Approximating the Quadratic Transportation Metric in Near-Linear Time

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Abstract
Computing the quadratic transportation metric (also called the 2-Wasserstein distance or root mean square distance) between two point clouds, or, more generally, two discrete distributions, is a fundamental problem in machine learning, statistics, computer graphics, and theoretical computer science. A long line of work has culminated in a sophisticated geometric algorithm due to Agarwal and Sharathkumar [2], which runs in time $\tilde{O}(n^{3/2})$, where $n$ is the number of points. However, obtaining faster algorithms has proven difficult since the 2-Wasserstein distance is known to have poor sketching and embedding properties, which limits the effectiveness of geometric approaches. In this paper, we give an extremely simple deterministic algorithm with $\tilde{O}(n)$ runtime by using a completely different approach based on entropic regularization, approximate Sinkhorn scaling, and low-rank approximations of Gaussian kernel matrices. We give explicit dependence of our algorithm on the dimension and precision of the approximation.

1 Introduction
Transportation metrics—known in various communities as Wasserstein distances, Kantorovich distances, and optimal transport distances—are a natural set of metrics on probability distributions supported on metric spaces with widespread applications throughout mathematics and statistics [55].

Given two distributions $p$ and $q$ on $\mathbb{R}^d$, we define

$$W_p(p, q) := \min_{\gamma \in \mathcal{M}(p, q)} \left( \int \|x - y\|^p d\gamma(x, y) \right)^{1/p},$$

where $\| \cdot \|$ is the Euclidean distance on $\mathbb{R}^d$ and where $\mathcal{M}(p, q)$ is the set of couplings between $p$ and $q$, that is, the set of all joint distributions on $\mathbb{R}^d \times \mathbb{R}^d$ whose projections

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onto the first and second component agree with $p$ and $q$, respectively (see, e.g., [43, 54] for background on Wasserstein distances and their properties). Wasserstein distances have recently witnessed a surge of interest from the computer science community in large part due to their effectiveness in a number of practical domains, including image processing and retrieval [34, 39, 44] and machine learning [8, 15, 33].

Of particular interest to applications is the 2-Wasserstein distance $W_2$, which has been used for barycenter computation [14, 22], shape interpolation [13, 51], shape reconstruction [23], triangulations [37], domain adaptation [19], synthesis of soft maps [50], blue-noise generation [24], and many more. For many such applications, $W_2$ gives better practical results than other $W_p$ distances (in particular $W_1$), see e.g. the discussions in [6, 19, 24, 37] and the references within.

There has been a great deal of work on the question of how fast $W_p$ can be computed between discrete distributions. Much of the focus, for computational reasons, has been on $W_1$, also known as earth mover’s distance. This research direction, inaugurated by embedding results into the $\ell_1$ metric [16, 32], has focused largely on efficiently sketching $W_1$ (see, e.g., [30]), and has resulted in an algorithm to compute a $(1 + \varepsilon)$ multiplicative approximation to $W_1$ between two distributions supported on $n$ atoms in time $\tilde{O}(n)$, that is, nearly linear in the size of the input [48] (see also [2, 5, 31]). These impressive results rely strongly on the fact that the cost $\|x - y\|$ appearing in the definition of $W_1$ is a metric.

In contrast to these results for $W_1$, the situation for $W_2$ – also known as the root mean square (RMS) distance or the transportation metric with quadratic cost – is much less complete. Breakthroughs due to Agarwal and Phillips [1] (for the $R^2$ case) and Agarwal and Sharathkumar [2] (for the general case) showed that this quantity can be approximated in time $\tilde{O}(n^{3/2})$, but no better results are known. This lack of progress is partially explained by the fact that the cost $\|x - y\|^2$ appearing in the definition of $W_2$ is not a metric. Moreover, strong evidence was given for the difficulty of approximating $W_2$ by Andoni et al. [6], who showed that, unlike the earth mover distance, the quadratic transportation metric cannot be effectively sketched. This impossibility result poses a fundamental obstacle to geometric algorithms for estimating $W_2$ in near-linear time, and raises the question of whether any algorithm can achieve this goal.

**Question.** Can an approximation of $W_2$ be computed in time $\tilde{O}(n)$?

In this work, we show that the answer is yes. We employ a radically different approach from prior work in the geometric algorithms community. Our technique, based on entropic regularization, bypasses embedding and sketching and leverages instead a low-rank approximation to the optimal coupling.

### 1.1 Problem statement

Let $\mathcal{X} := \{x_1, \ldots, x_n\} \subseteq \mathbb{R}^d$, and let $p$ and $q$ be two distributions supported on $\mathcal{X}$, given as two vectors in the simplex $\Delta_n := \{\lambda \in \mathbb{R}^n : \lambda \geq 0, \sum_{i=1}^n \lambda_i = 1\}$. We identify the set $\mathcal{M}(p, q)$ of couplings with nonnegative $n \times n$ matrices whose rows and columns sum to $p$ and $q$, respectively. This set $\mathcal{M}(p, q)$ is often called the transportation polytope. We

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1In this section, we suppress dependence on the dimension $d$ and precision $\varepsilon$ and defer detailed consideration to Section 1.4.
assume for normalization purposes throughout that \( X \) lies in the Euclidean ball of radius 1 centered at the origin; since the diameter of \( X \) can easily be estimated within a constant factor in \( O(n) \) time, this can always be achieved by translating and rescaling.

