\mu^m$ the following holds

$$
W_\mu(\hat{p}_\mu^m) - W_\mu(p^*_\mu) \leq \frac{4M^2}{\alpha\mu m}.
$$

Then from this and (14) we get

$$
W_\mu(p) - W_\mu(p^*_\mu) \leq \frac{4M^2}{\alpha\mu m} + W_\mu(p) - W_\mu(\hat{p}_\mu^m).
$$

From Lipschitz continuity of $W_\mu(p)$ we have

$$
W_\mu(p) - W_\mu(p^*_\mu) \leq M \|p - \hat{p}_\mu^m\|_2.
$$

(15)

From strong convexity of $W_\mu(p, q)$ we get

$$
\|p - \hat{p}_\mu^m\|_2 \leq \sqrt{\frac{2}{\mu} \left( \frac{1}{m} \sum_{k=1}^m W_\mu(p, q^k) - \frac{1}{m} \sum_{k=1}^m W_\mu(\hat{p}_\mu^m, q^k) \right)}.
$$

(16)

By using (15) and (16) and taking $p = \hat{p}_{\epsilon'}$ we get the first statement of the theorem

$$
W_\mu(\hat{p}_{\epsilon'}) - W_\mu(p^*_\mu) \leq \sqrt{\frac{2M^2}{\mu} \left( \frac{1}{m} \sum_{k=1}^m W_\mu(\hat{p}_{\epsilon'}, q^k) - \frac{1}{m} \sum_{k=1}^m W_\mu(\hat{p}_\mu^m, q^k) \right)} + \frac{4M^2}{\alpha\mu m}
$$

$$
\leq \sqrt{\frac{2M^2}{\mu} \epsilon' + \frac{4M^2}{\alpha\mu m}}.
$$

(17)

Then from the strong convexity we have

$$
\|\hat{p}_{\epsilon'} - p^*_\mu\|_2 \leq \sqrt{\frac{2}{\mu} \left( \sqrt{\frac{2M^2}{\mu} \epsilon' + \frac{4M^2}{\alpha\mu m}} \right)}.
$$

(18)
Equating (17) to epsilon we get the expressions for the number of measures \( m \) and auxiliary precision \( \varepsilon' \). Substituting both of these expressions in (18) we get the confidence region for \( p^*_\mu \).

To calculate the total complexity we refer to the Algorithm 6 in the paper [45] calculating \( \hat{p}_\varepsilon \). For the readers convenience we repeat the scheme of the proof. This algorithm was developed for dual problem to (11) and relates to the class of fast gradient methods for Lipschitz smooth functions and, consequently, required \( O\left(\sqrt{\frac{LR^2}{\varepsilon'}}\right) \) calculations of \( \nabla D_q(\lambda) \) per node [53]. Here \( L \) is the Lipschitz constant of smoothness for dual function \( D_q(\lambda) \) from [3] \( (L = \lambda_{\text{max}}/\mu, \text{where} \lambda_{\text{max}} - \text{maximum eigenvalue of communication network} \ [19 \text{ Lemma 1}]) \) and \( R \) is the radius for dual solution \( R^2 \leq M^2/\lambda^+_{\text{min}}, \text{where} \lambda^+_{\text{min}} - \text{minimal positive eigenvalue of communication network} \ (10 \text{ Lemma 10 }, [45 \text{ Lemma 8}] \text{ and } 34 \text{ Lemma 7}). \) Incorporating all of this we get the following number of \( \nabla D_q(\lambda) \) calculations per node \( (\chi = \lambda_{\text{max}}/\lambda^+_{\text{min}}) \)

\[
\tilde{N} = O \left( \kappa \sqrt{\frac{M^2}{\varepsilon'\mu}} \right),
\]

where \( \kappa \) is the parameter of the architecture. Multiplying this by the complexity of calculating the gradient for the dual function \( D_q(\lambda) \) (which is \( n^2 \)) and using the definition of \( \varepsilon' \) we get the following complexity per each node

\[
O \left( n^2 \tilde{N} \right) = O \left( n^2 \kappa \sqrt{\frac{M^2}{\mu\varepsilon'}} \right) = O \left( n^2 \kappa \frac{M^2}{\mu\varepsilon'} \right).
\]

Using the expression for the number of measures and by using \( \kappa \) for one-machine architecture we get the algorithm complexity and finish the proof.

From the recent results [21] we may expect that the dependence on \( \alpha \) in Theorem 3.2 is indeed much better (logarithmic) if \( \mu \) in these formulas is small (proportional to \( \varepsilon \)). Otherwise, it is still a hypothesis.

