Hardness results for Multimarginal Optimal Transport problems

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Abstract

Multimarginal Optimal Transport (MOT) is the problem of linear programming over joint probability distributions with fixed marginals. A key issue in many applications is the complexity of solving MOT: the linear program has exponential size in the number of marginals $k$ and their support sizes $n$. A recent line of work has shown that MOT is poly$(n, k)$-time solvable for certain families of costs that have poly$(n, k)$-size implicit representations. However, it is unclear what further families of costs this line of algorithmic research can encompass. In order to understand these fundamental limitations, this paper initiates the study of intractability results for MOT.

Our main technical contribution is developing a toolkit for proving \textsc{NP}-hardness and inapproximability results for MOT problems. We demonstrate this toolkit by using it to establish the intractability of a number of MOT problems studied in the literature that have resisted previous algorithmic efforts. For instance, we provide evidence that repulsive costs make MOT intractable by showing that several such problems of interest are \textsc{NP}-hard to solve—even approximately.

1 Introduction

Multimarginal Optimal Transport (MOT) is the problem of linear programming over joint probability distributions with fixed marginal distributions. That is, given $k$ marginal distributions $\mu_1, \ldots, \mu_k$ in the simplex $\Delta_n = \{ u \in \mathbb{R}^n : \sum_{i=1}^n u_i = 1 \}$ and a cost tensor $C$ in the $k$-fold tensor product space $(\mathbb{R}^n)^\otimes k = \mathbb{R}^n \otimes \cdots \otimes \mathbb{R}^n$, compute

$$\min_{P \in \mathcal{M}(\mu_1, \ldots, \mu_k)} \langle P, C \rangle$$

(MOT)

where $\mathcal{M}(\mu_1, \ldots, \mu_k)$ is the “transportation polytope” containing entrywise non-negative tensors $P \in (\mathbb{R}^n)^\otimes k$ satisfying the marginal constraints $\sum_{j_{i+1}, \ldots, j_k} p_{j_1, \ldots, j_{i-1}, j_{i+1}, \ldots, j_k} = [\mu_i]_j$ for all $i \in \{1, \ldots, k\}$ and $j \in \{1, \ldots, n\}$.

This MOT problem has recently attracted significant interest due to its many applications in data science, applied mathematics, and the natural sciences; see for instance [2, 6, 31, 32] and the many references within. However, a key issue that dictates the usefulness of MOT in applications is its complexity. Indeed, while MOT can be easily solved in $n^{\Theta(k)}$ time since it is a linear program in $n^k$ variables and $n^k + nk$ constraints, this is far from scalable.

In this paper and the literature, we are interested in “polynomial time” algorithms, where polynomial means in the number of marginals $k$ and their support sizes $n$ (as well as the scale-invariant quantity $\|C\|_{\max}/\varepsilon$ if we are considering $\varepsilon$ additive approximations). An obvious obstacle
is that in general, one cannot even read the input to \textit{MOT}—let alone solve \textit{MOT}—in \text{poly}(n, k) time since the cost tensor \(C\) has \(n^k\) entries.

Nevertheless, in nearly all applications of practical interest, the cost tensor \(C\) has a simple structure that enables it to be input implicitly via a \text{poly}(n, k)-sized representation. Moreover, a recent line of work has shown that in many applications where \(C\) has such a polynomial-size implicit representation, the \textit{MOT} problem can also be solved in polynomial time. A simple-to-describe illustrative example is cost tensors \(C\) which have constant rank and are given as input in factored form [2]. Other examples include computing generalized Euler flows [2, 6], computing low-dimensional Wasserstein barycenters [3, 14], solving MOT problems with tree-structured costs [25], and solving MOT problems with decomposable costs [2].

A fundamental question is: What further families of succinctly representable costs lead to tractable \textit{MOT} problems? As an illustrative example, can \textit{MOT} still be solved in \text{poly}(n, k) time if the cost \(C\) has rank that is low but not constant, say of size \text{poly}(n, k)? There are a number of MOT problems studied in the literature for which \(C\) has a \text{poly}(n, k)-sized representation but developing \text{poly}(n, k)-time algorithms has resisted previous efforts. The purpose of this paper is to understand the fundamental limitations of this line of algorithmic research.

1.1 Contributions

This paper initiates the study of intractability results for \textit{MOT}. Our main contributions are:

1. In §3, we develop a toolkit for proving \text{NP}-hardness and inapproximability results for \textit{MOT} problems on costs \(C\) that have \text{poly}(n, k)-size implicit representations. This is the main technical contribution of the paper.

2. In §4, §5, and §6, we demonstrate this toolkit by using it to establish the intractability of a number of \textit{MOT} problems studied in the literature that have resisted previous algorithmic efforts.

We elaborate on each point below.