The primary goal is to estimate the cost of an optimal matching with respect to the quadratic Euclidean cost.

**Problem 1.** Given \( X, p, q, \) and \( \varepsilon \in (0, 1) \), compute \( \hat{W} \) satisfying
\[
|\hat{W} - W_2^2(p, q)| \leq \varepsilon.
\]

Note that the elementary inequality \((a - b)^2 \leq |a^2 - b^2|\) for \( a, b \geq 0 \) implies that \( \sqrt{\hat{W}} \) provides a \( \sqrt{\varepsilon} \) approximation to \( W_2^2(p, q) \). This additive guarantee implies a multiplicative guarantee if \( W_2^2(p, q) = \Omega(1) \); however, we do not obtain a multiplicative guarantee when \( W_2^2(p, q) \) is very small. We discuss prospects for obtaining a multiplicative guarantee in Section 4.

We also consider the stronger goal of producing a near-optimal feasible coupling between \( p \) and \( q \).

**Problem 2.** Given \( X, p, q, \) and \( \varepsilon \in (0, 1) \), compute \( \hat{P} \in \mathcal{M}(p, q) \) satisfying
\[
\sum_{i,j=1}^{n} \hat{P}_{ij} \|x_i - x_j\|^2 \leq W_2^2(p, q) + \varepsilon.
\]

A solution \( \hat{P} \) to Problem 2 clearly yields a solution to Problem 1 as long as the cost \( \hat{W} = \sum_{i,j=1}^{n} \hat{P}_{ij} \|x_i - x_j\|^2 \) can be computed quickly. Note that since we are interested in algorithms with \( o(n^2) \) running time, we will not be able to represent a solution \( \hat{P} \) to Problem 2 explicitly, so we will focus on returning such a matrix in *factored* form, with rank \( r = o(n) \).

### 1.2 Our results

Our main result breaks the \( \tilde{O}(n^{3/2}) \) barrier for approximating the quadratic transportation cost and shows that Problems 1 and 2 can be solved in near-linear time.

**Theorem 1** (Informal, constants suppressed). There exists a universal constant \( C > 0 \) and an algorithm that, given two distributions supported on \( n \) points in \( \mathbb{R}^d \), can compute an additive \( \varepsilon \)-approximation to the quadratic transportation cost in time
\[
\tilde{O}\left(\frac{n}{\varepsilon^3} \left( \frac{C \log n}{\varepsilon} \right)^d \right).
\]

Moreover, the algorithm also computes a feasible coupling (in factored form) achieving this approximation.

The explicit version appears as Theorem 2 below.
1.3 Our techniques

Our algorithm is simple. We leverage the technique of entropic regularization, which has been used in the machine learning literature to approximate the optimal transportation between two distributions with arbitrary costs \[21\], and has yielded algorithms which are fast both in theory and in practice \[4, 25, 28, 40, 51\].

The entropic regularization approach is based on solving the program

\[
\min_{P \in \mathcal{M}(p, q)} \langle C, P \rangle - \eta^{-1} H(P),
\]

for a carefully chosen regularization parameter \(\eta\), where \(C_{ij} := \|x_i - x_j\|^2\) for \(i, j \in [n]\) and \(H(P) := \sum_{ij} P_{ij} \log \frac{P_{ij}}{r_{ij}}\) is the entrywise Shannon entropy of the matrix \(P\). This approach was popularized by Cuturi \[21\], though similar ideas date back to Wilson \[56\].

The benefit of this technique is that the solution to the regularized program \(2\) can be characterized explicitly.

**Fact 1** (Cuturi \[21\], Lemma 2). The minimizer of \(2\) is the unique matrix in \(\mathcal{M}(p, q)\) of the form \(D_1KD_2\) for positive matrices \(D_1\) and \(D_2\), where \(K_{ij} := e^{-\eta C_{ij}}\) for \(i, j \in [n]\).

Finding matrices \(D_1\) and \(D_2\) for which \(D_1KD_2 \in \mathcal{M}(p, q)\) is an instance of what is known as the matrix scaling problem, which has a long history in the optimization and computer science literature \[29, 36, 43\]. Several recent works have shown that the matrix scaling problem can be solved in \(O(n^2)\) time by second-order methods \[3, 17\], and this quadratic dependence on \(n\) is not improvable for general matrices \(K\).