### 3.3. Comparison of SA and SAA for population Wasserstein barycenter problem defined with respect to regularized OT

Next we compare the SA and the SAA approaches for problem [6]. For the readers convenience we skip the details about high probability bounds. The first reason is that we can fixed \( \alpha \), say as \( \alpha = 0.05 \), and consider it to be fixed parameter in the all bounds. The second reason is the intuition, which goes back to [61], that all bounds of this paper have logarithmic dependence on \( \alpha \) in fact and up to a \( \tilde{O}(\cdot) \) denotation we can ignore the dependence on \( \alpha \).

Table 1 presents the total complexity of the numerical algorithms from this section implementing SA and SAA approaches. We estimate \( M_{\infty} = O(\|C\|_{\infty}) \) and \( M \leq \sqrt{n}M_{\infty} \) in the complexity bounds by using Proposition 2.5.
Table 1. Total complexity of SA and SAA implementations for problem $\min_{p \in \mathbb{S}_n} \mathbb{E}_q W_\mu(p, q)$.

| Algorithm | Complexity |
|-----------|------------|
| Algorithm 1 (SA) | $\tilde{O}\left(n^3 \frac{\|C\|_2}{\mu \varepsilon} \min \left\{ \exp \left( \frac{\|C\|_{\infty}}{\mu} \right), \left( \frac{\|C\|_{\infty}}{\gamma \varepsilon^2} \right), \sqrt{\frac{n}{\gamma \mu \varepsilon^2}} \right\} \right)$ |
| Algorithm from [45] (SAA) | $O\left(n^4 \frac{\|C\|_4}{\mu^2 \varepsilon^2}\right)$ |

We conclude that when $\mu$ is not too large, SA has the complexity according to the second term under the minimum that is typically bigger than SAA complexity since $\gamma \ll \mu/n$. Hereby, SAA approach outperforms SA approach under this condition on the parameter $\mu$.

4. Population Wasserstein barycenter

In previous section, we were aim at computing the barycenter w.r.t. regularized OT. Now we refuse the regularization of OT and compare the SA and the SAA approaches for the problem of population Wasserstein barycenter defined w.r.t OT

$$p^* = \arg \min_{p \in \mathbb{S}_n(1)} \mathbb{E}_q W(p, q).$$ (20)

Throughout this section we use the following simplification for the objective

$$W_q(p) = \mathbb{E}_q W(p, q).$$

We notice that Proposition [25] is not completely valid for $W(p, q)$ since $W(p, q)$ is not strongly convex in $p$ w.r.t the 2-norm but still Lipschitz continuous. We assume that the Lipschitz constants for $W(p, q)$ in the 1-norm and the 2-norm are merely the same as for $W_\mu(p, q)$: $M_{\infty}$ and $M$ respectively.

4.1. Stochastic Approximation (SA)

Now we show how proper chose of $\mu$ ensures the application of the results from Sect. 3 to the problem (20). Let $p^*$ be the solution of (20) then for any $p \in \mathbb{S}_n(1)$ the following holds [26, 45, 56]

$$\mathbb{E}_q W(p, q) - \mathbb{E}_q W(p^*, q) \leq \mathbb{E}_q W_\mu(p, q) - \mathbb{E}_q W_\mu(p^*, q) + 2\mu \ln n$$

$$\leq \mathbb{E}_q \left( W_\mu(p, q) - W_\mu(p^*_\mu, q) \right) + 2\mu \ln n. \quad (21)$$

Let us choose $\mu = \frac{\varepsilon}{4 \ln n}$ that ensures the following

$$\mathbb{E}_q W(p, q) - \mathbb{E}_q W(p^*, q) \leq \mathbb{E}_q \left( W_\mu(p, q) - W_\mu(p^*_\mu, q) \right) + \varepsilon/2, \quad \forall p \in \mathbb{S}_n(1).$$

This means that solving the problem [6] with $\varepsilon/2$ precision, we get the solution of problem (20) with $\varepsilon$ precision. The next theorem is a modification of Theorem 3.1 for the problem (20).
Theorem 4.1. Let $\mu = \varepsilon / (2 \bar{R}^2)$ with $\bar{R}^2 = 2 \ln n$ and let $\tilde{p}^N$ be the average of $N$ online outputs of Algorithm 1. Then, with probability $\geq 1 - \alpha$ we have

$$\mathbb{E}_q \left[ W(\tilde{p}^N, q) - W(p^*, q) \right] = O \left( \frac{M^2 \ln(N/\alpha) \ln n}{\varepsilon N} + \delta \right).$$

