On Efficient Optimal Transport: An Analysis of Greedy and Accelerated Mirror Descent Algorithms

Tianyi Lin⋆,† Nhat Ho⋆,○ Michael I. Jordan○,†

Department of Electrical Engineering and Computer Sciences○
Department of Industrial Engineering and Operations Research†
Department of Statistics‡
University of California, Berkeley

January 18, 2019

Abstract

We provide theoretical analyses for two algorithms that solve the regularized optimal transport (OT) problem between two discrete probability measures with at most \( n \) atoms. We show that a greedy variant of the classical Sinkhorn algorithm, known as the Greenkhorn algorithm, can be improved to \( \tilde{O} \left( \frac{n^2}{\varepsilon^2} \right) \), improving on the best known complexity bound of \( \tilde{O} \left( \frac{n^2}{\varepsilon^3} \right) \). Notably, this matches the best known complexity bound for the Sinkhorn algorithm and helps explain why the Greenkhorn algorithm can outperform the Sinkhorn algorithm in practice. Our proof technique, which is based on a primal-dual formulation and a novel upper bound for the dual solution, also leads to a new class of algorithms that we refer to as adaptive primal-dual accelerated mirror descent (APDAMD) algorithms.

We prove that the complexity of these algorithms is \( \tilde{O} \left( \frac{n^2 \gamma^{1/2}}{\varepsilon} \right) \), where \( \gamma > 0 \) refers to the inverse of the strong convexity module of Bregman divergence with respect to \( \| \cdot \|_\infty \). This implies that the APDAMD algorithm is faster than the Sinkhorn and Greenkhorn algorithms in terms of \( \varepsilon \). Experimental results on synthetic and real datasets demonstrate the favorable performance of the Greenkhorn and APDAMD algorithms in practice.

1 Introduction

Optimal transport—the problem of finding minimal cost couplings between pairs of probability measures—has a long history in mathematics and operations research [40]. In recent years, it has been the inspiration for numerous applications in machine learning and statistics, including posterior contraction of parameter estimation in Bayesian nonparametrics models [29, 30], scalable posterior sampling for large datasets [36, 37], optimization models for clustering complex structured data [19], deep generative models and domain adaptation in deep learning [4, 18, 11, 38], and other applications [34, 32, 8, 25]. These large-scale applications have placed significant new demands on the efficiency of algorithms for solving the optimal transport problem, and a new literature has begun to emerge to provide new algorithms and complexity analyses for optimal transport.

The computation of the optimal-transport (OT) distance can be formulated as a linear programming problem and solved in principle by interior-point methods. The best known complexity bound in this formulation is \( \tilde{O} \left( n^{5/2} \right) \), achieved by an interior-point algorithm due to Lee and Sidford [24]. However, Lee and Sidford’s method requires as a subroutine a practical

---

* Tianyi Lin and Nhat Ho contributed equally to this work.
implementation of the Laplacian linear system solver, which is not yet available in the literature. Pele and Werman [31] proposed an alternative, implementable interior-point method for OT with a complexity bound is $\tilde{O}(n^3)$. Another prevalent approach for computing OT distance between two discrete probability measures involves regularizing the objective function by the entropy of the transportation plan. The resulting problem, referred to as entropic regularized OT or simply regularized OT [12, 5], is more readily solved than the original problem since the objective is strongly convex with respect to $\|\cdot\|_1$. The longstanding state-of-the-art algorithm for solving regularized OT is the Sinkhorn algorithm [35, 23, 21]. Inspired by the growing scope of applications for optimal transport, several new algorithms have emerged in recent years that have been shown empirically to have superior performance when compared to the Sinkhorn algorithm. An example includes the Greenkhorn algorithm [3, 9, 1], which is a greedy version of Sinkhorn algorithm. A variety of standard optimization algorithms have also been adapted to the OT setting, including accelerated gradient descent [16], quasi-Newton methods [14, 7] and stochastic average gradient [17]. The theoretical analysis of these algorithms is still nascent.

Very recently, Altschuler et al. [3] have shown that both the Sinkhorn and Greenkhorn algorithm can achieve the near-linear time complexity for regularized OT. More specifically, they proved that the complexity bounds for both algorithms are $\tilde{O}\left(\frac{n^2}{\varepsilon}\right)$, where $n$ is the number of atoms (or equivalently dimension) of each probability measure and $\varepsilon$ is a desired tolerance. Later, Dvurechensky et al. [16] improved the complexity bound for the Sinkhorn algorithm to $\tilde{O}\left(\frac{n^2}{\varepsilon^2}\right)$ and further proposed an adaptive primal-dual accelerated gradient descent (APDAGD), asserting a complexity bound of $\tilde{O}\left(\min\left\{\frac{n^{9/4}}{\varepsilon}, \frac{n^2}{\varepsilon^2}\right\}\right)$ for this algorithm. It is also possible to use a carefully designed Newton-type algorithm to solve the OT problem [2, 10], by making use of a connection to matrix-scaling problems. Blanchet et al. [6] and Quanrud [33] provided a complexity bound of $\tilde{O}\left(\frac{n^2}{\varepsilon}\right)$ for Newton-type algorithms. Unfortunately, these Newton-type methods are complicated and efficient implementations are not yet available. Nonetheless, this complexity bound can be viewed as a theoretical benchmark for the algorithms that we consider in this paper.

Our Contributions. The contribution of this work is three-fold and can be summarized as follows:

1. We improve the complexity bound for the Greenkhorn algorithm from $\tilde{O}\left(\frac{n^2}{\varepsilon^3}\right)$ to $\tilde{O}\left(\frac{n^2}{\varepsilon^2}\right)$, matching the best known complexity bound for the Sinkhorn algorithm. This analysis requires a new proof technique—the technique used in [16] for analyzing the complexity of Sinkhorn algorithm is not applicable to the Greenkhorn algorithm. In particular, the Greenkhorn algorithm only updates a single row or column at a time and its per-iteration progress is accordingly more difficult to quantify than that of the Sinkhorn algorithm. In contrast, we employ a novel proof technique that makes use of a novel upper bound for the dual optimal solution in terms of $\|\cdot\|_\infty$. Our results also shed light on the better practical performance of the Greenkhorn algorithm compared the Sinkhorn algorithm.

2. The smoothness of the dual regularized OT with respect to $\|\cdot\|_\infty$ allows us to formulate a novel adaptive primal-dual accelerated mirror descent (APDAMD) algorithm for the OT problem. Here the Bregman divergence is strongly convex and smooth with respect to $\|\cdot\|_\infty$. The resulting method involves an efficient line-search strategy [28] that is readily analyzed. It can be adapted to problems even more general than regularized OT. It can also be viewed as a primal-dual extension of [39, Algorithm 1] and a mirror descent extension of the APDAGD algorithm [16]. We establish a complexity bound
for the APDAMD algorithm of $\tilde{O}\left(\frac{n^2\gamma^{1/2}}{\varepsilon}\right)$, where $\gamma > 0$ refers to the inverse of the strong convexity module of the Bregman divergence with respect to $\|\cdot\|_\infty$. In particular, $\gamma = n$ if the Bregman divergence is simply chosen as $\frac{1}{2n}\|\cdot\|_2^2$. This implies that the APDAMD algorithm is faster than the Sinkhorn and Greenkhorn algorithms in terms of $\varepsilon$. Furthermore, we are able to provide a robustness result for the APDAMD algorithm (see Section 5).

3. We show that there is a limitation in the derivation by [16] of the complexity bound $\tilde{O}\left(\min\left\{\frac{n^{9/4}}{\varepsilon}, \frac{n^2}{\varepsilon^2}\right\}\right)$. More specifically, the complexity bound in [16] depends on a parameter which is not estimated explicitly. We provide a sharp lower bound for this parameter by a simple example (Proposition 4.8), demonstrating that this parameter depends on $n$. Due to the dependence on $n$ of that parameter, we demonstrate that the complexity bound of APDAGD algorithm is indeed $\tilde{O}(n^{2.5}/\varepsilon)$. This is slightly worse than the asserted complexity bound of $\tilde{O}\left(\min\left\{\frac{n^{9/4}}{\varepsilon}, \frac{n^2}{\varepsilon^2}\right\}\right)$ in terms of dimension $n$. Finally, our APDAMD algorithm potentially provides an improvement for the complexity of APDAGD algorithm as its complexity bound is $\tilde{O}(n^{3/2}/\varepsilon)$ and $\gamma$ can be smaller than $n$.

**Organization.** The remainder of the paper is organized as follows. In Section 2, we provide the basic setup for regularized OT in primal and dual forms, respectively. Based on the dual form, we analyze the worst-case complexity of the Greenkhorn algorithm in Section 3. In Section 4, we propose the APDAMD algorithm for solving regularized OT and provide a theoretical complexity analysis. Section 5 presents experiments that illustrate the favorable performance of the Greenkhorn and APDAMD algorithms. Proofs for several key results are presented in Section 6. Finally, we conclude in Section 7.

**Notation.** We let $\Delta^n$ denote the probability simplex in $n-1$ dimensions, for $n \geq 2$: $\Delta^n = \{u = (u_1, \ldots, u_n) \in \mathbb{R}^n : \sum_{i=1}^n u_i = 1, \ u \geq 0\}$. Furthermore, $[n]$ stands for the set $\{1, 2, \ldots, n\}$ while $\mathbb{R}_n^n$ stands for the set of all vectors in $\mathbb{R}^n$ with nonnegative components for any $n \geq 1$. For a vector $x \in \mathbb{R}^n$ and $1 \leq p \leq \infty$, we denote $\|x\|_p$ as its $\ell_p$-norm and $\text{diag}(x)$ as the diagonal matrix with $x$ on the diagonal. For a matrix $A \in \mathbb{R}^{n \times n}$, the notation $\text{vec}(A)$ stands for the vector in $\mathbb{R}^{n^2}$ obtained from concatenating the rows and columns of $A$. $\mathbf{1}$ stands for a vector with all of its components equal to 1. $\partial_x f$ refers to a partial gradient of $f$ with respect to $x$. Lastly, given the dimension $n$ and accuracy $\varepsilon$, the notation $a = \mathcal{O}(b(n, \varepsilon))$ stands for the upper bound $a \leq C \cdot b(n, \varepsilon)$ where $C$ is independent of $n$ and $\varepsilon$. Similarly, the notation $a = \tilde{\mathcal{O}}(b(n, \varepsilon))$ indicates the previous inequality may depend on the logarithmic function of $n$ and $\varepsilon$, and where $C > 0$.

## 2 Problem Setup

In this section, we review the formal problem of computing the OT distance between two discrete probability measures with at most $n$ atoms. We also discuss its regularized version, the entropic regularized OT problem. We then proceed to present the formulation of the dual regularized OT problem, which is vital for our theoretical analysis in the sequel.

### 2.1 (Regularized) OT

Approximating the OT distance amounts to solving a linear problem given by [22]:

$$
\min_{X \in \mathbb{R}^{n \times n}} \langle C, X \rangle \quad \text{s.t.} \quad X \mathbf{1} = r, \ X^\top \mathbf{1} = l, \ X \succeq 0,
$$

(1)
where \( X \) is called the \textit{transportation plan} while \( C = \{C_{ij}\} \in \mathbb{R}_+^{n \times n} \) is a cost matrix comprised of nonnegative elements. The vectors \( r \) and \( l \) are fixed vectors in the probability simplex \( \Delta^n \). Problem (1) can be solved in principle by the interior-point method, with a theoretical complexity of \( \tilde{O}(n^{5/2}) \) \cite{24}, and a practical complexity of \( \tilde{O}(n^3) \) \cite{31}. Unfortunately, even the practical method becomes inefficient in the setting of the kinds of large-scale problems that are currently being treated with OT methods. These include clustering models \cite{19} and Wasserstein barycenter computations \cite{13}. As an alternative to interior-point methods, Cuturi \cite{12} proposed a regularized version of problem (1) with the entropy of transportation plan \( X \) instead of the nonnegative constraints. The resulting regularized OT problem is formulated as follows:

\[
\min_{X \in \mathbb{R}_+^{n \times n}} \langle C, X \rangle - \eta H(X) \tag{2}
\]

s.t. \( X1 = r, \ X^\top 1 = l, \)

where \( \eta > 0 \) is the \textit{regularization parameter} and \( H(X) \) is the entropic regularization given by

\[
H(X) = -\sum_{i,j=1}^n X_{ij} \log(X_{ij}). \tag{3}
\]

The computational problem is to find \( \hat{X} \in \mathbb{R}_+^{n \times n} \) such that \( \hat{X}1 = r \) and \( \hat{X}^\top 1 = l \) and

\[
\langle C, \hat{X} \rangle \leq \langle C, X^* \rangle + \varepsilon, \tag{4}
\]

where \( X^* \) is an optimal transportation plan, i.e., an optimal solution to problem (1). In this formulation, \( \langle C, \hat{X} \rangle \) is referred to an \textit{\( \varepsilon \)-approximation} for the OT distance and \( \hat{X} \) is an \( \varepsilon \)-approximate transportation plan.