In this work, we adopt an older and simpler approach to the matrix scaling problem, known as Sinkhorn scaling (after Sinkhorn \[49\]) or the RAS method \[11\]. Sinkhorn scaling is a simple alternating minimization scheme, which alternates between renormalizing the rows and columns of \(K\) so that they have the desired marginals \(p\) and \(q\), respectively. For completeness, pseudocode for this procedure is provided in Appendix A.2. This algorithm iteratively builds positive diagonal matrices \(D_1\) and \(D_2\) such that \(D_1KD_2\) converges to an element of \(\mathcal{M}(p, q)\). This method has also been shown to solve the scaling problem in time \(O(n^2)\), albeit with polynomial (rather than logarithmic) dependence on the desired precision:

**Fact 2** (Altschuler et al. \[4, Theorem 2\], Dvurechensky et al. \[25, Theorem 1\]). Given a positive matrix \(K \in \mathbb{R}^{n \times n}\), Sinkhorn scaling (Algorithm 2) computes diagonal matrices \(\tilde{D}_1\) and \(\tilde{D}_2\) such that \(\tilde{P} := \tilde{D}_1K\tilde{D}_2\) satisfies \(\|P - p\|_1 + \|\tilde{P}^\top 1 - q\|_1 \leq \delta\) in \(O(\delta^{-1} \log \frac{n}{\min_{ij} K_{ij}})\) iterations. Moreover, the entries of \(\tilde{D}_1\) and \(\tilde{D}_2\) are polynomially bounded in \(\delta, \min_{ij} K_{ij}\), and \(n\) throughout the execution of the algorithm.

The benefit of using this algorithm rather than a second-order method is that Sinkhorn scaling can be implemented such that each iteration requires \(O(1)\) matrix-vector products with \(K\). The simple but key observation is that although computing these products takes \(\Theta(n^2)\) time for general positive matrices, if \(K\) can be written in factored form as \(V^\top V\) where \(V \in \mathbb{R}^{r \times n}\) for \(r = o(n)\), then each iteration takes time \(O(rn) = o(n^2)\). To exploit this property, we rely on the fact that when \(C_{ij} = \|x_i - x_j\|^2\), the matrix \(K\) is a Gaussian kernel.
matrix, with entries of the form $e^{-\eta \|x_i - x_j\|^2}$. We then appeal to the fact that Gaussian kernel matrices can be efficiently approximated by matrices of very low rank, with $r = \tilde{O}(1)$.

The main technical step is to show that Sinkhorn scaling can be used on this approximate matrix to produce a suitably good estimate of the optimal coupling. We then round the matrix obtained from approximate Sinkhorn scaling to the transport polytope and return the resulting matrix $\hat{P}$ and its cost $\tilde{W} = \sum_{ij} \hat{P}_{ij}\|x_i - x_j\|^2$. Once we establish that each step can be implemented in time $O(nr) = \tilde{O}(n)$, the proof is complete.

### 1.4 Related work

Approximating the Wasserstein distance between discrete distributions is a fundamental problem in optimization. In particular, since it is a special case of the transportation problem, it has been the focus of a great deal of work in the combinatorial optimization community. (See [47, Chapter 21] and references therein.) General optimal transportation problems are linear programs and can be solved in time $\tilde{O}(n^{2.5})$ by interior point techniques [35], or in time $\tilde{O}(n^3)$ by simple combinatorial methods [38]. In general, no algorithm for the optimal transport problem can run in time $o(n^2)$ without additional structural assumptions, since the matrix $(C_{ij})$ encoding the costs between locations has size $\Theta(n^2)$. Altschuler et al. [4] showed that this goal is (nearly) achievable by exhibiting an algorithm that obtained an additive $\varepsilon$ approximation to the optimal transport cost in time $\tilde{O}(n^2\varepsilon^{-3})$, which has been improved to $\tilde{O}(n^2\varepsilon^{-1})$ in subsequent work [12, 25, 41]. These results hold for any nonnegative cost matrix $C$ satisfying $\max_{ij} C_{ij} = O(1)$.

If the cost $C$ is metric, it is possible to obtain near-linear time algorithms. When $C_{ij}$ is an $\ell_p$ norm on $\mathbb{R}^d$—which includes the $W_1$ case—Sharathkumar and Agarwal [48] show that a $(1 + \varepsilon)$ multiplicative approximation can be obtained in $O(n \text{poly}(\log n, \varepsilon^{-1}))$ time in the special case where $p$ and $q$ are uniform distributions on $n$ points. Andoni et al. [5] gives an algorithm that can obtain an estimate of the $W_1$ distance between any two distributions in $\mathbb{R}^2$ in time $O(n^{1+\omega(1)})$, though this algorithm does not return a coupling. Both algorithms incur an exponential dependence on $d$ in the high-dimensional setting.