Let Algorithm 1 run with $\delta = O(\varepsilon)$ and $N = \tilde{O} \left( \frac{M^2}{\varepsilon^2} \right)$. Then, with probability $\geq 1 - \alpha$ the following holds

$$\mathbb{E}_q \left[ W(\tilde{p}^N, q) - W(p^*, q) \right] \leq \varepsilon$$

The total complexity of Algorithm 1 is

$$\tilde{O} \left( \left( \frac{Mn}{\varepsilon} \right)^2 \exp \left( \frac{\|C\|_\infty \ln n}{\varepsilon} \right) \left( \frac{\|C\|_\infty \ln n}{\varepsilon} + \ln \left( \frac{\|C\|_\infty \ln n}{\gamma \varepsilon^2} \right) \right) \sqrt{\frac{n}{\gamma \varepsilon^2}} \right).$$

Next we provide another algorithm for an implementation of SA approach which solves directly problem (20) without regularization of OT.

4.1.1. Stochastic Mirror Descent

Let $d(p)$ be a distance generating function and $D_d(t, p)$ be the Bregman divergence associated to $d(p)$:

$$D_d(t, p) = d(t) - d(p) - \langle \nabla d(p), t - p \rangle.$$

We consider stochastic mirror descent (MD) with simplex setup (see, e.g., [35, 50, 54] for MD with exact oracle, for inexact oracle see, e.g., [25, 38]):

$$p^{k+1} = \text{Prox}_{p^k}(\eta_k \nabla^\delta p^k W(p^k, q))$$

where $\text{Prox}_{p}(g)$ is the prox-mapping

$$\text{Prox}_{p}(g) = \arg \min_{t \in S_n(1)} (\langle g, t \rangle + D_d(t, p))$$

and $\nabla^\delta p W(p, q)$ is the gradient of $W(p, q)$ w.r.t. $p$ calculated with $\delta$ precision

$$\|\nabla^\delta p W(p, q) - \nabla_p W(p, q)\|_2 \leq \delta \quad \forall q \in S_n(1).$$

We take negative entropy as a distance generating function $d(p) = \sum_{j=1}^{n} p_j \ln p_j$, the corresponding Bregman divergence is given by Kullback–Leibler divergence in this case. This setting ensures that the prox mapping (23) and iterative formula of MD (22) can be rewritten in a closed form described in Algorithm 2. We have starting point $p^1 = \arg \min_{p \in S_n(1)} d(p) = (1/n, \ldots, 1/n)$ and $R^2 = \max_{p \in S_n(1)} d(p) - \min_{p \in S_n(1)} d(p) = \ln n$.

We take step size $\eta = \sqrt{2R} / Mn \sqrt{N}$ according to [50].

4By using dual averaging scheme [52] we can rewrite Alg. 2 in online regime [35, 54] without including $N$ in the step-size policy. Note, that mirror descent and dual averaging scheme are very close to each other [39].
Algorithm 2 Stochastic Mirror Descent

**Input:** starting point \( p_1 = (1/n, \ldots, 1/n)^T \), \( N \) – number of measures \( q^1, \ldots, q^N \), accuracy of gradient calculation \( \delta \)

1. \( \eta = \sqrt{2 \ln n \over M_\infty \sqrt{N}} \)
2. for \( k = 1, \ldots, N \) do
3. calculate component-wise

\[
p^{k+1}_i = \frac{p^k_i \exp \left( -\eta \nabla^\delta_{p_i} W(p^k, q^k) \right)}{\sum_{j=1}^n p^k_j \exp \left( -\eta \nabla^\delta_{p_j} W(p^k, q^k) \right)}.
\]

where indices \( i, j \) denote the \( i \)-th (or \( j \)-th) component of a vector, \( \nabla^\delta_{p_i} W(p^k, q^k) \) is calculated with \( \delta \)-precision \([24]\) (e.g., by Simplex Method or Interior Point Method)

**Output:** \( \hat{p}^N = \frac{1}{N} \sum_{k=1}^N p^k \)

The next theorem estimates the complexity of Algorithm 2

**Theorem 4.2.** Let \( \hat{p}^N \) be the output of Algorithm 2 processing \( N \) measures. Then, with probability \( \geq 1 - \alpha \) we have

\[
\mathbb{E}_q \left[ W(\hat{p}^N, q) - W(p^*, q) \right] \leq \frac{M_\infty (3R + 2D_1 \sqrt{\ln(\alpha^{-1})})}{\sqrt{2N}} + \delta D_1 = O \left( \frac{M_\infty \sqrt{\ln(n/\alpha)}}{\sqrt{N}} + 2\delta \right),
\]

where \( R = KL(p^*, p^1) \leq \sqrt{\ln n} \) and \( D_1 = \max_{p', p'' \in S_n(1)} \|p' - p''\|_1 = 2 \). Let Algorithm 2 run with \( \delta = 0 \) and \( N = \tilde{O} \left( M_\infty^2 / \varepsilon^2 \right) \) Then, with probability \( \geq 1 - \alpha \) the following holds

\[
\mathbb{E}_q \left[ W(\hat{p}^N, q) - W(p^*, q) \right] \leq \varepsilon.
\]