### 2.2 Dual regularized OT

While problem (2) involves optimizing a convex objective with several affine constraints, its dual problem is a unconstrained optimization problem, which simplifies both algorithm design and the complexity analysis. To derive the dual, we begin with a Lagrangian:

\[
\mathcal{L}(X, \alpha, \beta) = \langle C, X \rangle - \eta H(X) - \langle \alpha, X1 - r \rangle - \langle \beta, X^\top 1 - l \rangle,
\]

which can be rewritten as follows:

\[
\mathcal{L}(X, \alpha, \beta) = \langle \alpha, r \rangle + \langle \beta, l \rangle + \langle C, X \rangle - \eta H(X) - \langle \alpha, X1 \rangle - \langle \beta, X^\top 1 \rangle.
\]

The dual regularized OT is obtained by solving \( \min_{X \in \mathbb{R}_+^{n \times n}} \mathcal{L}(X, \alpha, \beta) \). Since \( \mathcal{L}(\cdot, \alpha, \beta) \) is strictly convex and differentiable, we can easily solve for the minimum by setting \( \partial_X \mathcal{L}(X, \alpha, \beta) \) to zero. More specifically, we have

\[
C_{ij} + \eta (1 + \log(X_{ij})) - \alpha_i - \beta_j = 0, \quad \forall i, j \in [n],
\]

implying that

\[
X_{ij} = e^{-\frac{C_{ij} + \alpha_i + \beta_j}{\eta}}, \quad \forall i, j \in [n].
\]
To simplify the notation, we perform a change of variables, setting $u_i = \frac{\alpha_i}{\eta} - \frac{1}{2}$ and $v_j = \frac{\beta_j}{\eta} - \frac{1}{2}$ from which we obtain $X_{ij} = e^{-\frac{C_{ij}}{\eta} + u_i + v_j}$. With this solution, we have

$$\min_{X \in \mathbb{R}^{n \times n}} L(X, \alpha, \beta) = \eta \left(- \sum_{i,j=1}^{n} e^{-\frac{C_{ij}}{\eta} + u_i + v_j} + \langle u, r \rangle + \langle v, l \rangle + 1 \right).$$

Thus, solving $\max_{\alpha, \beta \in \mathbb{R}^n} \min_{X \in \mathbb{R}^{n \times n}} L(X, \alpha, \beta)$ is equivalent to solving

$$\max_{u, v \in \mathbb{R}^n} - \sum_{i,j=1}^{n} e^{-\frac{C_{ij}}{\eta} + u_i + v_j} + \langle u, r \rangle + \langle v, l \rangle. \quad (5)$$

To simplify the notation further, let $B(u, v) \in \mathbb{R}^{n \times n}$ be defined as follows:

$$B(u, v) := \text{diag}(e^u) e^{-\frac{C}{\eta}} \text{diag}(e^v),$$

such that solving problem $(5)$ is equivalent to solving

$$\min_{u, v \in \mathbb{R}^n} f(u, v) := 1^T B(u, v) 1 - \langle u, r \rangle - \langle v, l \rangle. \quad (6)$$

We refer to problem $(6)$ to the dual regularized OT problem.

### 3 The Greenkhorn Algorithm

In this section, we present a complexity analysis for the Greenkhorn algorithm, which stands for a “greedy Sinkhorn” algorithm [3]. In particular, we improve the existing best known complexity bound $O\left(\frac{n^2\|C\|_\infty^3 \log(n)}{\epsilon^2} \right)$ in [3] to $O\left(\frac{n^2\|C\|_\infty^2 \log(n)}{\epsilon^2} \right)$, which matches the best known complexity bound for the Sinkhorn algorithm [16]. To facilitate the discussion later, we present the Greenkhorn algorithm in pseudocode form in Algorithm 1 and its application to regularized OT in Algorithm 2.

Both the Sinkhorn and Greenkhorn procedures are coordinate descent algorithms for the dual regularized OT problem $(6)$. However, while the Greenkhorn algorithm is a greedy coordinate descent algorithm, the Sinkhorn algorithm is block coordinate descent with only two blocks. It turns out to be easier to quantify the per-iteration progress of the Sinkhorn algorithm than that of the Greenkhorn algorithm, as suggested by the fact that the proof techniques in [16] are not applicable to the Greenkhorn algorithm. We thus explore a different strategy which will be elaborated in the sequel.

#### 3.1 Algorithm scheme

The Greenkhorn algorithm is presented in Algorithm 1 with the function $\rho : \mathbb{R}_+ \times \mathbb{R}_+ \to [0, +\infty]$ [3] given by

$$\rho(a, b) := b - a + a \log \left(\frac{a}{b}\right).$$

Note that $\rho$ measures the progress in the dual objective value between two consecutive iterates of the Greenkhorn algorithm. In particular, we have

$$\rho(a, b) \geq 0, \quad \forall a, b \in \mathbb{R}_+,$$
Algorithm 1: GREENKHORN(C, η, r, l, ε′)

Input: k = 0 and u₀ = v₀ = 0.
while Eᵏ > ε′ do
  r(uᵏ, vᵏ) = B(uᵏ, vᵏ)₁.
  l(uᵏ, vᵏ) = B(uᵏ, vᵏ)⊤₁.
  I = argmax₁≤i≤n ρ(rip, rᵢ(uᵏ, vᵏ)).
  J = argmax₁≤j≤n ρ(lⱼp, lⱼ(uᵏ, vᵏ)).
  if ρ(rip, rᵢ(uᵏ, vᵏ)) > ρ(lⱼp, lⱼ(uᵏ, vᵏ)) then
    uᵢ₊₁ = uᵢ + log (rip) − log (rᵢp(uᵏ, vᵏ)).
  else
    vⱼ₊₁ = vⱼ + log (lⱼp) − log (lⱼp(uᵏ, vᵏ)).
  end if
  k = k + 1.
end while
Output: B(uᵏ, vᵏ).

Algorithm 2: Approximating OT by GREENKHORN

Input: η = 4log(n) and ε′ = 8∥C∥∞.
Step 1: Let ˜r ∈ ∆ₙ and ˜l ∈ ∆ₙ be defined as
(˜r, ˜l) = (1 − ε′/8) (r, l) + ε′/8n (1, 1).
Step 2: Compute ˜X = GREENKHORN (C, η, ˜r, ˜l, ε′/2).
Step 3: Round ˜X to ˆX by Algorithm 2 [3] such that ˆX₁ = r and ˆX ⊤₁ = l.
Output: ˆX.

and the equality holds if and only if a = b.

On the other hand, we observe that the optimality condition of the dual regularized OT problem (6) is

B(u, v)₁ − r = 0, B(u, v)⊤₁ = 0.

This brings us to the following quantity which measures the error of the k-th iterate of the Greenkhorn algorithm [3]:

Eᵏ := ∥B(uᵏ, vᵏ)₁ − r∥₁ + ∥B(uᵏ, vᵏ)⊤₁ − l∥₁.

3.2 Complexity analysis—bounding dual objective values

Given the definition of Eᵏ, we first prove the following lemma which yields an upper bound for the objective values of the iterates.

Lemma 3.1. For each iteration k > 0 of the Greenkhorn algorithm, we have

f(uᵏ, vᵏ) − f(u*, v*) ≤ (2∥u*∥ₘ + 2∥v*∥ₘ) Eᵏ,

where (u*, v*) denotes an optimal solution pair for the dual regularized OT problem (6).
Proof. By the definition, we have
\[ f(u, v) = 1^\top B(u, v)1 - \langle u, r \rangle - \langle v, l \rangle = \sum_{i,j=1}^{n} e^{u_i + v_j - C_{ij}/\eta} - \sum_{i=1}^{n} r_i u_i - \sum_{j=1}^{n} l_j v_j \]

The gradients of \( f \) at \((u^k, v^k)\) are
\[ \nabla_u f(u^k, v^k) = B(u^k, v^k)1 - r, \]
\[ \nabla_v f(u^k, v^k) = B(u^k, v^k)^\top 1 - l. \]

Therefore, the quantity \( E_k \) can be rewritten as
\[ E_k = \|\nabla_u f(u^k, v^k)\|_1 + \|\nabla_v f(u^k, v^k)\|_1. \]

By using the fact that \( f \) is convex and globally minimized at \((u^*, v^*)\), we have
\[ f(u^k, v^k) - f(u^*, v^*) \leq (u^k - u^*)^\top \nabla_u f(u^k, v^k) + (v^k - v^*)^\top \nabla_v f(u^k, v^k). \]

Applying Hölder’s inequality yields
\[ f(u^k, v^k) - f(u^*, v^*) \leq \|u^k - u^*\|_\infty \|\nabla_u f(u^k, v^k)\|_1 + \|v^k - v^*\|_\infty \|\nabla_v f(u^k, v^k)\|_1 \]
\[ = \left( \|u^k - u^*\|_\infty + \|v^k - v^*\|_\infty \right) E_k. \]

Thus it suffices to show that
\[ \|u^k - u^*\|_\infty + \|v^k - v^*\|_\infty \leq 2 \|u^*\|_\infty + 2 \|v^*\|_\infty. \]

The next result is the key observation that makes our analysis work for the Greenkhorn algorithm. We use an induction argument to establish the following bound:
\[ \max\{\|u^k - u^*\|_\infty, \|v^k - v^*\|_\infty\} \leq \max\{\|u^0 - u^*\|_\infty, \|v^0 - v^*\|_\infty\}. \]
\[ \text{(9)} \]

It is easy to verify (9) for \( k = 0 \). Assuming that it holds true for \( k = k_0 \geq 0 \), we show that it also holds true for \( k = k_0 + 1 \). Without loss of generality, let \( I \) be the index chosen at the \( k_0 + 1 \)-th iteration. Then we have
\[ \|u^{k_0+1}_I - u^*_I\|_\infty \leq \max\{\|u^{k_0}_I - u^*_I\|_\infty, |u^{k_0+1}_I - u^*_I|\}, \]
\[ \|v^{k_0+1}_I - v^*_I\|_\infty = \|v^{k_0}_I - v^*_I\|_\infty. \]
\[ \text{(10)} \]

By the updating formula for \( u^{k_0+1}_I \) and the optimality condition for \( u^*_I \), we have
\[ e^{u^{k_0+1}_I} = \frac{r_I}{\sum_{j=1}^{n} e^{C_{ij}/\eta + v^0_j}} \]
\[ e^{u^*_I} = \frac{r_I}{\sum_{j=1}^{n} e^{C_{ij}/\eta + v^*_j}}. \]

This implies that
\[ |u^{k_0+1}_I - u^*_I| = \log \left( \frac{\sum_{j=1}^{n} e^{-C_{ij}/\eta + v^0_j}}{\sum_{j=1}^{n} e^{-C_{ij}/\eta + v^*_j}} \right) \leq \|v^0 - v^*\|_\infty, \]
\[ \text{(12)} \]
where the inequality comes from the following inequality:

\[
\frac{\sum_{i=1}^{n} a_i}{\sum_{i=1}^{n} b_i} \leq \max_{1 \leq j \leq n} \frac{a_i}{b_i}, \quad \forall a_i, b_i > 0.
\]

Combining (10) and (12) yields

\[
\|u^{k_0+1} - u^*\|_\infty \leq \max\{\|u^{k_0} - u^*\|_\infty, \|v^{k_0} - v^*\|_\infty\}.
\]

Therefore, we conclude that (9) holds true for \(k = k_0 + 1\) by combining (11) and (13). Since \(u^0 = v^0 = 0\), (9) implies that

\[
\|u^k - u^*\|_\infty + \|v^k - v^*\|_\infty \leq 2\|u^0 - u^*\|_\infty - 2\|v^0 - v^*\|_\infty,
\]

Finally, we obtain the result (7) by combining (8) and (14).