1.1.1 Reduction toolkit

Let \(\text{MOT}_C(\mu)\) denote the problem of computing the optimal value of \textit{MOT} for a cost tensor \(C \in (\mathbb{R}^n)^{\otimes k}\) and marginals \(\mu = (\mu_1, \ldots, \mu_k) \in (\Delta_n)^k\). Informally, our main result establishes that for any fixed cost \(C\), the following discrete optimization problem \(\text{MIN}_C\) can be (approximately) solved in polynomial time if \(\text{MOT}_C\) can be (approximately) solved in polynomial time.

\[\text{MIN}_C\]

For \(C \in (\mathbb{R}^n)^{\otimes k}\) and \(p = (p_1, \ldots, p_k) \in \mathbb{R}^{n \times k}\), the problem \(\text{MIN}_C(p)\) is to compute

\[\min_{(j_1, \ldots, j_k) \in \{1, \ldots, n\}^k} C_{j_1, \ldots, j_k} - \sum_{i=1}^k [p_i]_{j_i}.\]  

(1.1)

The upshot of our result is that it enables us to prove intractability results for \(\text{MOT}_C\) by instead proving intractability results for \(\text{MIN}_C\). This is helpful since \(\text{MIN}_C\) is more directly amenable to \text{NP}-hardness and inapproximability reductions because it is phrased as a more conventional combinatorial optimization problem; examples can be found in §4, §5, and §6.

We briefly highlight the primary insight behind the proof: The convex relaxation of \(\text{MIN}_C\) is exact and is a convex optimization problem whose objective can be evaluated by solving an auxiliary \(\text{MOT}_C\) problem. This means that if one can (approximately) solve \(\text{MOT}_C\), then one can use this in
a black-box manner to (approximately) solve $\text{MIN}_C$ via zero-th order optimization. In §3, we show how to perform this zero-th order optimization efficiently using the Ellipsoid algorithm if $\text{MOT}_C$ can be computed exactly, and otherwise using recent developments on zero-th order optimization of approximately convex functions [5, 34] if $\text{MOT}_C$ can be computed approximately.

We conclude this discussion with several remarks.

**Remark 1.2** (Converse). There is no loss of generality when using our results to reduce proving the intractability of $\text{MOT}_C$ to proving the intractability of $\text{MIN}_C$. This is because the $\text{MOT}_C$ and $\text{MIN}_C$ problems are polynomial-time equivalent—for any cost $C$, and for both exact and approximate solving—because the converse of this reduction also holds [2, §3].

**Remark 1.3** (Value vs solution for MOT). A desirable feature of our hardness results is that they apply regardless of how an MOT solution is computed and (compactly) represented. This is because we show hardness for (approximately) computing the optimal value of $\text{MOT}$.

**Remark 1.4** (Differences from classical LP theory). The intuition behind the MIN problem is that it is the feasibility problem for the dual LP to MOT; see the preliminaries section. However, it should be emphasized that our reductions rely on the particular structure of the LP defining MOT, and do not hold for a general LP and its dual feasibility oracle [23]. Moreover, our approximate reduction is even further from the purview of classical LP theory since it can be used to prove hardness of approximating to polynomially small error rather than exponentially small error.

**Remark 1.5** ($p = 0$). The $\text{MIN}_C(0)$ problem is to compute the minimum entry of the tensor $C$. Thus, as a special case of our reductions, it follows that if (approximately) computing the minimum entry of $C$ is $\text{NP}$-hard, then so is (approximately) computing $\text{MOT}_C$. In fact, in our applications in §§4, §5, and §6, we prove intractability of $\text{MIN}_C$—and thus of $\text{MOT}_C$—by showing intractability for this “simple” case $p = 0$. However, we mention that in general one cannot restrict only to the case $p = 0$: In §7, we give a concrete example where $\text{MIN}_C$ is tractable for $p = 0$ but not general $p$.

1.1.2 Applications

**Low-rank costs.** In §4, we demonstrate this toolbox on MOT problems with low-rank cost tensors given in factored form. Recent algorithmic work has shown that such MOT problems can be solved to arbitrary precision $\varepsilon > 0$ in $\text{poly}(n, k, C_{\text{max}}/\varepsilon)$ time for any fixed rank $r$ [2]. However, this algorithm’s dependence on $r$ is exponential, and it is a natural question whether such MOT problems can be solved in time that is also polynomial in $r$. We show that unless $P = \text{NP}$, the answer is no. Moreover, our hardness result extends even to approximate computation. This provides a converse to the aforementioned algorithmic result.

**Pairwise-interaction costs.** In §5, we consider MOT problems with costs $C$ that decompose into sums of pairwise interactions

$$C_{j_1, \ldots, j_k} = \sum_{1 \leq i < i' \leq k} g_{i, i'}(j_i, j_{i'}) \quad (1.2)$$

for some functions $g_{i, i'} : [n] \times [n] \to \mathbb{R}$. This cost structure appears in many applications; for instance in Wasserstein barycenters [4] and the MOT relaxation of Density Functional Theory [12, 15].

\[\text{Indeed, the representations produced by MOT algorithms often vary: e.g., the solution is polynomially-sparse for the Ellipsoid and Multiplicative Weights algorithms; and is fully dense but has a polynomial-size representation which supports certain efficient operations for the Sinkhorn algorithm. See [2] for details.}\]
Although these costs have poly\((n, k)\)-size implicit representations, we show that this cost structure alone is not sufficient for solving MOT in polynomial time.