The total complexity of Algorithm 2 is

\[
\tilde{O}(n^3 N) = \tilde{O} \left( n^3 \left( {M_\infty R \over \varepsilon} \right)^2 \right) = \tilde{O} \left( n^3 \left( {M_\infty \over \varepsilon} \right)^2 \right).
\]

**Proof.** For stochastic mirror descent with \( d(p) = \sum_{j=1}^n p_j \ln p_j \) the following holds for any \( p \in S_n(1) \)

\[
\eta \langle \nabla^\delta_p W(p^k, q^k), p^k - p \rangle \leq KL(p, p^k) - KL(p, p^{k+1}) + {\eta^2 \over 2} \| \nabla^\delta_p W(p^k, q^k) \|_\infty
\]

\[
\leq KL(p, p^k) - KL(p, p^{k+1}) + {\eta^2 M_\infty^2}.
\]

By adding and subtracting the terms \( \langle \nabla_p W(p, q^k), p - p^k \rangle \) and \( \langle \nabla^\delta_p W(p, q^k), p - p^k \rangle \)

---

5Notice, that Simplex method gives exact solution (\( \delta = 0 \)).
we get using Cauchy–Schwarz inequality

\[
\eta \langle \nabla_p W(p^k), p^k - p \rangle \leq \eta \langle \nabla_p W(p^k, q^k) - \nabla^\delta_p W(p^k, q^k), p^k - p \rangle + \eta \langle \nabla_p W(p^k) - \nabla_p W(p^k, q^k), p^k - p \rangle + KL(p, p^k) - KL(p, p^{k+1}) + \eta^2 M_\infty^2
\]

\[
\leq \eta \delta \max_{k=1, \ldots, N} \|p^k - p\|_1 + \eta \langle \nabla_p W(p^k) - \nabla_p W(p^k, q^k), p^k - p \rangle
\]

\[
+ KL(p, p^k) - KL(p, p^{k+1}) + \eta^2 M_\infty^2.
\]

Summing this for \(k = 1, \ldots, N\) and we get for \(p = p^*\)

\[
\sum_{k=1}^N \eta \langle \nabla_p W(p^k), p^k - p^* \rangle \leq KL(p^*, p^1) + \eta^2 M_\infty^2 + \eta \delta \max_{k=1, \ldots, N} \|p^k - p^*\|_1
\]

\[
+ \sum_{k=1}^N \eta \langle \nabla_p W(p^k) - \nabla_p W(p^k, q^k), p^k - p^* \rangle
\]

\[
\leq R^2 + \eta^2 M_\infty^2 N + \eta \delta N D_1 + \sum_{k=1}^N \eta \langle \nabla_p W(p^k) - \nabla_p W(p^k, q^k), p^k - p^* \rangle.
\]

Where we used \(KL(p^*, p^1) \leq R^2\) and \(\max_{k=1, \ldots, N} \|p^k - p^*\|_1 \leq D_1\). Then using convexity of \(W(p^k)\) and definition of output \(\hat{p}^N\) we have

\[
W(\hat{p}^N) - W(p^*) \leq \frac{R^2}{\eta N} + \eta M^2 + \delta D_1 + \frac{1}{N} \sum_{k=1}^N \langle \nabla_p W(p^k) - \nabla_p W(p^k, q^k), p^k - p^* \rangle.
\]

Next we use Azuma–Hoeffding’s [40] inequality and get for all \(\beta \geq 0\)

\[
P \left( \sum_{k=1}^{N+1} \langle \nabla_p W(p^k) - \nabla_p W(p^k, q^k), p^k - p^* \rangle \leq \beta \right) \geq 1 - \exp \left( -\frac{2\beta^2}{N(2M_\infty D_1)^2} \right) = 1 - \alpha
\]

since \(\langle \nabla_p W(p^k) - \nabla_p W(p^k, q^k), p^* - p^k \rangle\) is a martingale-difference and

\[
\left| \langle \nabla_p W(p^k) - \nabla_p W(p^k, q^k), p^* - p^k \rangle \right| \leq \|\nabla_p W(p^k) - \nabla_p W(p^k, q^k)\|_\infty \|p^* - p^k\|_1
\]

\[
\leq 2M_\infty \max_{k=1, \ldots, N} \|p^k - p^*\|_1 \leq 2M_\infty D_1.
\]