For the quadratic Euclidean cost—the $W_2$ case—no near-linear time algorithms are currently known. The first subquadratic algorithm was given by Agarwal and Phillips [1], who again consider the special case where $p$ and $q$ are uniform distributions on $n$ points in $\mathbb{R}^2$. They obtain a $(1 + \varepsilon)$ multiplicative approximation in time $\tilde{O}(n^{3/2}\varepsilon^{-3/2})$. This was extended to $\mathbb{R}^d$ by Agarwal and Sharathkumar [2] (though still under the condition that $p$ and $q$ are uniform distributions), who obtain a $(1 + \varepsilon)$ multiplicative approximation in $\tilde{O}(n^{3/2}\varepsilon^{-1}\tau(n, \varepsilon))$ time, where $\tau(n, \varepsilon)$ is the time required to query an $O(\varepsilon)$-approximate nearest neighbor data structure for $\ell_2$. Designing such data structures in high dimensions is a delicate matter [7], but if we require that query time be polylogarithmic in $n$ and that the data structure take $n^{O(1)}$ time to build, the best results incur dependence of order $O(d/\varepsilon^d)$ on the dimension [8]. No algorithms running in time $o(n^{3/2})$ are known, even for the case of uniform distributions in $\mathbb{R}^2$.

The idea of low-rank approximation to kernel matrices, which we exploit here, is common in machine learning [10, 23, 42, 46]. The use of low-dimensional couplings in optimal transport has been proposed for statistical purposes [27, 52], but, to our knowledge, has not been explored from an optimization perspective.
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2 Preliminaries

First, some notation. We use the matrix norms $\|A\|_\infty := \max_{ij} |A_{ij}|$ and $\|A\|_1 := \sum_{ij} |A_{ij}|$. For vectors, the notation $\|\cdot\|$ refers to the $\ell_2$ norm. We write $B^d_2$ to denote the unit $\ell_2$ ball around the origin in dimension $d$, $\mathbf{1}$ to denote the all-ones vector of dimension $n$, and $[k]$ to denote $\{1, \ldots, k\}$ for positive integers $k$. The Frobenius inner product between matrices is denoted by $\langle A, B \rangle$. The notation $\tilde{O}(\cdot)$ hides factors of the form $\log^{O(1)}(1/n\log^{O(1)}(1/\varepsilon))$.

2.1 Low-rank approximation of Gaussian kernel matrices

For the quadratic transport cost, the cost matrix $C_{ij} := \|x_i - x_j\|^2$ corresponds to the squared Euclidean distance, and thus the entrywise-exponentiated matrix $K_{ij} := \exp(-\eta C_{ij})$ in Fact 1 is a Gaussian kernel matrix (where $\eta = \frac{1}{2\sigma^2}$).

Definition 1. The Gaussian kernel matrix corresponding to points $x_1, \ldots, x_n \in \mathbb{R}^d$ and bandwidth parameter $\sigma > 0$ is the matrix $K := K(x_1, \ldots, x_n; \sigma) \in \mathbb{R}^{n \times n}$ with entries $K_{ij} := \exp(-\frac{\|x_i - x_j\|^2}{2\sigma^2})$.

Details about Gaussian kernel matrices can be found in, e.g., [18, 53]. Of critical importance to our approach is the fact that the spectrum of Gaussian kernel matrices decays exponentially fast, since this enables the approximation of Gaussian kernel matrices by low-rank matrices. We will use throughout the paper an explicit low-rank approximation obtained by truncating the Taylor expansion of the Gaussian kernel.

Lemma 1 (Cotter et al. [18]). There is a procedure $\text{TAYLORGKM}$ that, given any $x_1, \ldots, x_n \in B^d_2$, $\sigma > 0$, and $M \in \mathbb{N}$, takes time $O(n \binom{M-1+d}{M-1})$ to output a matrix $V_M \in \mathbb{R}^{\binom{M-1+d}{M-1} \times n}$ satisfying

$$\|K(x_1, \ldots, x_n; \sigma) - V_M^TV_M\|_\infty \leq \frac{1}{M!\sigma^{2M}}.$$

We write $V_M \leftarrow \text{TAYLORGKM}(x_1, \ldots, x_n; \sigma, M)$ to denote the procedure generating this low-rank factorization; for completeness, this is briefly described in Appendix A.1. We will choose $M = O(\varepsilon^{-1} \log n)$, so that the approximation $V_M^TV_M$ has rank $O(\varepsilon^{-1} \log n)^d$.

2.2 Rounding to transport polytope

It will be helpful to record the following simple guarantee about the rounding algorithm $\text{ROUND}$ due to Altschuler et al. [4]. The performance guarantee is a slight variation of [4, Lemma 7], and the runtime guarantee is immediate by definition of the algorithm. For completeness, Appendix A.3 includes a short proof of this as well as pseudocode for the $\text{ROUND}$ procedure.
Lemma 2. Given \( p, q \in \Delta_n \) and \( F \in \mathbb{R}^{n \times n}_{\geq 0} \) satisfying \( \| F \|_1 = 1 \), \( \text{ROUND}(F, p, q) \) outputs a matrix \( G \in M(p, q) \) of the form \( G = D_1 F D_2 + uw^\top \) for positive diagonal matrices \( D_1 \) and \( D_2 \) satisfying

\[
\| G - F \|_1 \leq \| F^1 - p \|_1 + \| F^T 1 - q \|_1.
\]

Moreover, the algorithm only uses \( O(1) \) matrix-vector products with \( F \) and \( O(n) \) additional processing time.