One implication of this NP-hardness result is a converse to the algorithmic result of [2] which shows that MOT problems can be solved in poly\((n, k)\) time for costs \(C\) which are decomposable into local interactions of low treewidth. This is a converse because the pairwise-interactions structure (1.2) also falls under the framework of MOT costs that decompose into local interactions, but has high treewidth.

**Repulsive costs.** In §6, we consider MOT problems with “repulsive costs”. Informally, these are costs \(C_{j_1, \ldots, j_k}\) which encourage diversity between the indices \(j_1, \ldots, j_k\); we refer the reader to the nice survey [17] for a detailed discussion of such MOT problems and their many applications. We provide evidence that repulsive costs lead to intractable MOT problems by proving that several such MOT problems of interest are NP-hard to solve. Again, our hardness results extend even to approximate computation.

Specifically, in §6.1 we show this for MOT problems with the determinantal cost studied in [13, 17], and in §6.3 we show this for the popular MOT formulation of Density Functional Theory [8, 12, 15] with the Coulomb-Buckingham potential. Additionally, in §6.2, we observe that the classical problem of evaluating the convex envelope of a discrete function is an instance of MOT, and we leverage this connection to point out that MOT is NP-hard to approximate with supermodular costs, yet tractable with submodular costs. This dichotomy provides further evidence for the intractability of repulsive costs, since the intractable former problem has a “repulsive” cost, whereas the tractable latter problem has an “attractive” cost.

To our knowledge, these are the first results that rigorously demonstrate intractability of MOT problems with repulsive costs. This provides the first step towards explaining why—despite a rapidly growing literature—there has been a lack of progress in developing polynomial-time algorithms with provable guarantees for many MOT problems with repulsive costs.

1.2 Related work

**Algorithms for MOT.** The many applications of MOT throughout data science, mathematics, and the sciences at large have motivated a rapidly growing literature around developing efficient algorithms for MOT. The algorithms in this literature can be roughly divided into two categories.

The first category consists of MOT algorithms which work for generic “unstructured” costs. While these algorithms work for any MOT problem, they inevitably cannot have polynomial runtime in \(n\) and \(k\) since they read all \(n^k\) entries of the cost tensor. A simple such algorithm is to solve MOT using an out-of-the-box LP solver; this has \(n^{\Theta(k)}\) runtime. An alternative popular algorithm is the natural multimarginal generalization of the Sinkhorn scaling algorithm, which similarly has \(n^{\Theta(k)}\) runtime but can be faster than out-of-the-box LP solvers in practice, see e.g., [6, 7, 8, 9, 19, 27, 28, 37] among many others. The exponential runtime dependence on \(n\) and \(k\) prohibits these algorithms from being usable beyond very small values of \(n\) and \(k\). For instance even \(n = k = 10\), say, is at the scalability limits of these algorithms.

The second category consists of MOT algorithms that can run in poly\((n, k)\) time\(^3\) for MOT problems with certain “structured” costs that have poly\((n, k)\)-sized implicit representations. This line of work includes for instance the algorithms mentioned earlier in the introduction, namely computing generalized Euler flows [2, 6], computing low-dimensional Wasserstein barycenters [3, 14],

\(^3\)Or poly\((n, k, C_{\text{max}}/\varepsilon)\) time for \(\varepsilon\)-approximate solutions.
solving MOT problems with tree-structured costs [25], and solving MOT problems with decomposable costs [2]. The purpose of this paper is to understand the fundamental limitations of this line of work.

Connection to fractional hypergraph matching and complexity of sparse solutions. Deciding whether MOT has a solution of sparsity exactly \( n \) is well-known to be \( \text{NP} \)-hard. This \( \text{NP} \)-hardness holds even in the special case where the number of marginals \( k = 3 \), the cost tensor \( C \) has all \( \{0, 1\} \) entries, and the marginals are uniform \( \mu_i = 1/n \). This is because in this special case, MOT is the natural convex relaxation of the \( \text{NP} \)-hard \( k \)-partite matching problem [21, 26], and in particular \( n \)-sparse solutions to this MOT problem are in correspondence with optimal solutions to this \( \text{NP} \)-hard problem. The \( \text{NP} \)-hardness of finding the sparsest MOT solution further extends to “structured” MOT problems whose costs have poly\((n, k)\)-size implicit representations, e.g., the Wasserstein barycenter problem [10].

However, it is important to clarify that finding an MOT solution which is polynomially sparse (albeit perhaps not the sparsest) is not necessarily \( \text{NP} \)-hard. Indeed, sparse such solutions can be computed in polynomial-time for e.g., low-dimensional Wasserstein barycenters [3] and MOT problems with decomposable costs [2].

We emphasize that a desirable property of our hardness results is that they entirely bypass this discussion about whether computing sparse solutions is tractable. This is because our results show that it is \( \text{NP} \)-hard to even compute the value of certain structured MOT problems (see Remark 1.3), which is clearly a stronger statement than \( \text{NP} \)-hardness of computing a sparse solution.