Our second lemma provides an upper bound for the \(\ell_\infty\)-norm of the optimal solution pair \((u^*, v^*)\) of the dual regularized OT problem. Note that this result is stronger than [16, Lemma 1] and generalize [6, Lemma 8] with fewer assumptions.

**Lemma 3.2.** For the dual regularized OT problem (6), there exists an optimal solution \((u^*, v^*)\) such that

\[
\|u^*\|_\infty \leq R, \quad \|v^*\|_\infty \leq R,
\]

where \(R > 0\) is defined as

\[
R := \frac{\|C\|_\infty}{\eta} + \log(n) - 2\log\left(\min_{1 \leq i, j \leq n} \{r_i, l_j\}\right).
\]

**Proof.** First, we claim that there exists an optimal solution pair \((\tilde{u}^*, \tilde{v}^*)\) such that

\[
\max_{1 \leq i \leq n} u_i^* \geq 0 \geq \min_{1 \leq i \leq n} u_i^*.
\]

Indeed, since the function \(f\) is convex with respect to \((u, v)\), the set of optima of problem (5) is not empty. Thus, we can choose an optimal solution \((\tilde{u}^*, \tilde{v}^*)\) where

\[
+\infty > \max_{1 \leq i \leq n} \tilde{u}_i^* \geq \min_{1 \leq i \leq n} \tilde{u}_i^* > -\infty,
+\infty > \max_{1 \leq i \leq n} \tilde{v}_i^* \geq \min_{1 \leq i \leq n} \tilde{v}_i^* > -\infty.
\]

Given the optimal solution \((\tilde{u}^*, \tilde{v}^*)\), we let \((u^*, v^*)\) be

\[
u^* = \tilde{u}^* - \frac{\max_{1 \leq i \leq n} u_i^* + \min_{1 \leq i \leq n} u_i^*}{2} \mathbf{1},
\]

\[
v^* = \tilde{v}^* + \frac{\max_{1 \leq i \leq n} u_i^* + \min_{1 \leq i \leq n} u_i^*}{2} \mathbf{1}.
\]

and observe that \((u^*, v^*)\) satisfies (16). It now suffices to show that \((u^*, v^*)\) is optimal; i.e.,

\[
f(u^*, v^*) = f(\tilde{u}^*, \tilde{v}^*).\]

Since \(\mathbf{1}^\top r = \mathbf{1}^\top l = 1\), we have

\[
\langle u^*, r \rangle = \langle \tilde{u}^*, r \rangle, \quad \langle v^*, l \rangle = \langle \tilde{v}^*, l \rangle.
\]
Therefore, we conclude that

\[ f(u^*, v^*) = \sum_{i,j=1}^{n} e^{-C_{ij}/\eta} + u_i^* + v_j^* - \langle u^*, r \rangle - \langle v^*, l \rangle \]

\[ = \sum_{i,j=1}^{n} e^{-C_{ij}/\eta} + \tilde{u}_i^* + \tilde{v}_j^* - \langle \tilde{u}^*, r \rangle - \langle \tilde{v}^*, l \rangle \]

\[ = f(\tilde{u}^*, \tilde{v}^*). \]

The next step is to establish the following bounds:

\[ \max_{1 \leq i \leq n} u_i^* - \min_{1 \leq i \leq n} u_i^* \leq \frac{\|C\|_{\infty}}{\eta} - \log \left( \min_{1 \leq i,j \leq n} \{r_i, l_j\} \right), \quad (17) \]

\[ \max_{1 \leq i \leq n} v_i^* - \min_{1 \leq i \leq n} v_i^* \leq \frac{\|C\|_{\infty}}{\eta} - \log \left( \min_{1 \leq i,j \leq n} \{r_i, l_j\} \right). \quad (18) \]

Indeed, for each \( 1 \leq i \leq n \), we have

\[ e^{-\|C\|_{\infty}/\eta + u_i^*} \left( \sum_{j=1}^{n} e^{v_j^*} \right) \leq \sum_{j=1}^{n} e^{-C_{ij}/\eta + u_i^* + v_j^*} = [B(u^*, v^*)]_i = r_i \leq 1, \]

implying that

\[ u_i^* \leq \frac{\|C\|_{\infty}}{\eta} - \log \left( \sum_{j=1}^{n} e^{v_j^*} \right). \quad (19) \]

On the other hand, we have

\[ e^{v_i^*} \left( \sum_{j=1}^{n} e^{v_j^*} \right) \geq \sum_{j=1}^{n} e^{-C_{ij}/\eta + u_i^* + v_j^*} = [B(u^*, v^*)]_i = r_i \geq \min_{1 \leq i,j \leq n} \{r_i, l_j\}, \]

implying that

\[ u_i^* \geq \log \left( \min_{1 \leq i,j \leq n} \{r_i, l_j\} \right) - \log \left( \sum_{j=1}^{n} e^{v_j^*} \right). \quad (20) \]

Combining (19) and (20) yields (17). In addition, (18) can be proved by a similar argument.

Finally, we proceed to prove that (15) holds true. We first assume that

\[ \max_{1 \leq i \leq n} v_i^* \geq 0, \quad \max_{1 \leq i \leq n} u_i^* \geq 0 \geq \min_{1 \leq i \leq n} u_i^*. \]

The optimality condition implies that

\[ \sum_{i,j=1}^{n} e^{-C_{ij}/\eta + u_i^* + v_j^*} = 1, \]

and

\[ \max_{1 \leq i \leq n} u_i^* + \max_{1 \leq i \leq n} v_i^* \leq \log \left( \max_{1 \leq i,j \leq n} e^{C_{ij}/\eta} \right) = \frac{\|C\|_{\infty}}{\eta}. \]
Equipped with the assumptions $\max_{1 \leq i \leq n} u^*_i \geq 0$ and $\max_{1 \leq i \leq n} v^*_i \geq 0$, we have

$$0 \leq \max_{1 \leq i \leq n} u^*_i \leq \frac{\|C\|_{\infty}}{\eta}, \quad 0 \leq \max_{1 \leq i \leq n} v^*_i \leq \frac{\|C\|_{\infty}}{\eta}.$$  \hfill (21)

Combining (21) with (17) and (18) yields

$$\min_{1 \leq i \leq n} u^*_i \geq -\frac{\|C\|_{\infty}}{\eta} + \log \left( \min_{1 \leq i,j \leq n} \{r_i, l_j\} \right),$$

$$\min_{1 \leq i \leq n} v^*_i \geq -\frac{\|C\|_{\infty}}{\eta} + \log \left( \min_{1 \leq i,j \leq n} \{r_i, l_j\} \right).$$

We conclude (15) by putting together the above inequalities.

We proceed to the alternative scenario, where

$$\max_{1 \leq i \leq n} v^*_i \leq 0, \quad \max_{1 \leq i \leq n} u^*_i \geq 0 \geq \min_{1 \leq i \leq n} u^*_i.$$

Combining with (17) yields

$$\max_{1 \leq i \leq n} u^*_i \leq \frac{\|C\|_{\infty}}{\eta} - \log \left( \min_{1 \leq i,j \leq n} \{r_i, l_j\} \right),$$

$$\min_{1 \leq i \leq n} u^*_i \geq -\frac{\|C\|_{\infty}}{\eta} + \log \left( \min_{1 \leq i,j \leq n} \{r_i, l_j\} \right).$$

Similar to (20), we have

$$\min_{1 \leq i \leq n} v^*_i \geq \log \left( \min_{1 \leq i,j \leq n} \{r_i, l_j\} \right) - \log \left( \sum_{i=1}^n e^{u^*_i} \right)$$

$$\geq 2 \log \left( \min_{1 \leq i,j \leq n} \{r_i, l_j\} \right) - \log(n) - \frac{\|C\|_{\infty}}{\eta},$$

and again we conclude that (15) holds. \hfill \Box

Putting together Lemma 3.1 and Lemma 3.2, we have the following straightforward consequence:

**Corollary 3.3.** Letting $\{(u^k, v^k)\}_{k \geq 0}$ denote the iterates returned by the Greenkhorn algorithm, we have

$$f(u^k, v^k) - f(u^*, v^*) \leq 4RE^k.$$  \hfill (22)

**Remark 3.4.** The constant R provides an upper bound both in this paper and in [16], where the same notation is used. The values in the two papers are of the same order since R in our paper only involves an additional term $\log(n) - \log(\min_{1 \leq i,j \leq n} \{r_i, l_j\})$.

**Remark 3.5.** We further comment on the proof techniques in this paper and [16]. The proof for [16, Lemma 2] depends on taking full advantage of the shift property of the Sinkhorn algorithm; namely, either $B(\overline{u}^k, \overline{v}^k) \mathbf{1} = r$ or $B(\overline{u}^k, \overline{v}^k)^\top \mathbf{1} = l$, where $(\overline{u}^k, \overline{v}^k)$ stands for the iterates of the Sinkhorn algorithm. Unfortunately, the Greenkhorn algorithm does not enjoy such a shift property. We have thus proposed a different approach for bounding $f(u^k, v^k) - f(u^*, v^*)$, based on the $\ell_{\infty}$-norm of the optimal solution $(u^*, v^*)$ of the dual regularized OT problem.
3.3 Complexity analysis—bounding the number of iterations

We proceed to provide an upper bound for the number of iterations $k$ to achieve a desired tolerance $\varepsilon'$ for the iterates of the Greenkhorn algorithm. First, we start with a lower bound for the difference of function values between two consecutive iterates of the Greenkhorn algorithm:

**Lemma 3.6.** Let $\{(u^k, v^k)\}_{k\geq 0}$ be the iterates returned by the Greenkhorn algorithm, we have

$$f(u^k, v^k) - f(u^{k+1}, v^{k+1}) \geq \frac{(E^k)^2}{28n},$$  \hspace{1cm} (23)

**Proof.** We observe that

$$f(u^k, v^k) - f(u^{k+1}, v^{k+1}) \geq \frac{1}{2n} \left( \rho \left( r, B(u^k, v^k)1 \right) + \rho \left( c, B(u^k, v^k)^\top 1 \right) \right) \geq \frac{1}{14n} \left( \| r - B(u^k, v^k)1 \|_1^2 + \| c - B(u^k, v^k)^\top 1 \|_1^2 \right),$$

where the first inequality comes from [3, Lemma 5] and the fact that the row or column update is chosen in a greedy manner, and the second inequality comes from [3, Lemma 6]. Therefore, by the definition of $E^k$, we conclude (23). \hfill \Box

We are now able to derive the iteration complexity of Greenkhorn algorithm based on Corollary 3.3 and Lemma 3.6.

**Theorem 3.7.** The Greenkhorn algorithm returns a matrix $B(u^k, v^k)$ that satisfies $E_k \leq \varepsilon'$ in the number of iterations $k$ satisfying

$$k \leq 2 + \frac{112nR}{\varepsilon'},$$  \hspace{1cm} (24)

where $R$ is defined in Lemma 3.2.

**Proof.** Denote $\delta_k = f(u^k, v^k) - f(u^*, v^*)$. Based on the results of Corollary 3.3 and Lemma 3.6, we have

$$\delta_k - \delta_{k+1} \geq \max \left\{ \frac{\delta_k^2}{448nR^2}, \frac{(\varepsilon')^2}{28n} \right\},$$

where $E_k \geq \varepsilon'$ as soon as the stopping criterion is not fulfilled. In the following step we apply a switching strategy introduced by Dvurechensky et.al. [16]. More specifically, given any $k \geq 1$, we have two estimates:

(i) Considering the process from the first iteration and the $k$-th iteration, we have

$$\frac{\delta_{k+1}^2}{448nR^2} \leq \frac{1}{k + \frac{448nR^2}{\delta_1^2}} \implies k \leq 1 + \frac{448nR^2}{\delta_k} - \frac{448nR^2}{\delta_1}.$$

(ii) Considering the process from the $(k + 1)$-th iteration to the $(k + m)$-th iteration for $\forall m \geq 1$, we have

$$\delta_{k+m} \leq \delta_k - \frac{(\varepsilon')^2m}{28n} \implies m \leq \frac{28n}{(\varepsilon')^2} (\delta_k - \delta_{k+m}).$$
We then minimize the sum of these two estimates by an optimal choice of a tradeoff parameter $s \in (0, \delta_1]$:

\[
  k \leq \min_{0<s<\delta_1} \left( \frac{2 + 448nR^2}{s} - \frac{448nR^2}{\delta_1} \frac{1}{(\varepsilon')^2} + \frac{28n\varepsilon}{(\varepsilon')^2} \right)
\]

\[
  = \begin{cases} 
    2 + \frac{224nR}{\varepsilon'} - \frac{448nR^2}{\delta_1}, & \delta_1 \geq 4R\varepsilon', \\
    2 + \frac{28n\delta_1}{(\varepsilon')^2}, & \delta_1 \leq 4R\varepsilon'.
  \end{cases}
\]

This implies that \( k \leq 2 + \frac{112nR}{\varepsilon'} \) in both cases. Therefore, we conclude that the number of iterations \( k \) satisfies (24).