In particular, if \( F \) is given explicitly in factored form, then the output of \( \text{ROUND}(F, p, q) \) also has an explicit factorization with at most one additional rank 1 term.

2.3 Computing the quadratic transportation cost of low-rank matrices

Given a matrix \( P \in M(p, q) \), computing the cost \( \sum_{i,j=1}^{n} P_{ij} \| x_i - x_j \|^2 \) naïvely takes \( \Omega(n^2) \) time. However, if \( P \) is given explicitly in low-rank form, this cost can be computed more quickly.

**Fact 3.** The matrix \( C \) given by \( C_{ij} = \| x_i - x_j \|^2 \) satisfies

\[
C = y 1^\top + 1 y^\top - 2 X^\top X,
\]

where \( X := [x_1 \ldots x_n] \in \mathbb{R}^{d \times n} \) and \( y := [[\| x_1 \|^2, \ldots, \| x_n \|^2]^\top] \in \mathbb{R}^n \).

**Lemma 3.** If \( P \in M(p, q) \) is given as \( \sum_{k=1}^{r} v_k w_k^\top \), then \( \sum_{i,j=1}^{n} P_{ij} \| x_i - x_j \|^2 \) can be computed in \( O(n d r) \) time.

**Proof.** The matrix \( X \) and the vector \( y \) can be computed in \( O(d n) \) time. Clearly \( \langle P, y 1^\top + 1 y^\top \rangle = y^\top (p + q) \) can be computed in \( O(n) \) time, and \( \langle P, X^\top X \rangle = \sum_{k=1}^{r} v_k X^\top X v_k \) can be computed in \( O(n d r) \) time. Therefore computing \( \sum_{i,j=1}^{n} P_{ij} \| x_i - x_j \|^2 = \langle P, C \rangle \) takes \( O(n d r) \) time.

3 Approximating \( W_2 \) in \( \tilde{O}(n) \) time

**Algorithm 1:** \( \tilde{O}(n) \) time algorithm for approximating 2-Wasserstein distance.

\[
\text{Input: } X := \{x_1, \ldots, x_n\} \subseteq \mathbb{R}^d, p, q \in \Delta_n, \varepsilon > 0
\]

\[
\text{Output: } \hat{P} \in M(p, q), \hat{W} \in \mathbb{R}
\]

1: \( \eta \leftarrow \frac{20 \log n}{\varepsilon}, M \leftarrow \frac{300 \log n}{\varepsilon} \)
2: \( V_M \leftarrow \text{TAYLORGKM}(x_1, \ldots, x_n; \frac{1}{\sqrt{2\eta}}, M) \) \quad \triangleright \text{Compute low-rank approximation}
3: \( (D_1, D_2) \leftarrow \text{SINKHORN}(V_M^\top V_M, p, q, \frac{\varepsilon}{10}) \) \quad \triangleright \text{Approximate Sinkhorn projection}
4: \( \hat{P} \leftarrow \text{ROUND}(D_1 V_M^\top D_2, p, q) \) \quad \triangleright \text{Round to feasible set}
5: \( \hat{W} \leftarrow \sum_{i,j=1}^{n} \hat{P}_{ij} \| x_i - x_j \|^2 \) \quad \triangleright \text{Compute objective value}
6: \text{return } \hat{P}, \hat{W}

Pseudocode for our proposed algorithm is given in Algorithm 1. It returns a feasible matrix \( \hat{P} \in M(p, q) \) as well as its objective value \( \hat{W} \). We emphasize that we never explicitly manipulate \( n \times n \) matrices in Algorithm 1 since even writing such a matrix would require \( \Omega(n^2) \)
time. Instead, the algorithm uses factored matrices (of rank at most $1 + \binom{M-1+d}{M-1}$) throughout, which allows lines 2-5 to be computed in $o(n^2)$ time. The coupling $\hat{P}$ is also returned in factored form, which may enable scalable implementation of algorithms that use $\hat{P}$ later in the computational pipeline. Moreover, since each step requires computing matrix-vector products, Algorithm 1 is easily parallelizable. Implementation details are deferred to Subsection 3.1.

The following theorem—the main result of the paper—shows that $\hat{W}$ is an additive $\varepsilon$ approximation of the true 2-Wasserstein distance between $p$ and $q$.