Other related work. We mention two tangentially related bodies of work in passing. First, the transportation polytope (a.k.a., the constraint set in the MOT problem) is an object of significant interest in discrete geometry and combinatorics, see e.g., [16, 39] and the references within. Second, linear programming problems over exponentially-sized joint probability distributions appear in various fields such as game theory [30] and variational inference [38]. However, it is important to note that the complexity of these linear programming problems is heavily affected by the specific linear constraints, which often differ between problems in different fields.

2 Preliminaries

Notation. The \( k \)-fold tensor product space \( \mathbb{R}^n \otimes \cdots \otimes \mathbb{R}^n \) is denoted by \( (\mathbb{R}^n)^\otimes k \), and similarly for \( (\mathbb{R}^n_{\geq 0})^\otimes k \). The set \( \{1, \ldots, n\} \) is denoted by \([n]\). The \( i \)-th marginal of a tensor \( P \in (\mathbb{R}^n)^\otimes k \) is the vector \( m_i(P) \in \mathbb{R}^n \) with \( j \)-th entry \( \sum_{j_1, \ldots, j_{i-1}, j_{i+1}, \ldots, j_k} P_{j_1, \ldots, j_{i-1}, j_{i+1}, \ldots, j_k} \), for \( i \in [k] \) and \( j \in [n] \). In this notation, the transportation polytope in (MOT) is \( \mathcal{M}(\mu_1, \ldots, \mu_k) = \{ P \in (\mathbb{R}^n_{\geq 0})^\otimes k : m_i(P) = \mu_i, \forall i \in [k] \} \). For shorthand, we often denote an index \( (j_1, \ldots, j_k) \) by \( \bar{j} \). For a tensor \( C \in (\mathbb{R}^n)^\otimes k \), we denote the maximum absolute value of its entries by \( C_{\text{max}} = \max_{\bar{j}} |C_{\bar{j}}| \). For shorthand, we write \( \text{poly}(t_1, \ldots, t_m) \) to denote a function that grows at most polynomially fast in those parameters.

MOT dual. The dual LP to (MOT-D) is

\[
\max_{p_1, \ldots, p_k \in \mathbb{R}^n} \sum_{i=1}^k (p_i, \mu_i) \quad \text{subject to} \quad \sum_{i=1}^k [p_i]_{j_i} \geq 0, \forall \bar{j} \in [n]^k. \tag{MOT-D}
\]

Observe that \( p = (p_1, \ldots, p_k) \in \mathbb{R}^{n\times k} \) is feasible for (MOT-D) if and only if the problem \( \text{MIN}_C(p) \) has non-negative value. This is the connection between the problem \( \text{MIN}_C \) and the feasibility oracle for (MOT-D) alluded to in Remark 1.4.
Bit complexity. Throughout, we assume for simplicity of exposition that all entries of the cost \( C \) and the weights \( p \in \mathbb{R}^{nk} \) inputted in the \( \text{MIN}_C \) problem have bit complexity at most \( \text{poly}(n,k) \). This implies that the distributions \( \mu \) on which the \( \text{MOT}_C \) oracle is queried in Theorems 3.1 and 3.2 also have polynomial bit complexity. The general case is a straightforward extension.

Computational complexity. BPP is the class of problems solvable by polynomial-time randomized algorithms with error probability that is \(< 1/3\) (or equivalently, any constant less than 1/2). The statement “\( \text{NP} \not\subseteq \text{BPP} \)” is a standard assumption in computational complexity and is the randomized version of \( \text{P} \not= \text{NP} \), i.e., that \( \text{NP} \)-hard problems do not have polynomial-time randomized algorithms.

3 Reducing \( \text{MIN} \) to \( \text{MOT} \)

Here we present the reduction toolkit overviewed in §1.1. Specifically, we show the following two reductions from \( \text{MIN}_C \) to \( \text{MOT}_C \). The first reduction is used for proving \( \text{NP} \)-hardness of exactly solving \( \text{MOT}_C \), and the second reduction is used for proving inapproximability. These two reductions are incomparable.

**Theorem 3.1** (Exact reduction). There is a deterministic algorithm that, given access to an oracle solving \( \text{MOT}_C \) and weights \( p \in \mathbb{R}^{n \times k} \), solves \( \text{MIN}_C(p) \) in \( \text{poly}(n,k) \) time and oracle queries.

**Theorem 3.2** (Approximate reduction). There is a randomized algorithm that, given \( \varepsilon > 0 \), access to an oracle solving \( \text{MOT}_C \) to additive accuracy \( \varepsilon \), and weights \( p \in \mathbb{R}^{n \times k} \), solves \( \text{MIN}_C(p) \) up to \( \varepsilon \cdot \text{poly}(n,k) \) additive accuracy with probability \( 2/3 \) in \( \text{poly}(n,k,\frac{\text{min}}{\varepsilon}) \) time and oracle queries.