Equipped with the result of Theorem 3.7 and the scheme of Algorithm 2, we are able to establish the following result for the complexity of the Greenkhorn algorithm:

**Theorem 3.8.** The Greenkhorn algorithm for approximating optimal transport (Algorithm 2) returns \( \hat{X} \in \mathbb{R}^{n \times n} \) satisfying \( \hat{X}1 = r, \hat{X}^\top 1 = l \) and (4) in

\[
  \mathcal{O} \left( \frac{n^2 \|C\|_\infty^2 \log(n)}{\varepsilon^2} \right)
\]

arithmetic operations.

The proof of Theorem 3.8 is in Section 6.1. The result of Theorem 3.8 improves the best known complexity bound \( \tilde{\mathcal{O}} \left( \frac{n^2}{\varepsilon^3} \right) \) for the Greenkhorn algorithm [3, 1], and further matches the best known complexity bound for the Sinkhorn algorithm [16]. This sheds light on the superior performance of the Greenkhorn algorithm in practice.

### 4 Adaptive Primal-Dual Accelerated Mirror Descent

In this section, we propose and analyze a novel adaptive primal-dual accelerated mirror descent (APDAMD) algorithm for a general class of problems that specializes to the regularized OT problem in (2).

APDAMD algorithm is an adaptive primal-dual optimization algorithm for finding a primal-dual optimal solution pair for a broad class of OT problems. The pseudocode for the APDAMD algorithm and its specialization to the regularized OT problem (2) are presented in Algorithm 4 and Algorithm 3, respectively. In Section 4.3 we show that the complexity of APDAMD is \( \mathcal{O} \left( \frac{n^2 \sqrt{\gamma} \|C\|_\infty \log(n)}{\varepsilon} \right) \), where \( \gamma > 0 \) refers to the inverse of the strong convexity module of Bregman divergence with respect to \( \|\cdot\|_\infty \).

#### 4.1 General setup

We consider the following generalization of the regularized OT problem:

\[
  \min_{x \in \mathbb{R}^n} f(x), \quad \text{s.t. } Ax = b,
\]

(25)
where $A \in \mathbb{R}^{n \times n}$ is a matrix and $b \in \mathbb{R}^n$. Here $f$ is assumed to be strongly convex with respect to the $\ell_1$-norm:

$$f(x_2) - f(x_1) - \langle \nabla f(x_1), x_2 - x_1 \rangle \geq \frac{\eta}{2} \|x_2 - x_1\|_1^2.$$  

The Lagrangian dual problem for (25) can be written as the following minimization problem:

$$\min_{\lambda \in \mathbb{R}^n} \varphi(\lambda) := \left\{ (\lambda, b) + \max_{x \in \mathbb{R}^n} \left\{ -f(x) - \langle A^\top \lambda, x \rangle \right\} \right\}. \tag{26}$$

A direct computation leads to $\nabla \varphi(\lambda) = b - Ax(\lambda)$ where

$$x(\lambda) := \arg\max_{x \in \mathbb{R}^n} \left\{ -f(x) - \langle A^\top \lambda, x \rangle \right\}.$$  

To analyze the complexity of the APDAMD algorithm, we start with the following result that establishes the smoothness of the dual objective function $\varphi$ with respect to the $\ell_\infty$-norm.

**Lemma 4.1.** The dual objective $\varphi$ is smooth with respect to $\ell_\infty$-norm:

$$\varphi(\lambda_1) - \varphi(\lambda_2) - \langle \nabla \varphi(\lambda_2), \lambda_1 - \lambda_2 \rangle \leq \frac{\|A\|_2^2}{2\eta} \|\lambda_1 - \lambda_2\|_\infty^2.$$  

**Proof.** The proof shares the same spirit with that used in [27, Theorem 1]. In particular, we first show that

$$\|\nabla \varphi(\lambda_1) - \nabla \varphi(\lambda_2)\|_1 \leq \frac{\|A\|_2^2}{\eta} \|\lambda_1 - \lambda_2\|_\infty. \tag{27}$$

Indeed, from the definition of $\nabla \varphi(\lambda)$, we have

$$\|\nabla \varphi(\lambda_1) - \nabla \varphi(\lambda_2)\|_1 = \|Ax(\lambda_1) - Ax(\lambda_2)\|_1 \leq \|A\|_1 \|x(\lambda_1) - x(\lambda_2)\|_1. \tag{28}$$

We also observe from the strong convexity of $f$ that

$$\eta \|x(\lambda_1) - x(\lambda_2)\|_1^2 \leq \langle \nabla f(x(\lambda_1)) - \nabla f(x(\lambda_2)), x(\lambda_1) - x(\lambda_2) \rangle$$

$$= \langle A^\top \lambda_2 - A^\top \lambda_1, x(\lambda_1) - x(\lambda_2) \rangle$$

$$\leq \|\lambda_1 - \lambda_2\|_\infty \|Ax(\lambda_1) - Ax(\lambda_2)\|_1$$

$$\leq \|A\|_1 \|x(\lambda_1) - x(\lambda_2)\|_1 \|\lambda_1 - \lambda_2\|_\infty,$$

which implies

$$\|x(\lambda_1) - x(\lambda_2)\|_1 \leq \frac{\|A\|_1}{\eta} \|\lambda_1 - \lambda_2\|_\infty. \tag{29}$$

We conclude (27) by combining (28) and (29). To this end, we have

$$\varphi(\lambda_1) - \varphi(\lambda_2) - \langle \nabla \varphi(\lambda_2), \lambda_1 - \lambda_2 \rangle = \int_0^1 \langle \nabla \varphi(t\lambda_1 + (1-t)\lambda_2) - \nabla \varphi(\lambda_2), \lambda_1 - \lambda_2 \rangle \, dt$$

$$\leq \left( \int_0^1 \|\nabla \varphi(t\lambda_1 + (1-t)\lambda_2) - \nabla \varphi(\lambda_2)\|_1 \, dt \right) \|\lambda_1 - \lambda_2\|_\infty$$

$$\leq \left( \int_0^1 t \, dt \right) \frac{\|A\|_2^2}{\eta} \|\lambda_1 - \lambda_2\|_\infty^2$$

$$= \frac{\|A\|_2^2}{2\eta} \|\lambda_1 - \lambda_2\|_\infty^2.$$  

13
This completes the proof of the lemma. □

To facilitate the ensuing discussion, we assume that the dual problem (25) has a solution \( \lambda^* \in \mathbb{R}^n \). Now, the Bregman divergence \( B_\phi : \mathbb{R}^n \times \mathbb{R}^n \to [0, +\infty] \) is given by

\[
B_\phi(z, z') := \phi(z) - \phi(z') - \langle \phi(z'), z - z' \rangle,
\]

for any \( z, z' \in \mathbb{R}^n \). Here, \( \phi \) is \( \frac{1}{\gamma} \)-strongly convex and 1-smooth on \( \mathbb{R}^n \) with respect to the \( \ell_{\infty} \)-norm; i.e., for any \( z, z' \in \mathbb{R}^n \), we have

\[
\frac{1}{2\gamma} \|z - z'\|_{\infty}^2 \leq \phi(z) - \phi(z') - \langle \nabla \phi(z'), z - z' \rangle \leq \frac{1}{2} \|z - z'\|_{\infty}^2.
\]

(30)

In particular, one useful choice of \( \phi \) for the APDAMD algorithm is

\[
\phi(z) = \frac{1}{2n} \|z\|_2^2, \quad B_\phi(z, z') = \frac{1}{2n} \|z - z'\|_2^2.
\]

In this case, \( \gamma = n \) since \( \phi \) is \( \frac{1}{n} \)-strongly convex and 1-smooth with respect to the \( \ell_{\infty} \)-norm. In general, \( \gamma \) is a function of \( n \). It is worth noting that the value of \( \gamma \) will affect the complexity bound of the APDAMD algorithm for approximating optimal transport problem (see Theorem 4.6). We make no attempt to optimize the value of \( \gamma \) as a function of \( n \) in the current manuscript.

**Algorithm 3: Approximating OT by APDAMD**

**Input:** \( \eta = \frac{\varepsilon}{4 \log(n)} \) and \( \varepsilon' = \frac{\varepsilon}{8\|c\|_{\infty}} \).

**Step 1:** Let \( \tilde{r} \in \Delta_n \) and \( \tilde{l} \in \Delta_n \) be defined as

\[
\left( \tilde{r}, \tilde{l} \right) = \left( 1 - \frac{\varepsilon'}{8} \right) (r, l) + \frac{\varepsilon'}{8n} (1, 1).
\]

**Step 2:** Let \( A \in \mathbb{R}^{2n \times n^2} \) and \( b \in \mathbb{R}^{2n} \) be defined by

\[
\text{Vec}(X) = \begin{pmatrix} X_1 \\ X^\top 1 \end{pmatrix}, \quad b = \begin{pmatrix} \tilde{r} \\ \tilde{l} \end{pmatrix}
\]

**Step 3:** Compute \( \tilde{X} = \text{APDAMD}(\varphi, A, b, \varepsilon'/2) \) with \( \varphi \) defined in (26) with \( f(x) = \text{vec}(C)^\top \text{vec}(X) - \eta H(X) \).

**Step 4:** Round \( \tilde{X} \) to \( \hat{X} \) by Algorithm 2 [3] such that \( \hat{X} 1 = r, \hat{X}^\top 1 = l \).

**Output:** \( \hat{X} \).

### 4.2 Properties of the APDAMD algorithm

In this section we present several important properties of the APDAMD algorithm that can be used later for regularized OT problems. First, we prove the following result regarding the number of line search iterations in the APDAMD algorithm:

**Lemma 4.2.** For the APDAMD algorithm, the number of line search iterations in the line search strategy is finite. Furthermore, the total number of gradient oracle calls after the \( k \)-th iteration is bounded as

\[
N_k \leq 4k + 4 + \frac{2 \log \left( \frac{\|A\|_2^2}{2n} \right)}{\log 2} - 2 \log(L_0),
\]

(31)
Algorithm 4: APDAMD($\varphi, A, b, \varepsilon'$)

Input: $k = 0$.
Initialization: $\alpha^0 = \alpha^0 = 0$, $z^0 = \mu^0 = \lambda^0$ and $L^0 = 1$
repeat
  Set $M^k = \frac{L^k}{2}$.
  repeat
    Set $M^k = 2M^k$.
    Compute
    \[
    \alpha^{k+1} = \frac{1 + \sqrt{1 + 4\gamma M^k \tilde{\alpha}^k}}{2\gamma M^k} \quad \text{(Step Size)}
    \]
    \[
    \tilde{\alpha}^{k+1} = \tilde{\alpha}^k + \alpha^{k+1} \quad \text{(Accumulating Parameter)}
    \]
  Compute
  \[
  \mu^{k+1} = \frac{\alpha^{k+1} z^k + \lambda^k}{\tilde{\alpha}^{k+1}} \quad \text{(Averaging Step)}
  \]
Compute
\[
 z^{k+1} = \arg\min_{z \in \mathbb{R}^n} \left\{ \langle \nabla \varphi(\mu^{k+1}), z - \mu^{k+1} \rangle + \frac{B_\varphi(z, z^k)}{\alpha^{k+1}} \right\} \quad \text{(Mirror Descent Step)}
\]
Compute
\[
 \lambda^{k+1} = \frac{\alpha^{k+1} z^{k+1} + \lambda^k}{\tilde{\alpha}^{k+1}} \quad \text{(Averaging Step)}
\]
until
\[
\varphi(\lambda^{k+1}) - \varphi(\mu^{k+1}) - \langle \nabla \varphi(\mu^{k+1}), \lambda^{k+1} - \mu^{k+1} \rangle \leq \frac{M^k}{2} \| \lambda^{k+1} - \mu^{k+1} \|_\infty^2 \quad \text{(Stopping Criterion)}
\]
Set
\[
 x^{k+1} = \frac{\alpha^{k+1} x(\mu^{k+1}) + \lambda^k x^k}{\tilde{\alpha}^{k+1}} \quad \text{(Averaging Step)}
\]
Set $L^{k+1} = \frac{M^k}{2}$.
Set $k = k + 1$.
until $\|Ax^k - b\|_1 \leq \varepsilon'$
Output: $X^k$ where $x^k = \text{vec}(X^k)$.