**Theorem 2.** For any $\{x_1, \ldots, x_n\} \subseteq B_d^2$, any $p, q \in \Delta_n$, and any $\varepsilon \in (0, 1)$, Algorithm 4 returns a feasible matrix $\hat{P} \in M(p, q)$ (in factored form) and scalar $\hat{W} = \sum_{i,j=1}^n \hat{P}_{ij} \|x_i - x_j\|^2$ such that $\hat{W} \leq W_2^2(p, q) + \varepsilon$ in time

$$O\left(n \frac{d \log n}{\varepsilon^2} \left( e + \frac{900 \log n}{\varepsilon d} \right)^{d+1}\right).$$

The proof of Theorem 2 requires a simple lemma showing that the low-rank approximation computed in line 2 is a sufficiently good approximation to the Gaussian kernel matrix. For the rest of this section, $x_1, \ldots, x_n \in B_d^2$ are fixed, $C \in \mathbb{R}^{n \times n}$ denotes the cost matrix with entries $C_{ij} := \|x_i - x_j\|^2$, and $K \in \mathbb{R}^{n \times n}$ denotes the kernel matrix $K_{ij} := \exp(-\eta C_{ij})$. We write $\tilde{K} := V_M^TV_M$ and define $\tilde{C}_{ij} := \eta^{-1} \log \tilde{K}_{ij}$.

**Lemma 4.** For all $i, j \in [n]$, the matrices $\tilde{K}$ and $\tilde{C}$ satisfy $\tilde{K}_{ij} \geq \frac{1}{2} e^{-\eta}$ and $|C_{ij} - \tilde{C}_{ij}| \leq \frac{\varepsilon}{10}$.

**Proof.** By Lemma 1, Stirling’s inequality, and our choice of $M = \frac{300 \log n}{\varepsilon} \geq 2e^2 \eta$, we have $\|K - \tilde{K}\|_{\infty} \leq \frac{(2n)^M}{M!} \leq \frac{1}{\sqrt{2\pi M}} \frac{2n^e}{M} \leq \frac{1}{2} e^{-2e^2 \eta} \leq \frac{1}{2} e^{-\eta}$. Since the smallest element of $K$ has size at least $e^{-\eta}$, we obtain $\tilde{K}_{ij} \geq \frac{1}{2} e^{-\eta}$, which implies in particular that $\tilde{K}$ is strictly positive and that $\tilde{C}$ is well defined.

Next, the bound $|\log K_{ij} - \log \tilde{K}_{ij}| \leq \frac{|K_{ij} - \tilde{K}_{ij}|}{\min(K_{ij}, \tilde{K}_{ij})} \leq \frac{e^{-\eta}}{\frac{1}{2} e^{-\eta}} = 1$ implies $|C_{ij} - \tilde{C}_{ij}| = \eta^{-1} |\log K_{ij} - \log \tilde{K}_{ij}| \leq \eta^{-1} \frac{\varepsilon}{20 \log n} \leq \frac{\varepsilon}{10}$. \qed

We will also use the following standard bound on the entropy of a discrete distribution.

**Fact 4.** [20, Theorem 2.6.4] Let $P \in \mathbb{R}^{n \times n}_{\geq 0}$ such that $\sum_{ij} P_{ij} = 1$. Then $H(P) \in [0, 2 \log n]$.

### 3.1 Proof of Theorem 2

**Approximation guarantee.** Let $P^* \in \arg\min_{P \in M(p, q)} \langle P, C \rangle$ be any optimal solution for the original problem, $\hat{P} := \arg\min_{P \in M(p, q)} \langle P, \hat{C} \rangle - \eta^{-1} H(P)$ be the (unique) optimal solution to the regularized problem with the cost matrix $\hat{C}$, and $P' := D_1\hat{K}D_2$ be the approximately scaled matrix obtained in line 3. We bound the suboptimality gap $\langle \hat{P}, C \rangle - \langle P^*, C \rangle$ by decomposing it as:

$$\langle \hat{P}, C \rangle - \langle P^*, C \rangle = \langle P' - \hat{P}, \hat{C} \rangle + \langle \hat{P} - P', \hat{C} \rangle + \langle \hat{P}, C - \hat{C} \rangle + \langle \hat{P}, C - \hat{C} \rangle$$

We now bound each of these terms individually so that their sum is bounded above by $\varepsilon$. 

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(i) By definition of \( \bar{P} \), \( \langle \bar{P}, \bar{C} \rangle - \eta^{-1}H(\bar{P}) \leq \langle P^*, \bar{C} \rangle - \eta^{-1}H(P^*) \). Thus \( \langle \bar{P}, \bar{C} \rangle - \langle P^*, C \rangle \leq \eta^{-1}(H(\bar{P}) - H(P^*)) + \langle P^*, C - \bar{C} \rangle \leq 2\eta^{-1}\log n + \| \bar{C} - C \|_{\infty} \leq \frac{\epsilon}{\delta} \) where we have used Fact 1, Hölder’s inequality, and Lemma 3.