We make two remarks in passing about these theorems. First, they hold unchanged if the \( \text{MIN}_C \) problem is modified to require computing the minimizing tuple rather than the minimum value in (1.1). This is because these two problems are polynomial-time equivalent [2, Appendix A.1]. Second, the inapproximability reduction is probabilistic\(^4\), and thus shows inapproximability under the standard complexity assumption \( \text{NP} \not\subseteq \text{BPP} \), which is informally the stronger “randomized version” of \( \text{P} \not= \text{NP} \).

3.1 Proof overview

As described briefly in §1.1, the main idea is to reduce \( \text{MIN}_C \) to a convex optimization problem for which the objective function can be evaluated by solving an auxiliary \( \text{MOT}_C \) problem. Formally, embed \( [n]^k \) into \( \mathbb{R}^{nk} \) via

\[
\phi((j_1, \ldots, j_k)) := (e_{j_1}, \ldots, e_{j_k})^T,
\]

where \( e_j \) denotes the vector in \( \mathbb{R}^n \) with a 1 on entry \( j \), and 0’s on all other entries. Then \( \text{MIN}_C \) is equivalent to minimizing \( f(x) := C_{\phi^{-1}(x)} - \langle p, x \rangle \) over the discrete set

\[
S := \phi([n]^k) = \{ x = (x_1, \ldots, x_k)^T \in \{0,1\}^{nk} : \lVert x_1 \rVert_1 = \cdots = \lVert x_k \rVert_1 = 1 \},
\]

where here we abuse notation slightly by viewing \( p = (p_1, \ldots, p_k) \in \mathbb{R}^{n \times k} \) as the vector in \( \mathbb{R}^{nk} \) formed by concatenating its columns \( p_1, \ldots, p_k \). Let \( F : \mathbb{R}^{nk} \rightarrow \mathbb{R} \) denote the convex envelope of \( f \), i.e., the pointwise largest convex function over \( \mathbb{R}^{nk} \) that is pointwise below \( f \) on the domain \( S \) of \( f \).

\(^4\)It is an interesting question whether the approximate reduction in Theorem 3.2 can be de-randomized. This would enable showing our inapproximability results under the assumption \( \text{P} \not= \text{NP} \) rather than \( \text{NP} \not\subseteq \text{BPP} \).
By explicitly computing $F$ as the Fenchel bi-conjugate of $f$, we obtain the following two useful characterizations of $F$ (proved in §3.2). Below, let $\Delta_S$ denote the set of probability distributions over $S$.

**Lemma 3.3** (MOT$_C$ is convex envelope of MIN$_C$). For all $\mu = (\mu_1, \ldots, \mu_k) \in (\Delta_n)^k$,

$$F(\mu) = \min_{D \in \Delta_S \text{ s.t. } \mathbb{E}_{x \sim D} x = \mu} \mathbb{E}_{x \sim D} f(x)$$  

(3.1)

$$= -\langle \mu, p \rangle + \text{MOT}_C(\mu).$$  

(3.2)

The first representation (3.1) of $F$ gives a Choquet integral representation of $F$ in terms of $f$. Importantly, it implies that in order to (approximately) minimize $f$ over its discrete domain $S$—i.e., solve the (approximate) MIN$_C$ oracle—it suffices to (approximately) minimize $F$ over its continuous domain, namely the convex hull $\text{conv}(S) = (\Delta_n)^k$. See Corollary 3.5.

Now to (approximately) minimize $F$, we appeal to algorithmic results from zero-th order convex optimization since the second representation (3.2) of $F$ shows that (approximately) evaluating $F$ amounts to (approximately) solving an auxiliary MOT$_C$ problem. Specifically, we show how to implement the zero-th order optimization using the Ellipsoid algorithm in the case of exact oracle evaluations, and otherwise using the recent results [5, 34] on zero-th order optimization of approximately convex functions in the case of approximate oracle evaluations.

**Remark 3.4** (Connection to submodular optimization). *This proof is inspired by the classical idea of minimizing a submodular function by minimizing its Lovász extension [22], which is a special case of Theorem 3.1 for $n=2$ and submodular costs $C$. In fact, in light of the equivalence between MOT$_C$ and the Lovász extension in that special case (described in §6.2), this is arguably the appropriate generalization thereof to optimizing general discrete functions over general ground sets of size $n \geq 2$.*

### 3.2 Proofs

**Proof of Lemma 3.3.** The convex envelope $F$ of $f$ is equal to the Fenchel bi-conjugate $f^{**}$ of $f$ [35]. The Fenchel conjugate of $f$ is $f^* : \mathbb{R}^{nk} \to \mathbb{R}$ where $f^*(y) = \max_{x \in S} \langle x, y \rangle - f(x) = \max_{x \in S} \langle x, y + p \rangle - C_{\phi^{-1}}(x)$. Thus the Fenchel bi-conjugate $f^{**}$ is

$$F(\mu) = f^{**}(\mu) = \max_{y \in \mathbb{R}^{nk}} \langle y, \mu \rangle - f^*(y) = \max_{y \in \mathbb{R}^{nk}} \min_{x \in S} \langle y, \mu - x \rangle - \langle x, p \rangle + C_{\phi^{-1}}(x).$$