Hence with probability \(\geq 1 - \alpha\) the following holds

\[
W(\hat{p}^N) - W(p^*) \leq \frac{R^2}{\eta N} + \eta M^2 + \delta D_1 + \frac{\beta}{N}.
\]

(25)

Expressing \(\beta\) through \(\alpha\) and substituting \(\eta = \frac{R}{M_\infty} \sqrt{\frac{2}{N}}\), that minimize RHS of (25) on
\[ W(\hat{p}^N) - W(p^*) \leq \frac{M_\infty R}{\sqrt{2N}} + \frac{M_\infty R \sqrt{2}}{\sqrt{N}} + \delta D_1 + \frac{M_\infty D_1 \sqrt{2 \ln \frac{1}{\alpha}}}{\sqrt{N}} \]

Using \( R \leq \sqrt{\ln n} \) and \( D_1 \leq 2 \) we have

\[ W(\hat{p}^N) - W(p^*) \leq \frac{M_\infty (3 \sqrt{\ln n} + 4 \sqrt{\ln \frac{1}{\alpha}})}{\sqrt{2N}} + 2\delta. \]  

(26)

Squaring the l.h.s of (26), using Caushi–Schwartz inequality and then extracting the root, we get the first statement of the theorem

\[ W(\hat{p}^N) - W(p^*) \leq \frac{M_\infty \sqrt{6 \ln n + 8 \ln \frac{1}{\alpha}}}{\sqrt{2N}} + 2\delta. = O \left( \frac{M_\infty \sqrt{\ln (n/\alpha)}}{\sqrt{N}} + 2\delta \right). \]

The second statement of the theorem directly follows from this and the condition \( W(\hat{p}^N) - W(p^*) \leq \varepsilon \). To get the complexity bounds we notice that the complexity for ‘exact’ calculating \( \nabla_p W(p^k, q^k) \) is \( \tilde{O}(n^3) \) (see [1, 15, 16, 24] and references therein), multiplying this by \( N \) we get the last statement of the theorem.

We notice that complexity bound for Algorithm 2 is \( \tilde{O}(\sqrt{n}) \)-times better than the bound for Algorithm 1 with Euclidean set up.

4.2. Sample Average Approximation (SAA)

Similar to SA approach for problem (20), we use regularization parameter \( \mu = \frac{\varepsilon}{4 \ln n} \) in Theorem 3.2 and formulate the following theorem.

**Theorem 4.3.** Let \( \mu = \varepsilon/(2\bar{R}^2) \) with \( \bar{R}^2 = 2 \ln n \) and let \( \hat{p}_{\varepsilon'} \) satisfies (12) with precision \( \varepsilon' \), where \( m \) is the number of measures in empirical average (11). Then, with probability \( \geq 1 - \alpha \) we have

\[ \mathbb{E}_q [W_{\mu}(\hat{p}_{\varepsilon'}, q) - W_{\mu}(p^*, q)] \leq \sqrt{\frac{4M^2 \ln n}{\varepsilon} \varepsilon' + \frac{8M^2 \ln n}{\alpha \varepsilon m}}. \]

Let \( \varepsilon' = \tilde{O} \left( \frac{\varepsilon}{M^2} \right) \) and \( m = \tilde{O} \left( \frac{M^2}{\alpha \varepsilon} \right) \). Then, with probability \( \geq 1 - \alpha \) the following holds

\[ \mathbb{E}_q [W_{\mu}(\hat{p}_{\varepsilon'}, q) - W_{\mu}(p^*, q)] \leq \varepsilon. \]

The total complexity of offline algorithm from [45] computing \( \hat{p}_{\varepsilon'} \) on one machine
(without parallelization/decentralization) that satisfies \[O\left(\frac{1}{\sqrt{\alpha}} \frac{n^2 M^3 \bar{R}^2}{\varepsilon^3}\right) = \tilde{O}\left(\frac{1}{\sqrt{\alpha}} \frac{n^2 M^3}{\varepsilon^3}\right).\]

5. Penalized Wasserstein barycenters

In this section, we consider alternative regularization of problem \[\text{(20)}\] by adding a strongly convex penalization

\[
\min_{p \in S_n(1)} \{\mathbb{E}_q W(p, q) + \lambda r(p)\}, \tag{27}
\]

where \(r(p)\) is a strongly convex penalty function: \(S_n(1) \rightarrow \mathbb{R}_+\) and \(\lambda > 0\).