Proof. We follow [20] but we provide the proof details for the reader’s convenience. First, we observe that multiplying $M^k$ by two will not stop until the line search stopping criterion is satisfied. Therefore, we must have
\[
M^k \geq \frac{\|A\|_1^2}{2\eta}.
\]
By using Lemma 4.1, we obtain that the number of line search iterations in the line search strategy is finite. Letting $i_j$ denote the total number of multiplication at the $j$-th iteration, we have
\[
i_0 \leq 1 + \log \left( \frac{M^0}{L^0} \right) \log 2, \quad i_j \leq 2 + \log \left( \frac{M^{j-1}}{M^{j-1+1}} \right) \log 2.
\]
Proof. We follow the proof path [16] with APDAMD algorithm. Therefore, we have
\[ M^j \geq \frac{\|A\|_1^2}{\eta}, \]
which implies that the line search stopping criterion will be satisfied with \( \frac{M^j}{2} \) and proceed to the line search in the next iteration. Therefore, the total number of line search can be bounded by
\[
\sum_{j=0}^{k} i_j \leq 1 + \frac{\log \left( \frac{M^0}{L} \right)}{\log 2} + \sum_{j=1}^{k} \left( 2 + \frac{\log \left( \frac{M^j}{M^{j-1}} \right)}{\log 2} \right) 
\leq 2k + 1 + \frac{\log (M^k) - \log(L^0)}{\log 2} 
\leq 2k + 1 + \frac{\log \left( \frac{\|A\|_1^2}{2\eta} \right) - \log(L^0)}{\log 2}.
\]
Since each line search contains two gradient oracle calls, we conclude (31).

The next lemma presents a property of the dual objective function at the iterates of the APDAMD algorithm.

Lemma 4.3. For each iteration \( k \) of the APDAMD algorithm and any \( z \in \mathbb{R}^n \), we have
\[
\alpha^k \varphi(\lambda^k) \leq \sum_{j=0}^{k} \left[ \alpha^j \left( \varphi(\mu^j) + \langle \nabla \varphi(\mu^j), z - \mu^j \rangle \right) \right] + \|z\|_\infty^2. \tag{32}
\]

Proof. We follow the proof path \([16]\) with \( \ell_\infty \)-norm instead of \( \ell_2 \)-norm. First, we claim that
\[
\alpha^{k+1} \left\langle \nabla \varphi(\mu^{k+1}), z^k - z \right\rangle \leq \alpha^{k+1} \left( \varphi(\mu^{k+1}) - \varphi(\lambda^{k+1}) \right) + B_\phi(z, z^k) - B_\phi(z, z^{k+1}), \tag{33}
\]
for any \( z \in \mathbb{R}^n \). Indeed, it follows from the optimality condition in the mirror descent step that, for any \( z \in \mathbb{R}^n \), we have
\[
\left\langle \nabla \varphi(\mu^{k+1}) + \frac{\nabla \phi(z^{k+1}) - \nabla \phi(z^k)}{\alpha^{k+1}}, z - z^{k+1} \right\rangle \geq 0. \tag{34}
\]
Recall the celebrated generalized triangle inequality for the Bregman divergence:
\[
B_\phi(z, z^k) - B_\phi(z, z^{k+1}) - B_\phi(z^{k+1}, z^k) = \left\langle \nabla \phi(z^{k+1}) - \nabla \phi(z^k), z - z^{k+1} \right\rangle. \tag{35}
\]
Therefore, we have
\[
\alpha^{k+1} \left\langle \nabla \varphi(\mu^{k+1}), z^k - z \right\rangle = \alpha^{k+1} \left\langle \nabla \varphi(\mu^{k+1}), z^k - z^{k+1} \right\rangle + \alpha^{k+1} \left\langle \nabla \varphi(\mu^{k+1}), z^{k+1} - z \right\rangle 
\leq \alpha^{k+1} \left\langle \nabla \varphi(\mu^{k+1}), z^k - z^{k+1} \right\rangle + B_\phi(z, z^k) - B_\phi(z, z^{k+1}) - B_\phi(z^{k+1}, z^k) 
\leq \alpha^{k+1} \left\langle \nabla \varphi(\mu^{k+1}), z^k - z^{k+1} \right\rangle + B_\phi(z, z^k) - B_\phi(z, z^{k+1}) - \frac{1}{2\gamma} \|z^{k+1} - z^k\|_\infty^2, \tag{36}
\]
where the last inequality comes from the fact that $\phi$ is $\frac{1}{\gamma}$-strongly convex with respect to $\ell_\infty$-norm. Furthermore, we observe from the update formula of $\mu^{k+1}$ and $\lambda^{k+1}$ that

$$
\lambda^{k+1} - \mu^{k+1} = \frac{\bar{\alpha}^{k+1}}{\bar{\alpha}^{k+1}}(z^{k+1} - z^k), \tag{37}
$$

and the update formula of $\alpha^{k+1}$ and $\bar{\alpha}^{k+1}$ yields

$$
\gamma M^k (\alpha^{k+1})^2 = \bar{\alpha}^k + \alpha^{k+1} = \bar{\alpha}^{k+1}. \tag{38}
$$

Therefore, we have

$$
\alpha^{k+1} \langle \nabla \phi(\mu^{k+1}), z^k - z^{k+1} \rangle \overset{(37)}{=} \bar{\alpha}^{k+1} \langle \nabla \phi(\mu^{k+1}), \mu^{k+1} - \lambda^{k+1} \rangle.
$$

In addition, the following equality holds:

$$
\|z^{k+1} - z^k\|_\infty^2 \overset{(37)}{=} \left(\frac{\bar{\alpha}^{k+1}}{\bar{\alpha}^{k+1}}\right)^2 \|\mu^{k+1} - \lambda^{k+1}\|_\infty^2 \overset{(38)}{=} \gamma M^k \bar{\alpha}^{k+1} \|\mu^{k+1} - \lambda^{k+1}\|_\infty^2.
$$

Plugging all the above equations into (36) yields that

$$
\alpha^{k+1} \langle \nabla \phi(\mu^{k+1}), z^k - z \rangle
\leq \bar{\alpha}^{k+1} \langle \nabla \phi(\mu^{k+1}), \mu^{k+1} - \lambda^{k+1} \rangle + B_\phi(z, z^k) - B_\phi(z, z^{k+1}) - \frac{\bar{\alpha}^{k+1} M^k}{2} \|\mu^{k+1} - \lambda^{k+1}\|_\infty^2
\leq \bar{\alpha}^{k+1} \langle \varphi(\mu^{k+1}) - \varphi(\lambda^{k+1}) \rangle + B_\phi(z, z^k) - B_\phi(z, z^{k+1}),
$$

where the last inequality comes from the stopping criterion in the line search strategy. Therefore, we conclude the desired inequality (33).

The next step is to bound the iterative objective gap, i.e., for $z \in \mathbb{R}^n$,

$$
\bar{\alpha}^{k+1} \varphi(\lambda^{k+1}) - \bar{\alpha}^{k} \varphi(\lambda^{k})
\leq \alpha^{k+1} \left( \varphi(\mu^{k+1}) + \langle \nabla \varphi(\mu^{k+1}), z - \mu^{k+1} \rangle \right) + B_\phi(z, z^k) - B_\phi(z, z^{k+1}), \tag{39}
$$

Indeed, we observe from the update formula of $\mu^{k+1}$ that

$$
\alpha^{k+1} (\mu^{k+1} - z^k) \overset{(38)}{=} \left(\frac{\bar{\alpha}^{k+1}}{\bar{\alpha}^{k}}\right) \mu^{k+1} - \alpha^{k+1} z^k
= \bar{\alpha}^{k+1} z^k + \bar{\alpha}^{k} \lambda^k - \bar{\alpha}^{k} \mu^{k+1} - \alpha^{k+1} z^k
= \bar{\alpha}^{k} \left( \lambda^k - \mu^{k+1} \right). \tag{40}
$$

Thus, we have

$$
\alpha^{k+1} \langle \nabla \varphi(\mu^{k+1}), \mu^{k+1} - z \rangle
= \alpha^{k+1} \langle \nabla \varphi(\mu^{k+1}), \mu^{k+1} - z^k \rangle + \alpha^{k+1} \langle \nabla \varphi(\mu^{k+1}), z^k - z \rangle
\overset{(40)}{=} \bar{\alpha}^{k} \langle \nabla \varphi(\mu^{k+1}), \lambda^k - \mu^{k+1} \rangle + \alpha^{k+1} \langle \nabla \varphi(\mu^{k+1}), z^k - z \rangle
= D.
$$
Furthermore, given the results of (33) and (38), the following results hold:

\[
D \leq \bar{\alpha}^k \left( \varphi(\lambda^k) - \varphi(\mu^{k+1}) \right) + \alpha^{k+1} \left\langle \nabla \varphi(\mu^{k+1}), z^k - z \right\rangle \\
\leq \bar{\alpha}^k \left( \varphi(\lambda^k) - \varphi(\mu^{k+1}) \right) + \alpha^{k+1} \left( \varphi(\mu^{k+1}) - \varphi(\lambda^{k+1}) \right) + B_\phi(z, z^k) - B_\phi(z, z^{k+1}) \\
= \bar{\alpha}^k \varphi(\lambda^k) - \bar{\alpha}^{k+1} \varphi(\lambda^{k+1}) + \alpha^{k+1} \left( \varphi(\mu^{k+1}) - \varphi(\lambda^{k+1}) \right) + B_\phi(z, z^k) - B_\phi(z, z^{k+1}).
\]

Summing up (39) over \( k = 0, 1, \ldots, N - 1 \) yields that

\[
\bar{\alpha}^N \varphi(\lambda^N) - \bar{\alpha}^0 \varphi(\lambda^0) \leq \sum_{k=0}^{N-1} \left[ \alpha^{k+1} \left( \varphi(\mu^{k+1}) + \left\langle \nabla \varphi(\mu^{k+1}), z - \mu^{k+1} \right\rangle \right) \right] + B_\phi(z, z^0) - B_\phi(z, z^N).
\]

Finally, we observe that \( \alpha^0 = \bar{\alpha}^0 = 0, \ B_\phi(z, z^N) \geq 0 \) and \( \phi \) is 1-smooth with respect to \( \ell_\infty \)-norm, and conclude that, for any \( z \in \mathbb{R}^n \)

\[
\bar{\alpha}^N \varphi(\lambda^N) \leq \sum_{k=0}^{N} \left[ \alpha^{k} \left( \varphi(\mu^{k}) + \left\langle \nabla \varphi(\mu^{k}), z - \mu^{k} \right\rangle \right) \right] + \| z - z^0 \|_\infty^2.
\]

The desired inequality (32) directly follows by changing the counter from \( k \) to \( i \) and the iteration count \( N \) to \( k \). \( \square \)

The final lemma provides us with a key lower bound for the accumulating parameter.