By performing a convex relaxation over the inner minimization (to distributions $D$ over the set $S$) and then invoking LP strong duality, we obtain

$$F(\mu) = \min_{D \in \Delta_S} \max_{y \in \mathbb{R}^{nk}} \langle y, \mu - \mathbb{E}_{x \sim D} x \rangle - \langle \mathbb{E}_{x \sim D} x, p \rangle + \mathbb{E}_{x \sim D} C_{\phi^{-1}}(x)$$

Note that the inner maximization over $y$ has unbounded cost $+\infty$ unless $\mathbb{E}_{x \sim D} x = \mu$. Thus

$$F(\mu) = -\langle \mu, p \rangle + \min_{D \in \Delta_S \text{ s.t. } \mathbb{E}_{x \sim D} x = \mu} \mathbb{E}_{x \sim D} C_{\phi^{-1}}(x).$$

This proves (3.1) by definition of $f$. Now (3.2) follows since distributions $D$ over $S$ with expectation $\mu$ are in correspondence with joint distributions $P \in \mathcal{M}(\mu_1, \ldots, \mu_k)$, and under this correspondence $\mathbb{E}_{x \sim D} C_{\phi^{-1}}(x)$ simply amounts to $(P, C)$. 

**Corollary 3.5** (Minimizing $F$ suffices for minimizing $f$). *The minimum value of $F$ over $(\Delta_n)^k$ is equal to the minimum value of $f$ over $S$.*

**Proof.** By the Choquet representation (3.1) of $F$ in Lemma 3.3, the set of minimizers of $F$ over $(\Delta_n)^k$ is equal to the convex hull of the minimizers of $f$ over $S$. 


3.2.1 Hardness of computation

Proof of Theorem 3.1. By Corollary 3.5, it suffices to minimize \( F \) over \((\Delta_n)^k\) in the desired runtime.

To this end, we claim that \( F \) is the maximum of a finite number of linear functions, each of which has polynomial encoding length in the sense of [23, §6.5]. To show this statement, it suffices to show the same statement for the function \( \mu \mapsto \text{MOT}_C(\mu) \) by the representation (3.2) of \( F \) in Lemma 3.3 that equates \( F \) to a linear function plus \( \text{MOT}_C \). This latter statement follows by the dual MOT formulation (MOT-D) and a standard LP argument. Specifically, the function \( \mu \mapsto \text{MOT}_C(\mu) \) is a linear function in \( \mu \) with finitely many pieces, one for each vertex of the polyhedral feasible set defining (MOT-D) by the Minkowski-Weyl Theorem; and furthermore, the vertices are solutions to linear systems in the constraints, and thus have polynomial bit complexity by Cramer’s Theorem.

Therefore, since \((\Delta_n)^k\) is a “well-described polyhedron” in the sense of [23, Definition 6.2.2], we may apply the Ellipsoid algorithm in [23, Theorem 6.5.19]. That theorem shows that \( F \) can be minimized over \((\Delta_n)^k\) using polynomially many evaluations of \( F \) and polynomial additional processing time. By appealing again to the representation (3.2) of \( F \) in Lemma 3.3, each evaluation of \( F \) can be performed via a single \( \text{MOT}_C \) computation and polynomial additional processing time.

\[ \square \]

3.2.2 Hardness of approximation

Proof of Theorem 3.2. By Corollary 3.5, it suffices to compute the minimum value of \( F \) over \((\Delta_n)^k\) to additive accuracy \( \Theta(\varepsilon nk) \). By the representation of \( F \) in (3.2), this amounts to approximately computing

\[ \min_{\mu \in (\Delta_n)^k} \text{MOT}_C(\mu) - \langle \mu, p \rangle. \tag{3.3} \]

to that accuracy. Note that a query to the oracle computing \( \text{MOT}_C \) to \( \varepsilon \) accuracy (plus polynomial-time additional computation) computes the objective function in (3.3) to \( \varepsilon \) additive accuracy. Therefore, this is an instance of the zero-th order optimization problem for approximately convex functions studied in [5, 34]. The claimed runtime and approximation accuracy follow from their results once we check that \( F \) has polynomial Lipschitz parameter, done next (we give a tighter bound than needed since it may be of independent interest).

\[ \square \]

Lemma 3.6 (\( \ell_1 \)-Lipschitzness of \( \text{MOT}_C \) w.r.t. marginals). The function \( \mu \mapsto \text{MOT}_C(\mu) \) on \((\Delta_n)^k\) is Lipschitz with respect to the entrywise \( \ell_1 \) norm with parameter \( 2C_{\max} \).