The SAA approach suggests to approximate this problem \[(27)\] by its empirical counterpart

\[
\hat{p}_m^\lambda = \arg \min_{p \in S_n(1)} \left\{\frac{1}{m} \sum_{k=1}^{m} W(p, q^k) + \lambda r(p)\right\}.
\]

The standard way for choosing \(r(p)\) is the squared norm penalty \(\frac{1}{2} \|p - p^1\|_2^2\) \((p^1\) is some vector from \(S_n(1)) [61]. In this case, the objective in \[(27)\] under the expectation is \(\lambda\)-strongly convex. This allows us to apply Theorem 3.2 replacing \(\mu\) by \(\lambda\), Lipschitz constant \(M\) by \(M + \lambda R\), where \(R = \max_{p \in S_n(1)} \|p - p^1\|_2 \leq \sqrt{2}6\) Consider \(m\) to be big enough, we choose \(\lambda = \sqrt{\frac{8M^2}{\alpha R^2 m}} [61]\) and obtain the following with probability \(\geq 1 - \alpha\)

\[
W(\hat{p}_{\varepsilon'}) - W(p^*) = O\left(\sqrt{MR \sqrt{m\varepsilon'}} + \sqrt{\frac{M^2 R^2}{\alpha m}}\right), \tag{28}
\]

where \(\hat{p}_{\varepsilon'}\) satisfies the following inequality

\[
\frac{1}{m} \sum_{k=1}^{m} W(\hat{p}_{\varepsilon'}, q^k) + \lambda r(\hat{p}_{\varepsilon'}) - \left(\frac{1}{m} \sum_{k=1}^{m} W(\hat{p}_m^\lambda, q^k) + \lambda r(\hat{p}_m^\lambda)\right) \leq \varepsilon'. \tag{29}
\]

Next, we present our new regularization \(r(p)\) in \[(27)\] to improve the results with standard penalization \(\frac{1}{2} \|p - p^1\|_2^2\).

5.1. New regularization for Wasserstein barycenter

Consider Bregman divergence \(B_d(p, p^1)\)

\[
B_d(p, p^1) = d(p) - d(p^1) - \langle \nabla d(p^1), p - p^1\rangle,
\]

\[\text{Note, that in [61] instead of } (M + \lambda R) \text{ it was used simple } M. \text{ For the moment we do not know how to justify this replacement. That is why we write } (M + \lambda R). \text{ Fortunately, when } m \text{ is big enough } (\lambda \sim 1/\sqrt{m} \text{ is small enough) it does not matter.}\]
with distance generating function \[3\]

\[
d(p) = \frac{1}{2(a - 1)}\|p\|^2_a, \quad a = 1 + \frac{1}{2\ln n}.
\]

Then, we choose \( r(p) = B_d(p, p^1) \) that leads to the following problem

\[
\min_{p \in S_n(1)} \left\{ \mathbb{E}_q W(p, q) + \lambda B_d(p, p^1) \right\}.
\] (30)

\( B_d(p, p^1) \) is 1-strongly convex in the 1-norm and \( \tilde{O}(1) \)-Lipschitz continuous in the 1-norm on \( S_n(1) \). One of the advantages of this penalization compared to the negative entropy penalization, proposed in \[2, 6\], is that we get the upper bound on the Lipschitz constant, the properties of strong convexity in the 1-norm on \( S_n(1) \) remain the same.

We consider empirical counterpart of problem (30) and redefine \( \hat{p}_\lambda^m \) as follows:

\[
\hat{p}_\lambda^m = \arg \min_{p \in S_n(1)} \left\{ \frac{1}{m} \sum_{k=1}^{m} W(p, q^k) + \lambda B_d(p, p^1) \right\}
\] (31)

and assume that \( \hat{p}_{\varepsilon'} \) such that

\[
\frac{1}{m} \sum_{k=1}^{m} W(\hat{p}_{\varepsilon'}, q^k) + \lambda B_d(\hat{p}_{\varepsilon'}, p^1) - \left( \frac{1}{m} \sum_{k=1}^{m} W(\hat{p}_\lambda^m, q^k) + \lambda B_d(\hat{p}_\lambda^m, p^1) \right) \leq \varepsilon'.
\] (32)

We summarize the result in the next theorem.

**Theorem 5.1.** Let \( \hat{R} \simeq \max_{p \in S_n(1)} B_d(p, p^1) = O(\ln n) \), \( \lambda = \sqrt{\frac{8M^2}{\alpha R^2 m}} \) (where \( m \) is big enough) and let \( \hat{p}_{\varepsilon'} \) satisfies (32) with accuracy \( \varepsilon' \). Then, with probability \( \geq 1 - \alpha \) we have

\[
\mathbb{E}_q [W_\mu(\hat{p}_{\varepsilon'}, q) - W_\mu(p^*, q)] = O \left( \sqrt{M_\infty \hat{R} \sqrt{m} \varepsilon'} + \sqrt{\frac{M^2_\infty \hat{R}^2}{\alpha m}} \right).
\]