**Lemma 4.4.** For each iteration \( k \) of the APDAMD algorithm, we have

\[
\bar{\alpha}^k \geq \frac{\eta(k + 1)^2}{8\gamma \| A \|_1^2}. \tag{41}
\]

**Proof.** For \( k = 1 \), we have

\[
\bar{\alpha}^1 = \bar{\alpha}^1 \overset{(38)}{=} \frac{1}{\gamma M^1} \geq \frac{\eta}{2\gamma \| A \|_1^2},
\]

where \( M^1 \leq \frac{2\| A \|_1^2}{\eta} \) has been proven in Lemma 4.2. So (41) holds true for \( k = 1 \). Then we
proceed to prove (41) for \( k \geq 1 \) by using the mathematical induction. Indeed, we have
\[
\bar{\alpha}^{k+1} = \bar{\alpha}^k + \frac{2\gamma M}{\bar{\alpha}^k + 1 + 4\gamma M^2} + \frac{\alpha^{k+1}}{\gamma M^k}
\]
\[
\geq \bar{\alpha}^k + \frac{\eta}{2\gamma M} + \sqrt{\alpha^k + 1 + 4\gamma M^2} + \frac{\eta\alpha^k}{\gamma M^k}
\]
\[
\geq \bar{\alpha}^k + \frac{\eta}{2\gamma M} + \frac{\eta\alpha^k}{2\gamma M^k},
\]
where \( M^k \leq \frac{2\|A\|_1^2}{\eta} \) was also proven in Lemma 4.2. Now, we assume that (41) hold true for \( k \). Then, we find that
\[
\bar{\alpha}^{k+1} \geq \frac{\eta(k + 1)^2}{8\gamma\|A\|_1^2} + \frac{\eta\gamma^2(k + 1)^2}{16\gamma^2\|A\|_1^2} + \frac{\eta\alpha^k}{2\gamma\|A\|_1^2},
\]
which implies that (41) holds true for \( k + 1 \). \( \square \)

4.3 Complexity analysis for the APDAMD algorithm

With the key properties of APDAMD algorithm for the general setup in (25) at hand, we are now ready to analyze the complexity of the APDAMD algorithm for solving the regularized OT problem.

We start with the setting of the dual objective \( \varphi \). In particular, different from dual problem (5), we set \( \varphi(\lambda) \) as the objective in the original dual OT problem in which \( \lambda := (\alpha, \beta) \), given by
\[
\min_{\alpha, \beta \in \mathbb{R}^n} \varphi(\alpha, \beta) := \eta \sum_{i,j=1}^n e^{-\frac{C_{ij} - u_i - \beta_j}{\eta}} - \langle \alpha, r \rangle - \langle \beta, l \rangle.
\]
(42)
The above dual form was also considered in [16] to establish the complexity bound of APDAGD algorithm. By means of transformations \( u_i = \frac{\alpha_i + \eta - \frac{1}{2}}{\eta} \) and \( v_j = \frac{\beta_j + \eta - \frac{1}{2}}{\eta} \), we follow from Lemma 3.2 that
\[
\|\alpha^*\|_\infty \leq \eta \left( R + \frac{1}{2} \right), \quad \|\beta^*\|_\infty \leq \eta \left( R + \frac{1}{2} \right)
\]
(43)
Theorem 4.5. The APDAMD algorithm for approximating optimal transport (Algorithm 3) returns an output \( X^k \) that satisfies \( \| A \, \text{vec}(X^k) - b \|_1 \leq \varepsilon' \) in a number of iterations \( k \) bounded as follows:

\[
k \leq 1 + 4\sqrt{2} \| A \|_1 \sqrt{\frac{\gamma (R + 1/2)}{\varepsilon'}}
\]

where \( R \) is defined in Lemma 3.2.

Proof. From Lemma 4.3, we have

\[
\tilde{\alpha}^k \varphi(\lambda^k) \leq \min_{z \in \mathbb{R}^n} \left\{ \sum_{j=0}^{k} \left[ \alpha^j \left( \varphi(\mu^j) + \langle \nabla \varphi(\mu^j), z - \mu^j \rangle \right) \right] + \| z \|_2^2 \right\}
\]

\[
\leq \min_{z \in B_{\infty}(2\hat{R})} \left\{ \sum_{j=0}^{k} \left[ \alpha^j \left( \varphi(\mu^j) + \langle \nabla \varphi(\mu^j), z - \mu^j \rangle \right) \right] + \| z \|_2^2 \right\},
\]

where \( \hat{R} = \eta(R + 1/2) \) is the upper bound for \( \ell_\infty \)-norm of optimal solutions of dual regularized OT problem (42) and \( B_{\infty}(r) \) is defined as

\[
B_{\infty}(r) := \{ \lambda \in \mathbb{R}^n \mid \| \lambda \|_\infty \leq r \}.
\]

This implies that

\[
\tilde{\alpha}^k \varphi(\lambda^k) \leq \min_{z \in B_{\infty}(2\hat{R})} \left\{ \sum_{j=0}^{k} \left[ \alpha^j \left( \varphi(\mu^j) + \langle \nabla \varphi(\mu^j), z - \mu^j \rangle \right) \right] \right\} + 4\hat{R}^2.
\]

By the definition of the dual objective function \( \varphi(\lambda) \), we further have

\[
\varphi(\mu^j) + \langle \nabla \varphi(\mu^j), z - \mu^j \rangle = \langle \mu^j, b - Ax(\mu^j) \rangle - f(x(\mu^j)) + \langle z - \mu^j, b - Ax(\mu^j) \rangle
\]

\[
= -f(x(\mu^j)) + \langle z, b - Ax(\mu^j) \rangle.
\]

Therefore, we conclude that

\[
\tilde{\alpha}^k \varphi(\lambda^k) \leq \min_{z \in B_{\infty}(2\hat{R})} \left\{ \sum_{j=0}^{k} \left[ \alpha^j \left( \varphi(\mu^j) + \langle \nabla \varphi(\mu^j), z - \mu^j \rangle \right) \right] \right\} + 4\hat{R}^2
\]

\[
\leq 4\hat{R}^2 - \tilde{\alpha}^k f(x^k) + \min_{z \in B_{\infty}(2\hat{R})} \left\{ \tilde{\alpha}^k \left\langle z, b - Ax^k \right\rangle \right\}
\]

\[
= 4\hat{R}^2 - \tilde{\alpha}^k f(x^k) - 2\tilde{\alpha}^k \hat{R} \| Ax^k - b \|_1,
\]

where the second inequality comes from the convexity of \( f \) and the last equality comes from the fact that \( \ell_1 \)-norm is the dual norm of \( \ell_\infty \)-norm. That is to say,

\[
f(x^k) + \varphi(\lambda^k) + 2 \tilde{\alpha}^k \| Ax^k - b \|_1 \leq \frac{4\hat{R}^2}{\tilde{\alpha}^k}.
\]
By the definition of $\varphi(\lambda)$ and the fact that $\lambda^*$ is an optimal solution, we have
\[
f(x^k) + \varphi(\lambda^*) \geq f(x^k) + \varphi(\lambda^*)
= f(x^k) + \langle \lambda^*, b \rangle + \max_{x \in \mathbb{R}^n} \left\{ -f(x) - \left\langle A^\top \lambda^*, x \right\rangle \right\}
\geq f(x^k) + \langle \lambda^*, b \rangle - f(x^k) - \left\langle \lambda^*, Ax^k \right\rangle
= \langle \lambda^*, b - Ax^k \rangle
\geq -\hat{R} \left\| Ax^k - b \right\|_1,
\]
where the last inequality comes from the Hölder inequality and $\|\lambda\|_\infty \leq \hat{R}$. We conclude that
\[
\left\| Ax^k - b \right\|_1 \leq \frac{4\hat{R}}{\alpha^k} \leq \frac{32\gamma(R + 1/2)\|A\|_1^2}{(k + 1)^2},
\]
and obtain the desired bound on the number of iterations $k$ required to satisfy the bound $\|A \text{ vec}(X^k) - b\|_1 \leq \varepsilon'$.

Now, we are ready to present the complexity bound of APDAMD algorithm for approximating the OT problem.

**Theorem 4.6.** The APDAMD algorithm for approximating optimal transport (Algorithm 3) returns $\hat{X} \in \mathbb{R}^{n \times n}$ satisfying $\hat{X} 1 = r$, $\hat{X}^\top 1 = l$ and (4) in a total of
\[
O \left( \frac{n^2 \sqrt{\gamma} \|C\|_\infty \log(n)}{\varepsilon} \right)
\]
arithmetic operations.

The proof of Theorem 4.6 is provided in Section 6.2. The complexity bound of the APDAMD algorithm in Theorem 4.6 suggests an interesting feature of the (regularized) OT problem. Indeed, the dependence of that bound on $\gamma$ manifests the necessity of using $\|\cdot\|_\infty$ in the understanding of the complexity of the regularized OT problem. This view is also in harmony with the proof technique of running time for the Greenkhorn algorithm in Section 3, where we rely on the $\|\cdot\|_\infty$ of optimal solutions of the dual regularized OT problem to measure the progress in the objective value among the successive iterates.

### 4.4 Revisiting the APDAGD algorithm

In this section, we revisit the adaptive primal-dual accelerated gradient descent (APDAGD) [16] for the regularized OT. We first point out that the complexity bound of the APDAGD algorithm for regularized OT is not $\tilde{O} \left( \min \left\{ \frac{n^{9/4}}{\varepsilon^2}, \frac{n^2}{\varepsilon^2} \right\} \right)$ as claimed from their current theoretical analysis before. Then, we provide a new complexity bound of the APDAGD algorithm based on our results in Section 4.3. Finally, despite the issue with regularized OT, we wish to emphasize that the APDAGD algorithm is still an interesting and efficient accelerated method for general setup (25) with theoretical guarantee under the certain conditions. More precisely, while [16, Theorem 3] can not be applied to regularized OT since there exists no dual solution with a constant bound in $\|\cdot\|_2$, this theorem is still valid and can be used for other regularized problems with bounded optimal dual solution.

To facilitate the ensuing discussion, we first present the complexity bound for regularized OT from [16], using the notation from the current paper.
Theorem 4.7 (Theorem 4 in [16]). The APDAGD algorithm [16] for approximating optimal transport returns \( \hat{X} \in \mathbb{R}^{n \times n} \) satisfying \( \hat{X} 1 = r, \hat{X}^\top 1 = l \) and (4) in a number of arithmetic operations bounded as

\[
O \left( \min \left\{ \frac{n^{9/4} \sqrt{R} \| C \|_\infty \log(n)}{\varepsilon}, \frac{n^2 R \| C \|_\infty \log(n)}{\varepsilon^2} \right\} \right),
\]

where \( \| (u^*, v^*) \|_2 \leq R \) and \( (u^*, v^*) \) denotes an optimal solution pair for the dual regularized OT problem (6).

This theorem suggests that the complexity bound for the APDAGD algorithm is at the order \( \mathcal{O} \left( \min \left\{ \frac{n^{9/4} \sqrt{R} \| C \|_\infty \log(n)}{\varepsilon}, \frac{n^2 R \| C \|_\infty \log(n)}{\varepsilon^2} \right\} \right) \). However, there are two issues:

1. The upper bound \( R \) is assumed to be bounded and independent of \( n \), which is not correct; see our counterexample in Proposition 4.8.

2. The known upper bound \( R \) is based on \( \min_{1 \leq i, j \leq n} \{ r_i, l_j \} \) (cf. Lemma 3.2 or [16, Lemma 1]). This implies that the valid algorithm needs to take the rounding error with weight vectors \( r \) and \( l \) into account.

Corrected upper bound \( \tilde{R} \). The upper bounds from (43) imply that a straightforward upper bound for \( R \) is \( \mathcal{O} \left( n^{1/2} \right) \). Furthermore, given \( \varepsilon \in (0, 1) \), we can show that \( \tilde{R} \) is indeed \( \Omega \left( n^{1/2} \right) \) by using the following specific regularized OT problem (2).

Proposition 4.8. Assume that all the entries of the ground cost matrix \( C \in \mathbb{R}^{n \times n} \) are 1 and the weight vectors \( r = l = 1/n \). Given \( \varepsilon \in (0, 1) \) and the regularization term \( \eta = \frac{\varepsilon}{4 \log(n)} \), the optimal solution \((\alpha^*, \beta^*)\) of the dual regularized OT problem (42) satisfies \( \| (\alpha^*, \beta^*) \|_2 \geq n^{1/2} \).