Proof. Let \( \mu, \mu' \in (\Delta_n)^k \). By symmetry, it suffices to show that

\[ \min_{P \in M(\mu_1', \ldots, \mu_k')} \langle P', C \rangle \leq \min_{P \in M(\mu_1, \ldots, \mu_k)} \langle P, C \rangle + 2C_{\max} \| \mu - \mu' \|_1. \]

Let \( P^* \) be an optimal solution for the optimization over \( M(\mu_1, \ldots, \mu_k) \). By the rounding algorithm in [27], there exists \( \hat{P} \in M(\mu_1', \ldots, \mu_k') \) such that the entrywise \( \ell_1 \) norm \( \| \hat{P} - P^* \|_1 \leq 2\| \mu - \mu' \|_1 \). Thus

\[ \min_{P \in M(\mu_1', \ldots, \mu_k')} \langle P', C \rangle \leq \langle \hat{P}, C \rangle = \langle P^*, C \rangle + \langle \hat{P} - P^*, C \rangle. \]

By construction of \( P^* \), the first term \( \langle P^*, C \rangle = \min_{P \in M(\mu_1, \ldots, \mu_k)} \langle P, C \rangle \). By Hölder’s inequality and the construction of \( \hat{P} \), the second term \( \langle \hat{P} - P^*, C \rangle \leq C_{\max} \| \hat{P} - P^* \|_1 \leq 2C_{\max} \| \mu - \mu' \|_1. \]

\[ \square \]
4 Application: costs with super-constant rank

Recent work has given a polynomial time algorithm for approximate MOT when the cost is a constant-rank tensor given in factored form [2]. A natural algorithmic question is whether the dependence on the rank can be improved: is there an algorithm whose runtime is simultaneously polynomial in \( n, k, \) and the rank \( r \)? Here we show that, under standard complexity theory assumptions, the answer is no. Our result provides a converse to [2], and justifies the constant-rank regime studied in [2].

**Proposition 4.1** (Hardness of MOT for low-rank costs). Assuming \( P \neq NP \), there does not exist a \( poly(n, k, r) \)-time deterministic algorithm for solving MOT\(_C\) for costs \( C \) given by a rank-\( r \) factorization.

Our impossibility result further extends to approximate computation.

**Proposition 4.2** (Hardness of approximate MOT for low-rank costs). Assuming \( NP \not\in BPP \), there does not exist a \( poly(n, k, r, C_{\text{max}}) \)-time randomized algorithm for approximating MOT\(_C\) to \( \varepsilon \) additive accuracy for costs \( C \) given by a rank-\( r \) factorization.

The proof encodes the hard problem of finding a large clique in a \( k \)-partite graph as an instance of MOT\(_C\) in which \( C \) has an explicit low-rank factorization. We define the following notation: for a \( k \)-partite graph \( G \) on \( nk \) vertices \( v_{i,j} \) for \( i \in [k] \) and \( j \in [n] \), let \( T_G \in (\mathbb{R}^n)^\otimes k \) denote the tensor with \((j_1, \ldots, j_k)\)-th entry equal to the number of edges in the induced subgraph of \( G \) with vertices \( \{v_{1,j_1}, \ldots, v_{k,j_k}\} \).

**Lemma 4.3** (\( T_G \) is low-rank). For any \( k \)-partite graph \( G \) on \( nk \) vertices, \( \text{rank}(T_G) \leq n^2k^2 \). Moreover, a factorization of \( T_G \) with this rank is computable from \( G \) in \( poly(n, k) \) time.

**Proof.** Consider an edge \((v_{i,j}, v_{i',j'})\) between partitions \( i, i' \in [k] \). Consider the rank-1 tensor formed by the outer product of the indicator vectors \( e_j \) and \( e_{j'} \) on respective slices \( i \) and \( i' \), and the all-ones vector \( 1_n \) on all other slices \( \ell \in [k] \setminus \{i, i'\} \). This tensor takes value 1 on all tuples in \([n]^k\) with \( i \)-th coordinate \( j \) and \( i' \)-th coordinate \( j' \), and takes value 0 elsewhere. Summing up such a rank-1 tensor for each edge of \( G \)—of which there are at most \((nk)^2\)—yields the desired factorization. \( \square \)

**Lemma 4.4** (Hardness of MIN for low-rank costs). Assuming \( P \neq NP \), there is no \( poly(n, k, r) \)-time deterministic algorithm for solving MIN\(_C\) for costs \( C \) given by a rank-\( r \) factorization. Moreover, assuming \( NP \not\in BPP \), there is \( poly(n, k, r, C_{\text{max}}) \)-time randomized algorithm for \( \varepsilon \)-approximate additive computation.

**Proof.** Deciding whether there exists a \( k \)-clique in a \( k \)-partite graph \( G \) on \( nk \) vertices is NP-hard. This problem reduces to computing the maximal entry in \( T_G \), which is equivalent to solving MIN\(_C(0)\) for \( C = -T_G \). The first statement then follows since a low-rank factorization of \(-T_G\) can be found in \( poly(n, k) \) time by Lemma 4.3. For the second statement, note that since the entries of \(-T_G\) are integral, it is also NP-hard to solve MIN\(_C(0)\) to additive error \( C_{\text{max}}/10k^2 \leq 0.1 \). \( \square \)

**Proof of Proposition 4.1.** By Theorem 3.1, a \( poly(n, k, r) \)-time deterministic algorithm for MOT\(_C\) on rank-\( r \) costs implies a \( poly(n, k, r) \)-time deterministic algorithm for MIN\(_C\) on rank-\( r \) costs. Assuming \( P \neq NP \), this contradicts Lemma 4.4. \( \square \)