Let

\[
\varepsilon' = O \left( \frac{\varepsilon^2}{M_\infty \hat{R} \sqrt{m}} \right) = \tilde{O} \left( \frac{\varepsilon^3 \sqrt{\alpha}}{M^2_\infty} \right)
\]

and

\[
m = O \left( \frac{M^2_\infty \hat{R}^2}{\alpha \varepsilon^2} \right) = \tilde{O} \left( \frac{M^2_\infty}{\alpha \varepsilon^2} \right).
\]

\[\text{Note, that to solve (31) we may use the same dual distributed tricks like in [13] if we put composite term in a separate node. But before, we should regularized} \ W(p, q) \text{ with } \mu = \frac{4\ln n}{\varepsilon'}. \text{ The complexity in terms of } O(\cdot) \text{ will be the same as in Theorem 5.2} \]

\[\text{Dual function for } B_d(p, p^1) \text{ can be calculated with the complexity } \tilde{O}(n) \]

\[\text{[27].} \]

\[\text{[See [4, Lemma 6.1].} \]

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Then, with probability $\geq 1 - \alpha$ the following holds

$$E_q [W_\mu(\hat{p}_\varepsilon', q) - W_\mu(p^*, q)] \leq \varepsilon.$$  

The total complexity of properly corrected algorithm from \cite{45} computing $\hat{p}_\varepsilon'$ on one machine (without parallelization/decentralization) that satisfies \cite{12} with $\mu = \varepsilon/(4 \ln n)$ is

$$O \left( mn^2 \sqrt{\frac{M^2}{\mu \varepsilon'}} \right) = \tilde{O} \left( \frac{n^{2.5} M^4}{\alpha^{1.25} \varepsilon^4} \right).$$

**Proof.** Let us define $f(p, q) \triangleq W(p, q) + \lambda B_d(p, p^1)$ and $F(p) \triangleq E_q[f(p, q)]$. Note, that $F(p, q)$ is $\lambda$-strongly convex in $p$ w.r.t. the 1-norm since $B_d \triangleq M_\infty + \lambda \tilde{R}$ by definition. Therefore, for $f(p, q)$ we can apply \cite{61, Theorem 6} (formulated in the 2-norm but also valid for the 1-norm) stated that with probability $\geq 1 - \alpha$

$$F(\hat{p}^m) - F(p^*) \leq \frac{4M^2 f}{\alpha \lambda m} = \frac{4(M_\infty + \lambda \tilde{R})^2}{\alpha \lambda m}.$$  

(33)

Denoting empirical average by $\hat{F}(p) \triangleq \frac{1}{m} \sum_{k=1}^{m} W(p, q_k) + \lambda B_d(p, p^1)$ we get the following consequence of \cite{33}

$$F(p) - F(p^*) \leq \sqrt{\frac{2(M_\infty + \lambda \tilde{R})^2}{\lambda} \left( \hat{F}(p) - \hat{F}(\hat{p}^m) \right)} + \frac{4(M_\infty + \lambda \tilde{R})^2}{\alpha \lambda m}.$$  

Therefore, from this we get

$$W(\hat{p}_\varepsilon') - W(p^*) \leq \sqrt{\frac{2(M_\infty + \lambda \tilde{R})^2 \varepsilon'}{\lambda}} + \frac{4(M_\infty + \lambda \tilde{R})^2}{\alpha \lambda m} - \lambda B_d(\hat{p}_\varepsilon', p^1) + \lambda B_d(p^*, p^1)$$

$$\leq \sqrt{\frac{2(M_\infty + \lambda \tilde{R})^2 \varepsilon'}{\lambda}} + \frac{4(M_\infty + \lambda \tilde{R})^2}{\alpha \lambda m} + \lambda \tilde{R}.$$  

Choosing $\lambda \approx \frac{\sqrt{8M^2}}{\tilde{R} m}$ we get the following

$$W(\hat{p}_\varepsilon') - W(p^*) = O \left( \sqrt{M_\infty \tilde{R} \sqrt{m \varepsilon'}} + \sqrt{\frac{M^2 \tilde{R}^2}{\alpha m}} \right).$$  

(34)

The other statements follows from this and the condition $W(\hat{p}_\varepsilon') - W(p^*) \leq \varepsilon$. \hfill \Box

\footnote{\textsuperscript{9}See \cite{13}. Recall that $\mu = \varepsilon^2/\tilde{R}^2$, $\tilde{R}^2 = 2 \ln n$. Note also that $\lambda$ after substituting of $m$ will be $\lambda = O \left( \varepsilon/\tilde{R}^2 \right) = \tilde{O}(\mu)$.}
Since $\frac{M}{M_\infty} \simeq \sqrt{n}$ we may conclude that (34) is $\tilde{O}(\sqrt{n})$-times better than (28).