Proof. Given the choices of \( r, l \) and \( \eta \), we can rewrite the dual function \( \varphi(\alpha, \beta) \) in (42) as follows:

\[
\varphi(\alpha, \beta) = \frac{\varepsilon}{4 e \log(n)} \sum_{1 \leq i, j \leq n} e^{-\frac{4 \log(n)}{\varepsilon} (1 - \alpha_i - \beta_j)} - \frac{\sum_{i=1}^n \alpha_i}{n} - \frac{\sum_{i=1}^n \beta_i}{n}.
\]

Since \((\alpha^*, \beta^*)\) is the optimal solution of dual regularized OT problem (42), we have

\[
e^{\frac{4 \log(n) \alpha_i^*}{\varepsilon}} \sum_{j=1}^n e^{-\frac{4 \log(n)}{\varepsilon} (1 - \beta_j^*)} = e^{\frac{4 \log(n) \beta_j^*}{\varepsilon}} \sum_{j=1}^n e^{-\frac{4 \log(n)}{\varepsilon} (1 - \alpha_j^*)} = \frac{e}{n}, \quad \forall i \in [n]. \tag{44}
\]

This implies that \( \alpha_i^* = \alpha_j^* \) and \( \beta_i^* = \beta_j^* \) for all \( i, j \in [n] \). So we can define \( A \) and \( B \) such that

\[
A \equiv e^{\frac{4 \log(n) \alpha_i^*}{\varepsilon}}, \quad B \equiv e^{\frac{4 \log(n) \beta_j^*}{\varepsilon}}.
\]

By the optimality condition (44), \( AB e^{-4 \log(n)/\varepsilon} = e/n^2 \). Equivalently, \( AB = \frac{e^{4 \log(n)/\varepsilon}}{n^2} \). So we have

\[
\alpha_i^* + \beta_i^* = \frac{\varepsilon (\log(A) + \log(B))}{4 \log(n)} = \frac{\varepsilon}{4 \log(n)} \left( \frac{4 \log(n)}{\varepsilon} + 1 - 2 \log(n) \right) = 1 + \frac{\varepsilon}{4 \log(n)} - \frac{\varepsilon}{2}.
\]

Therefore, we conclude that

\[
\| (\alpha^*, \beta^*) \|_2 \geq \sqrt{\sum_{i=1}^n (\alpha_i^* + \beta_i^*)^2} = \sqrt{\frac{n}{2} \left( 1 + \frac{\varepsilon}{4 \log(n)} - \frac{\varepsilon}{2} \right)} \geq n^{1/2}.
\]

As a consequence, we achieve the conclusion of the proposition. \( \square \)
Algorithm 5: Approximating OT by APDAGD

**Input:** \( \eta = \frac{\varepsilon}{4 \log(n)} \) and \( \varepsilon' = \frac{\varepsilon}{8 \|C\|_{\infty}} \).

**Step 1:** Let \( \tilde{r} \in \Delta_n \) and \( \tilde{l} \in \Delta_n \) be defined as

\[
\left( \tilde{r}, \tilde{l} \right) = \left( 1 - \frac{\varepsilon'}{8} \right) (r, l) + \frac{\varepsilon'}{8n} (1, 1).
\]

**Step 2:** Let \( A \in \mathbb{R}^{2n \times n^2} \) and \( b \in \mathbb{R}^{2n} \) be defined by

\[
A \text{vec}(X) = \begin{bmatrix} X & X^\top \end{bmatrix}, \quad b = \begin{bmatrix} \tilde{r} \\ \tilde{l} \end{bmatrix}.
\]

**Step 3:** Compute \( \tilde{X} = \text{APDAGD} (\varphi, A, b, \varepsilon'/2) \) with \( \varphi \) defined in (26) with \( f(x) = \text{vec}(C)^\top \text{vec}(X) - \eta H(X) \).

**Step 4:** Round \( \tilde{X} \) to \( \hat{X} \) by [3, Algorithm 2] such that \( \hat{X} \mathbf{1} = r, \hat{X}^\top \mathbf{1} = l \).

**Output:** \( \hat{X} \).

Approximation algorithm for OT by APDAGD. Algorithm 4 in [16] can be improved by incorporating the rounding procedure, which is summarized in Algorithm 5. Here, the APDAGD algorithm used in Algorithm 5 stands for Algorithm 3 in [16]. Given the corrected upper bound \( T \) and Algorithm 5 for approximating OT, we provide a new complexity bound of the APDAGD algorithm in the following proposition.

**Proposition 4.9.** The APDAGD algorithm for approximating optimal transport (Algorithm 5) returns \( \hat{X} \in \mathbb{R}^{n \times n} \) satisfying \( \hat{X} \mathbf{1} = r, \hat{X}^\top \mathbf{1} = l \) and (4) in a total of

\[
O \left( \frac{n^{5/2} \sqrt{\|C\|_{\infty} \log(n)}}{\varepsilon} \right)
\]

arithmetic operations.

The proof of Proposition 4.9 is provided in Section 6.3. As indicated in Proposition 4.9, the corrected complexity bound of APDAGD algorithm for the regularized OT is similar to that of our APDAMD algorithm when we choose the Bregman divergence to be \( \frac{1}{2n} \| \cdot \|_2^2 \), which leads to \( \gamma = n \). It is still unclear whether the upper bound \( n \) of \( \gamma \) can be further improved [26]. From this perspective, our APDAMD algorithm can be viewed as a generalization of the APDAGD algorithm. Finally, since our APDAMD algorithm utilizes \( \| \cdot \|_{\infty} \) in its line search criterion, it will be more robust than the APDAGD algorithm (see the experimental results in Section 5).

5 Experiments

In this section, we conduct the extensive comparative experiments with the Greenkhorn and APDAMD algorithms on both synthetic images and real images from MNIST Digits dataset\(^1\). The baseline algorithms include the Sinkhorn algorithm [12, 3], the APDAGD algorithm [16] and the GCPB algorithm [17]. The Greenkhorn and APDAGD algorithms have been shown outperform the Sinkhorn algorithm in [3] and [16], respectively. However, we repeat some of

\(^1\)http://yann.lecun.com/exdb/mnist/
these comparisons to ensure that our evaluation is systematic and complete. Finally, we utilize the default linear programming solver in MATLAB to obtain the optimal value of the original optimal transport problem without entropic regularization.

-1000 0 1000 2000 3000 4000 5000 Row/Col Updates
-0.2 0 0.2 0.4 0.6 0.8 1 1.2 1.4 1.6 1.8 |r(P)−r|1 + |c(P)−c|1 Distance to Polytope GREENKHORN SINKHORN

0 500 1000 1500 2000 2500 3000 3500 4000 Row/Col Updates 0 0.5 1 1.5 2 2.5 3 ln(compet ratio for error) Speed of ln(compet ratio for error) Max Median Min

0 500 1000 1500 2000 2500 3000 3500 4000 4500 Row/Col Updates
0 0.2 0.25 0.3 0.35 0.4 0.45 0.5 0.55 0.6 0.65 0.7 Value of OT SINKHORN vs GREENKHORN for OT True optimum SINKHORN, \( \eta = 1 \) SINKHORN, \( \eta = 5 \) SINKHORN, \( \eta = 9 \) GREENKHORN, \( \eta = 1 \) GREENKHORN, \( \eta = 5 \) GREENKHORN, \( \eta = 9 \)

0 1000 2000 3000 4000 Row/Col Updates
0 0.5 1 1.5 2 ln(compet ratio for error)

Figure 1: Performance of the Sinkhorn and Greenkhorn algorithms on the synthetic images. In the top two images, the comparison is based on using the distance \( d(P) \) to the transportation polytope, and the maximum, median and minimum of competitive ratios \( \log(d(P_S)/d(P_G)) \) on ten random pairs of images. Here, \( d(P_S) \) and \( d(P_G) \) refer to the Sinkhorn and Greenkhorn algorithms, respectively. In the bottom left image, the comparison is based on varying the regularization parameter \( \eta \in \{ 1, 5, 9 \} \) and reporting the optimal value of the original optimal transport problem without entropic regularization. Note that the foreground covers 10% of the synthetic images here. In the bottom right image, we compare by using the median of competitive ratios with varying coverage ratio of foreground in the range of 10%, 50%, and 90% of the images.

5.1 Synthetic images

We follow the setup in [3] in order to compare different algorithms on the synthetic images. In particular, the transportation distance is defined between a pair of randomly generated synthetic images and the cost matrix is comprised of \( \ell_1 \) distances among pixel locations in the images.

Image generation: Each of the images is of size 20 by 20 pixels and is generated based on
randomly positioning a foreground square in otherwise black background. We utilize a uniform distribution on $[0, 1]$ for the intensities of the background pixels and a uniform distribution on $[0, 50]$ for the foreground pixels. To further evaluate the robustness of all the algorithms to the ratio with varying foreground, we vary the proportion of the size of this square in $\{0.1, 0.5, 0.9\}$ of the images and implement all the algorithms on different kind of synthetic images.

**Evaluation metrics:** Two metrics proposed by [3] are used here to quantitatively measure the performance of different algorithms. The first metric is the distance between the output of the algorithm, $X$, and the transportation polytope, i.e.,

$$d(X) = \|r(X) - r\|_1 + \|l(X) - l\|_1,$$

(45)

where $r(X)$ and $l(X)$ are the row and column marginal vectors of the output $X$ while $r$ and $l$ stand for the true row and column marginal vectors. The second metric is the competitive ratio, defined by $\log(d(X_1)/d(X_2))$ where $d(X_1)$ and $d(X_2)$ refer to the distance between the outputs of two algorithms and the transportation polytope.
**Experimental setting:** We perform three pairwise comparative experiments: Sinkhorn versus Greenkhorn, APDAGD versus APDAMD, and Greenkhorn versus APDAMD by running these algorithms with ten randomly selected pairs of synthetic images. We also evaluate all the algorithms with varying regularization parameter $\eta \in \{1, 5, 9\}$ and the optimal value of the original optimal transport problem without entropic regularization, as suggested by [3].

Figure 3: Performance of the Greenkhorn and APDAMD algorithms on the synthetic images. All the four images correspond to those in Figure 1, showing that the Greenkhorn algorithm is faster than the APDAMD algorithm in terms of iterations. Note that $\log(d(P_G)/d(P_{MD}))$ on ten random pairs of images is consistently used, where $d(P_G)$ and $d(P_{MD})$ refer to the Greenkhorn and APDAMD algorithms, respectively.

**Experimental results:** We present the experimental results in Figure 1, Figure 2, and Figure 3 with different choices of regularization parameters and different choices of coverage ratio of the foreground. Figure 1 and 3 show that the Greenkhorn algorithm performs better than the Sinkhorn and APDAMD algorithms in terms of iteration numbers, illustrating the improvement achieved by using greedy coordinate descent on the dual regularized OT problem. This also supports our theoretical assertion that the Greenkhorn algorithm has the complexity bound as good as the Sinkhorn algorithm (cf. Theorem 3.7). Figure 2 shows that the APDAMD algorithm with $\gamma = n$ and the Bregman divergence equal to $\frac{1}{2\gamma} \|\cdot\|_2^2$ is not faster than the APDAGD algorithm but is more robust. This makes sense since their complexity bounds are the same in terms of $n$ and $\epsilon$ (cf. Theorem 4.6 and Proposition 4.9). On the other hand, the
robustness comes from the fact that the APDAMD algorithm can stabilize the training by using $\|\cdot\|_\infty$ in the line search criterion.

Figure 4: Performance of the Sinkhorn, Greenkhorn, APDAGD and APDAMD algorithms on the MNIST real images. In the first row of images, we compare the Sinkhorn and Greenkhorn algorithms in terms of iteration counts. The leftmost image specifies the distances $d(P)$ to the transportation polytope for two algorithms; the middle image specifies the maximum, median and minimum of competitive ratios $\log(d(P_S)/d(P_G))$ on ten random pairs of MNIST images, where $P_S$ and $P_G$ stand for the outputs of APDAGD and APDAMD, respectively; the rightmost image specifies the values of regularized OT with varying regularization parameter $\eta \in \{1, 5, 9\}$. In addition, the second and third rows of images present comparative results for APDAGD versus APDAMD and Greenkhorn versus APDAMD. In summary, the experimental results on the MNIST images are consistent with that on the synthetic images.
5.2 MNIST images

We proceed to the comparison between different algorithms on real images, using essentially the same evaluation metrics as in the synthetic images.

**Image processing:** The MNIST dataset consists of 60,000 images of handwritten digits of size 28 by 28 pixels. To understand better the dependence on $n$ for our algorithms, we add a very small noise term ($10^{-6}$) to all the zero elements in the measures and then normalize them such that their sum becomes one.