(ii) Let \( p' := P'1 \) and let \( q' := (P')^\top 1 \). By Lemma 2 there exists a matrix \( G \in \mathcal{M}(p', q') \) such that \( \| G - \bar{P} \|_1 \leq \| p - p' \|_1 + \| q - q' \|_1 \). Now by Fact 1, \( P' = \arg\min_{P \in \mathcal{M}(p', q')} \langle P, \bar{C} \rangle - \eta^{-1}H(P) \), thus \( \langle P', \bar{C} \rangle - \eta^{-1}H(P') \leq \langle G, \bar{C} \rangle - \eta^{-1}H(G) \). Rearranging yields \( \langle P' - \bar{P}, \bar{C} \rangle \leq \eta^{-1}(H(P') - H(G)) + \langle G - \bar{P}, \bar{C} \rangle \). The first term is bounded above by \( \frac{\epsilon}{\delta} \) by Fact 1 and the second is bounded above by

\[
\| \bar{C} \|_{\infty}(\| p - p' \|_1 + \| q - q' \|_1) \leq \frac{\epsilon}{\delta}, \tag{3}
\]

since \( \| p - p' \|_1 + \| q - q' \|_1 \leq \frac{\epsilon}{\delta} \) by line 3 and since \( \| \bar{C} \|_{\infty} \leq \| C \|_{\infty} + \| C - \bar{C} \|_{\infty} \leq 2 \) by Lemma 3. We conclude that term (ii) is bounded above by \( \frac{9\delta}{\epsilon} \).

(iii) By Hölder’s inequality and then Lemma 2, \( \langle \bar{P} - D_1 \tilde{K}D_2, \bar{C} \rangle \leq \| \bar{C} \|_{\infty}\| \bar{P} - D_1 \tilde{K}D_2 \|_1 \leq \| \bar{C} \|_{\infty}(\| p - p' \|_1 + \| q - q' \|_1) \). This is bounded above by \( \frac{\epsilon}{\delta} \) by (3).

(iv) By Hölder’s inequality and Lemma 4, \( \langle \bar{P}, C - \bar{C} \rangle \leq \| \bar{P} \|_1\| C - \bar{C} \|_{\infty} \leq \frac{\epsilon}{\delta} \).

**Runtime guarantee.** All computations in Algorithm 1 are done implicitly by only maintaining the matrices \( D_1 V_M^T V_M D_2 \) and \( \bar{P} \) in factored form. Let \( r := (M^{-1+d}) \leq \frac{(M+d)^{\delta}}{d} \leq (e + \frac{900\log n}{\epsilon \delta})^d \). Line 2 takes \( O(nr) \) time by Lemma 1. Now since \( V_M^T V_M \) is in rank-\( r \) factored form, multiplying it by a vector takes \( O(nr) \) operations, and by Fact 2 the algorithm manipulates numbers with at most \( O(\log \frac{1}{\delta} + \eta + \log n) = O(\frac{\log n}{\delta}) \) bits. Line 3 therefore takes \( O(nr \log^2 n) \) time by Fact 2 and Lemma 4. Line 4 takes \( O(nr) \) time by Lemma 2 and line 5 takes \( O(nrd) \) time by Lemma 3. The entire algorithm therefore takes \( O(nrd + \frac{nr \log n}{\delta^2}) \) time.

\[\Box\]

4 Conclusion

In this paper, we have given a simple algorithm based on entropic regularization that approximates the quadratic transport metric in near-linear time.

One interesting direction for future work is whether this result can be leveraged to obtain \( 1 + \epsilon \) multiplicative approximations to \( W_2 \) in near-linear time. We compute in this work a coupling with low-rank structure, and this approach naturally lends itself to additive guarantees. For instance, if \( p = q \), then the unique optimal coupling has cost 0, whereas any low-rank coupling is bound to incur nonzero cost. Obtaining a multiplicative guarantee may therefore require additional techniques.

Another interesting question is whether our techniques extend to other metrics. More generally, exploring the connection between low-rank approximation and geometric algorithms seems a promising direction for future research.
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A Deferred details about subroutines

A.1 Explicit low-rank approximation of Gaussian kernel matrices

Here, we briefly recall an explicit low-rank approximation of Gaussian kernel matrices obtained by truncating the Taylor series of the Gaussian kernel. For details, see [18].

First consider two vectors \( x, y \in \mathbb{R}^d \). Take a truncation of the Taylor expansion

\[
\exp\left(\frac{\langle x, y \rangle}{\sigma^2}\right) = \sum_{m=0}^{\infty} \frac{1}{m!} \left(\frac{\langle x, y \rangle}{\sigma^2}\right)^m,
\]

expand \( \langle x, y \rangle^m \) into monomials, group like-terms, and then multiply both sides by \( \exp\left(-\|x\|^2/2\sigma^2 + \|y\|^2/2\sigma^2\right) \) to obtain the approximation

\[
\exp\left(\frac{-\|x - y\|^2/2}{2\sigma^2}\right) \approx \sum_{\vec{v} \in \mathbb{N}^d, \sum_{i=1}^d v_i \leq M} \psi_{\vec{v}}(x; \sigma) \psi_{\vec{v}}(y; \sigma),
\]

where \( \psi_{\vec{v}}(x; \sigma) \propto \exp\left(-\|x\|^2/2\sigma^2\right) \prod_{j=1}^d x_j^{v_j} \). Concatenating these features \( \{\psi_{\vec{v}}(x; \sigma) : \vec{v} \in \mathbb{N}^d, \sum_{i=1}^d v_i < M\} \) into a so-called “feature vector” \( \Phi_M(x; \sigma) \), the right hand side of (4) can be re-written simply as \( \Phi_M(x; \sigma)^T \Phi_M(y; \sigma) \). Extending to Gaussian kernel matrices is now simple: approximate \( K(x_1, \ldots, x_n; \sigma) \) by the Gram matrix \( V_M^T V_M \) where \( V_M := [\Phi_M(x_1; \sigma), \ldots, \Phi_M(x_n; \sigma)] \). This subroutine for forming \( V_M \) will be denoted in the paper by \( \text{TAYLORGKM}(x_1, \ldots, x_n; \sigma, M) \).