From the recent results [21] we may expect that the dependence on $\alpha$ in Theorems 4.3, 5.1 is indeed much better (logarithmic). For the moment we do not possess an accurate prove of it, but we suspect that ideas from [21] allow to prove it.

### 5.2. Comparison of SA and SAA for population Wasserstein barycenter problem.

Now we compare the SA and the SAA approaches for problem (20).

Table 2 presents the total complexity for the numerical algorithms from this Sections 4 and 5 implementing SA and SAA approaches. We estimate $M_\infty = O(\|C\|_\infty)$ and $M \leq \sqrt{n}M_\infty$ in the complexity bounds by using Proposition 2.5.

| Algorithm | Complexity |
|-----------|------------|
| Algorithm 1 (SA) with $\mu = \varepsilon 4 \ln \frac{\varepsilon}{n}$ | $\tilde{O} \left( n^3 \left( \frac{\|C\|_\infty}{\varepsilon} \right)^2 \min \left\{ \exp \left( \frac{\|C\|_\infty \ln n}{\varepsilon} \right) \left( \frac{\|C\|_\infty \ln n}{\varepsilon} + \ln \left( \frac{\|C\|_\infty \ln n}{\gamma \varepsilon} \right) \right), \frac{1}{\varepsilon} \sqrt{\frac{n}{\gamma}} \right\} \right)$ |
| Algorithm from [45] (SAA), with $\mu = \varepsilon 4 \ln \frac{\varepsilon}{n}$ | $\tilde{O} \left( n^4 \left( \frac{\|C\|_\infty}{\varepsilon} \right)^4 \right)$ |
| Algorithm 2 (SA) | $\tilde{O} \left( n^3 \left( \frac{\|C\|_\infty}{\varepsilon} \right)^2 \right)$ |
| Regularized ERM + Algorithm from [45] (SAA) | $\tilde{O} \left( n^{2.5} \left( \frac{\|C\|_\infty}{\varepsilon} \right)^4 \right)$ |

We do not make any conclusion about comparison of Algorithm 2 and Regularized ERM (empirical risk minimization from Sect. 5 with our new regularization) + Algorithm from [45] since it depends on comparison of $\sqrt{n}$ and $(\|C\|_\infty/\varepsilon)^2$. However, both of these methods are definitely outperform (according to complexity results) Algorithm 1 and Algorithm from [45] approaches based on entropic regularization of OT with proper $\mu$.

Note, that recent Algorithm from [18] allows to improve the complexity of Algorithm from [45] $\sqrt{n}$-times. So it may reduce $n^{2.5}$ to $n^2$.

Also note, that in the case $\mu > 0$ we can compare SAA approach with SA approach by using rate of convergence in argument rather than in function. In this case SAA approach will have additional $\sqrt{n}$-factor advantage due to the possibility of more accurate investigation of the relation $\varepsilon'(\varepsilon)$ [30].

### 6. Numerical Experiments

Now we show the experiments performed on MNIST data set to support the results of Section 3. Each image from MNIST data set is a hand-written digit with the value from 0 to 9 of the size $28 \times 28$ pixels. We are interested in the convergence of estimated barycenter of digits 3 to its true counterpart. Since the true population barycenter $p^*_\mu$ of all hand-written digits 3 is unknown, we approximate it by the barycenter of all digits 3 in MNIST (7141 images) and then we study the convergence of estimated barycenter to $p^*_\mu$ as the number of measure grows. We estimate $p^*_\mu$ by Iterative Bregman Projection since it showed relatively good results. Figure 1 compares Algorithm 1 (SA
Figure 1. Quality of the estimate for population Wasserstein barycenter w.r.t regularized OT.

approach) and Iterative Bregman Projection (SAA approach)\[5\] in two metrics: the convergence in the 2-norm $\|p - p^*_\mu\|_2$ (Theorems 3.1 and 3.2) and the convergence in optimal transport distance $W_\mu(p, p^*_\mu)$. The entropy regularization parameter is set to $\mu = 0.01$. Despite the fact that our results guarantee the convergence only in the 2-norm, OT distance is a natural metric to compare two measures (‘true’ barycenter and its estimation).

We do not provide any experiments for Sect. 4 since we cannot exactly calculate the decrease in function value $W(p) - W(p^*)$ which was studied in Sect. 4. Recall that $W(p) = E_q W(p, q)$. Thus, we only limit ourselves by supporting the results about arguments convergence: $\|p - p^*_\mu\|_2$ (Sect. 3).

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