![Figure 5: Performance of the GCPB, APDAGD and APDAMD algorithms in term of time on the MNIST real images. These three images specify the values of regularized OT with varying regularization parameter $\eta \in \{1, 5, 9\}$, showing that the APDAMD algorithm is faster and more robust than the APDAGD and GCPB algorithms.](image)

Experimental results: We present the experimental results in Figure 4 and Figure 5 with different choices of regularization parameters as well as the coverage ratio of the foreground on the real images.

Figure 4 shows that the Greenkhorn algorithm is the fastest among all the candidate algorithms in terms of iteration count. Also, the APDAMD algorithm outperforms the APDAGD algorithm in terms of robustness and efficiency. All the results on real images are consistent with those on the synthetic images. Figure 5 shows that the APDAMD algorithm is faster and more robust than the APDAGD and GCPB algorithms. We conclude that APDAMD algorithm has a more favorable performance profile than APDAGD algorithm for solving the regularized OT problem.

6 Proofs

In this section, we provide the proofs for the remaining results in the paper.

6.1 Proof of Theorem 3.8

We follow the same steps as in the proof of Theorem 1 in [3] and obtain

$$
\langle C, \hat{X} \rangle - \langle C, X^* \rangle \leq 2\eta \log(n) + 4 \left( \left\| \hat{X} \mathbf{1} - r \right\|_1 + \left\| \hat{X}^\top \mathbf{1} - l \right\|_1 \right) \|C\|_\infty
$$

$$
\leq \frac{\varepsilon}{2} + 4 \left( \left\| \hat{X} \mathbf{1} - r \right\|_1 + \left\| \hat{X}^\top \mathbf{1} - l \right\|_1 \right) \|C\|_\infty,
$$

28
where $\hat{X}$ is the output of Algorithm 2, $X^*$ is a solution to the optimal transport problem and $\tilde{X}$ is the matrix returned by the Greenkhorn algorithm (Algorithm 1) with $\hat{r}$, $\tilde{l}$ and $\varepsilon'/2$ in Step 3 of Algorithm 2. The last inequality in the above display holds since $\eta = \frac{\varepsilon}{4\log(n)}$. Furthermore, we have

$$
\left\| \hat{X} - r \right\|_1 + \left\| \hat{X}^T - l \right\|_1 \leq \left\| \hat{X} - \tilde{r} \right\|_1 + \left\| \hat{X}^T - \tilde{l} \right\|_1 + \left\| r - \tilde{r} \right\|_1 + \left\| l - \tilde{l} \right\|_1 \\
\leq \frac{\varepsilon'}{2} + \frac{\varepsilon'}{4} + \frac{\varepsilon'}{2} = \varepsilon'.
$$

We conclude that $\langle C, \hat{X} \rangle - \langle C, X^* \rangle \leq \varepsilon$ from that $\varepsilon' = \frac{\varepsilon}{8\|C\|_{\infty}}$. The remaining task is to analyze the complexity bound. It follows from Theorem 3.7 that

$$
k \leq 2 + \frac{112nR}{\varepsilon'} \\
\leq 2 + \frac{96n\|C\|_{\infty}}{\varepsilon\eta} \left( \|C\|_{\infty} + \log(n) - 2\log \left( \min_{1 \leq i,j \leq n} \{r_i, l_j\} \right) \right) \\
\leq 2 + \frac{96n\|C\|_{\infty}}{\varepsilon} \left( 4\|C\|_{\infty} \log(n) + \log(n) - 2\log \left( \frac{\varepsilon}{64n\|C\|_{\infty}} \right) \right) \\
= O \left( \frac{n\|C\|^2_{\infty} \log(n)}{\varepsilon^2} \right).
$$

Therefore, the total iteration complexity of the Greenkhorn algorithm can be bounded by $O \left( \frac{n\|C\|^2_{\infty} \log(n)}{\varepsilon^2} \right)$. Combining with the fact that each iteration of Greenkhorn algorithm requires $O(n)$ arithmetic operations yields a total amount of arithmetic operations equal to $O \left( \frac{n^2\|C\|^2_{\infty} \log(n)}{\varepsilon^2} \right)$. On the other hand, $\tilde{r}$ and $\tilde{l}$ in Step 2 of Algorithm 2 can be found in $O(n)$ arithmetic operations [3, Algorithm 2], requiring $O(n^2)$ arithmetic operations. We conclude that the total number of arithmetic operations required for the Greenkhorn algorithm is $O \left( \frac{n^2\|C\|^2_{\infty} \log(n)}{\varepsilon^2} \right)$.

### 6.2 Proof of Theorem 4.6

We follow the same steps as those in the proof of Theorem 1 in [3] and obtain

$$
\langle C, \hat{X} \rangle - \langle C, X^* \rangle \leq 2\eta \log(n) + 4 \left( \left\| \hat{X} - r \right\|_1 + \left\| \hat{X}^T - l \right\|_1 \right) \|C\|_{\infty} \\
\leq \varepsilon' + 4 \left( \left\| \hat{X} - r \right\|_1 + \left\| \hat{X}^T - l \right\|_1 \right) \|C\|_{\infty},
$$

where $\hat{X}$ is the output of Algorithm 3, $X^*$ is a solution to the optimal transport problem and $\tilde{X}$ is the matrix returned by the APDAMD algorithm (Algorithm 4) with $\tilde{r}$, $\tilde{l}$ and $\varepsilon'/2$ in Step 3 of this algorithm. The last inequality in this display holds since $\eta = \frac{\varepsilon}{4\log(n)}$. Furthermore, we have

$$
\left\| \hat{X} - r \right\|_1 + \left\| \hat{X}^T - l \right\|_1 \leq \left\| \hat{X} - \tilde{r} \right\|_1 + \left\| \hat{X}^T - \tilde{l} \right\|_1 + \left\| r - \tilde{r} \right\|_1 + \left\| l - \tilde{l} \right\|_1 \\
\leq \frac{\varepsilon'}{2} + \frac{\varepsilon'}{4} + \frac{\varepsilon'}{2} = \varepsilon'.
$$
We conclude that \( \langle C, \hat{X} \rangle - \langle C, X^* \rangle \leq \varepsilon \) given that \( \varepsilon' = \frac{\varepsilon}{8\|C\|_{\infty}} \). The remaining step is to analyze the complexity bound. We obtain from Lemma 3.2 and \( \tilde{r} \) and \( \tilde{l} \) in Algorithm 3 that

\[
R = \frac{\|C\|_{\infty}}{\eta} + \log(n) - 2 \log \left( \min_{1 \leq i, j \leq n} \{ \tilde{r}_i, \tilde{l}_j \} \right) \leq \frac{4 \|C\|_{\infty} \log(n)}{\varepsilon} + \log(n) - 2 \log \left( \frac{\varepsilon}{64n\|C\|_{\infty}} \right). \tag{46}
\]

Since \( \|A\|_1 \) equals to the maximum \( \ell_1 \)-norm of a column of \( A \) and each column of \( A \) contains only two nonzero elements which are equal to one, we have \( \|A\|_1 = 2 \). We conclude by Lemma 4.2 and Theorem 4.5 that

\[
N_k \leq 4k + 4 + \frac{2 \log \left( \frac{\|A\|_1^2}{2\eta} \right) - 2 \log(L^0)}{\log 2}
\leq 8 + 16\sqrt{2} \|A\|_1 \sqrt{\gamma} \left( R + 1/2 \right) \|C\|_{\infty} \log(n) + \frac{2 \log \left( \frac{\log(n)}{\varepsilon} \right)}{\log 2}.
\]

Plugging (46) into the above inequality yields that

\[
N_k \leq 8 \sqrt{\varepsilon} \sqrt{\gamma} \left( R + 1/2 \right) \|C\|_{\infty} \log(n) + \frac{2 \log \left( \frac{\log(n)}{\varepsilon} \right)}{\log 2}.
\]

Therefore, the total number of iterations for the APDAMD algorithm can be bounded by \( O \left( \sqrt{\gamma} \|C\|_{\infty} \log(n) \right) \). Combined with the fact that each iteration of APDAMD algorithm requires \( O(n^2) \) arithmetic operations we find that the total number of arithmetic operations is \( O \left( n^2 \sqrt{\gamma} \|C\|_{\infty} \log(n) \right) \). Furthermore, \( \tilde{r} \) and \( \tilde{l} \) in Step 2 of Algorithm 3 can be found in \( O(n) \) arithmetic operations and Algorithm 2 in [3] requires \( O(n^2) \) arithmetic operations. Therefore, we conclude that the total number of arithmetic operations is \( O \left( n^2 \sqrt{\gamma} \|C\|_{\infty} \log(n) \right) \).

### 6.3 Proof of Proposition 4.9

The proof of Proposition 4.9 is a modification of the proof for [16, Theorem 4]. Therefore, we only give a proof sketch to ease the presentation. More specifically, we follow the argument of [16, Theorem 4] and obtain that the number of iterations for Algorithm 5 required to reach the tolerance \( \varepsilon \) is

\[
k \leq \max \left\{ O \left( \min \left\{ \frac{n^{1/4} \sqrt{R} \|C\|_{\infty} \log(n)}{\varepsilon}, \frac{R \|C\|_{\infty} \log(n)}{\varepsilon^2} \right\} \right), O \left( \frac{R \sqrt{\log n}}{\varepsilon} \right) \right\}. \tag{47}
\]
Plugging the tight upper bound $\bar{R} \leq \sqrt{n}$ into (47) yields that

$$k = \mathcal{O}\left(\sqrt{n\|C\|_\infty \log(n)} \over \varepsilon\right).$$

Since each iteration of the APDAGD algorithm requires $O(n^2)$ arithmetic operations, the total number of arithmetic operations is bounded by $\mathcal{O}\left(n^{5/2}\|C\|_\infty \log(n)\over \varepsilon\right)$. Furthermore, $\bar{r}$ and $\bar{l}$ in Step 2 of Algorithm 5 can be found in $O(n)$ arithmetic operations and Algorithm 2 in [3] requires $O(n^2)$ arithmetic operations. Therefore, we conclude that the total number of arithmetic operations required is $\mathcal{O}\left(n^{5/2}\sqrt{\|C\|_\infty \log(n)} \over \varepsilon\right)$.

7 Discussion

We have provided detailed analyses of convergence rates for two algorithms for solving regularized OT problems. First, we established that the complexity bound of the Greenkhorn algorithm can be improved to $\mathcal{O}\left(n^2\varepsilon^2\right)$, which matches the best known complexity bound of the Sinkhorn algorithm. We believe that this helps to explain why the Greenkhorn algorithm outperforms the Sinkhorn algorithm in practice. Second, we have proposed a novel adaptive primal-dual accelerated mirror descent (APDAMD) algorithm for solving regularized OT problems. We showed that the complexity bound of our algorithm is $\mathcal{O}\left(n^2\gamma^{1/2} \varepsilon^{-1}\right)$, where $\gamma$ is the inverse of the strongly convex module of the Bregman divergence with respect to $\|\cdot\|_\infty$. Finally, we pointed out that an existing complexity bound for the APDAGD algorithm from the literature is not valid in general by providing a concrete counterexample. We instead established a complexity bound for the APDAGD algorithm is $\mathcal{O}\left(n^{5/2} \varepsilon^{-1}\right)$, by exploiting the connection between the APDAMD and APDAGD algorithms.

There are many interesting directions for further research. First, the complexity bound of the APDAMD algorithm heavily depends on $\gamma$. As we mentioned earlier, a simple upper bound for $\gamma$ is the dimension $n$. However, this results in a complexity bound for the APDAMD algorithm of $\mathcal{O}\left(n^{5/2} \varepsilon^{-1}\right)$, which is unsatisfactory. It is of significant theoretical interest to investigate whether we can improve the dependence of $\gamma$ on $n$, such as $n^\tau$ for some $\tau < 1$. Another possible direction is to extend the APDAMD algorithm to the computation of Wasserstein barycenters. That computation has been proposed for a variety of applications in machine learning and statistics [19, 36, 37], but its theoretical understanding is limited despite recent developments in fast algorithms for solving the problem [13, 15].

Acknowledgements

We would like to thank Pavel Dvurechensky, Alexander Gasnikov, and Alexey Kroshnin for helpful discussion with the complexity bounds of APDAMD and APDAGD algorithms. This work was supported in part by the Mathematical Data Science program of the Office of Naval Research under grant number N00014-18-1-2764.
References