The approximation error in (4) is controlled by Taylor’s Theorem. This immediately yields an infinity-norm guarantee on the approximation error \( K \approx V_M^T V_M \). These guarantees are recorded in Lemma 1; proofs can be found in [18].
A.2 Pseudocode for Sinkhorn algorithm

Input: $\tilde{K}$ (in factored form $V^TV$), $p, q \in \Delta_n$, $\delta > 0$  
Output: Positive diagonal matrices $D_1, D_2 \in \mathbb{R}^{n \times n}$

1: $\tau \leftarrow \frac{\delta}{8}$, $D_1, D_2 \leftarrow I_{n \times n}$, $k \leftarrow 0$
2: $p' \leftarrow (1 - \tau)p + \frac{\tau}{n}1$, $q' \leftarrow (1 - \tau)q + \frac{\tau}{n}1$  \text{\hspace{1cm}} \triangleright Round $p$ and $q$
3: while $\|D_1 \tilde{K} D_2 1 - p'\|_1 + \|(D_1 \tilde{K} D_2)^\top 1 - q'\|_1 \leq \frac{\delta}{2}$ do
4: \hspace{0.5cm} $k \leftarrow k + 1$
5: \hspace{0.5cm} if $k$ odd then
6: \hspace{1cm} $(D_1)_{ii} \leftarrow p'_i/(D_1 \tilde{K} D_2 1)_i$ for $i = 1, \ldots, n$. \hspace{1cm} \triangleright Renormalize rows
7: \hspace{1cm} else
8: \hspace{1.5cm} $(D_2)_{jj} \leftarrow q'_j/((D_1 \tilde{K} D_2)^\top 1)_j$ for $j = 1, \ldots, n$. \hspace{1cm} \triangleright Renormalize columns
9: \hspace{0.5cm} end if
10: end while
11: return $D_1, D_2$

Algorithm 2: SINKHORN

A.3 Pseudocode for rounding algorithm

For completeness, here we briefly recall the rounding algorithm ROUND from [4] and give a short proof of Lemma [2] by adapting slightly their proof of Lemma 7.

It will be convenient to develop a little notation. For a vector $x \in \mathbb{R}^n$, $\mathbb{D}(x)$ denotes the $n \times n$ diagonal matrix with diagonal entries $[\mathbb{D}(x)]_{ii} = x_i$. For a matrix $A$, $r(A) := A1$ and $c(A) := A^T 1$ denote the row and column marginals of $A$, respectively. We further denote $r_i(A) = [r(A)]_i$ and similarly $c_j(A) = [c(A)]_j$.

Input: $F \in \mathbb{R}^{n \times n}$ and $p, q \in \Delta_n$  
Output: $G \in \mathcal{M}(p, q)$
1: $X \leftarrow \mathbb{D}(x)$, where $x_i := \frac{p_i}{r_i(F)} \wedge 1$
2: $F' \leftarrow XF$
3: $Y \leftarrow \mathbb{D}(y)$, where $y_j := \frac{q_j}{c_j(F)} \wedge 1$
4: $F'' \leftarrow F'Y$
5: $\text{err}_r \leftarrow p - r(F'')$, $\text{err}_c \leftarrow q - c(F'')$
6: Output $G \leftarrow F'' + \text{err}_r e^T / \|	ext{err}_r\|_1$

Algorithm 3: ROUND (from Algorithm 2 in [4])

Proof of Lemma [2] The runtime claim is clear. Next, let $\Delta := \|F\|_1 - \|F''\|_1 = \sum_{i=1}^n (r_i(F) - p_i) + \sum_{j=1}^n (c_j(F') - q_j) +$ denote the amount of mass removed from $F$ to create $F''$. Observe that $\sum_{i=1}^n (r_i(F) - p_i) = \frac{1}{2} \|r(F) - p\|_1$. Since $F' \leq F$ entrywise, we also have $\sum_{j=1}^n (c_j(F') - q_j) \leq \sum_{j=1}^n (c_j(F) - q_j) = \frac{1}{2} \|c(F) - q\|_1$. Thus $\Delta \leq \frac{1}{2}(\|r(F) - p\|_1 + \|c(F) - q\|_1)$. The proof is complete since $\|F - G\|_1 \leq \|F - F''\|_1 + \|F'' - G\|_1 = 2\Delta$.

\[ \square \]