**Proof of Proposition 4.2.** By Theorem 3.2, a \( poly(n, k, r, C_{\text{max}}) \)-time randomized algorithm for MOT\(_C\) on rank-\( r \) costs \( C \) implies a \( poly(n, k, r, C_{\text{max}}) \)-time randomized algorithm for MIN\(_C\) on rank-\( r \) costs \( C \). Assuming \( NP \not\in BPP \), this contradicts Lemma 4.4. \( \square \)
5 Application: costs with full pairwise interactions

Many studied MOT costs, such as the Wasserstein barycenter cost and Coulomb cost, have the following structure: they decompose into a sum of pairwise interactions, as

$$C_{j_1,...,j_k} = \sum_{1 \leq i < i' \leq k} g_{i,i'}(j_i,j_{i'})$$  (5.1)

for some functions $g_{i,i'}: [n] \times [n] \to \mathbb{R}$. This decomposability structure allows for a polynomial-size implicit representation of the cost tensor. It is a natural question whether this generic structure can be exploited to obtain polynomial-time algorithms for MOT. We show that the answer is no: there are MOT costs that are decomposable into pairwise interactions, but are NP-hard to solve.

**Proposition 5.1** (Hardness of MOT for pairwise-decomposable costs). Assuming $P \neq NP$, there does not exist a $poly(n,k)$-time deterministic algorithm for solving $MOT_C$ for costs $C$ of the form (5.1).

Our impossibility result further extends to approximate computation.

**Proposition 5.2** (Hardness of approximate MOT for pairwise-decomposable costs). Assuming $NP \not\subseteq BPP$, there does not exist a $poly(n,k,\varepsilon)$-time randomized algorithm for approximating $MOT_C$ to $\varepsilon$ additive accuracy for costs $C$ of the form (5.1).

**Proof of Propositions 5.1 and 5.2.** The proofs of Propositions 5.1 and 5.2 are the same as the proofs of Propositions 4.1 and 4.2 using the fact that for any graph $G = (V,E)$, the tensor $-T_G$ can be written as a sum of pairwise interactions: $(-T_G)_{j_1,...,j_k} = \sum_{1 \leq i < i' \leq k-1} [((v_{i,j_i},v_{i',j_{i'}}) \in E]$. □

Propositions 5.1 and 5.2 provides converses to the result of [2]. Specifically, [2, §4], considers MOT costs $C$ that decompose into local interactions as $C_{j_1,...,j_k} = \sum_{S \in S} g_S(\{j_i\}_{i \in S})$, and gives a polynomial-time algorithm in the case that the graph with vertices $[k]$ and edges $\{(i,i'): i,i' \in S \text{ for some } S \in S\}$ has constant treewidth. Conversely, our hardness results in Propositions 4.1 and 4.2 show that bounded treewidth is necessary for polynomial-time algorithms. This is because costs of the form (5.1) fall under the framework of decomposable costs in [2] with non-constant treewidth of size $k - 1$.

6 Application: repulsive costs

In this section, we investigate several MOT problems with repulsive costs that are of interest in the literature. We prove intractability results that clarify why—despite a growing literature (see, e.g., the survey [17] and the references within)—these problems have resisted algorithmic progress.

6.1 Determinantal cost

A repulsive cost of interest in the MOT literature is the determinant cost (e.g., [13, 17]). This cost is given by:

$$C_{j_1,...,j_k} = -|\det(x_{j_1},...,x_{j_k})|,$$  (6.1)

where $x_1,\ldots,x_n \in \mathbb{R}^k$ and $\det(x_{j_1},...,x_{j_k})$ is the determinant of the $k \times k$ matrix whose columns are $x_{j_1},\ldots,x_{j_k}$. This is a repulsive cost in the sense that tuples with “similar” vectors are penalized with higher cost, see the survey [17]. We prove that the MOT problem with this cost is NP-hard. For convenience of notation, we think of the marginal distributions $\mu_1,\ldots,\mu_k$ as distributions in the simplex $\Delta_n$, and write $[\mu_i]_j$ to mean the mass of $\mu_i$ on $x_j$. 

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Proposition 6.1 (Hardness of MOT with determinant cost). Assuming $P \neq NP$, then there is no poly$(n,k)$-time algorithm that given $x_1, \ldots, x_n \in \mathbb{R}^k$ solves $MOT_C$ for the cost $C$ in (6.1).

Proof. By Theorem 3.1, it suffices to prove that the $MIN_C$ problem is NP-hard. We show this is true even if the input weights $p$ are identically 0: in this case the $MIN_C$ problem is to compute $\min_j C_j = -\max_j |\det(x_j, \ldots, x_{jk})|$ given $x_1, \ldots, x_n \in \mathbb{R}^k$. This is NP-hard by [29].

Rather than show additive inapproximability of MOT with determinant costs, we consider log-determinant costs since additive error on the logarithmic scale amounts to multiplicative error on the natural scale, which is more standard in the combinatorial-optimization literature on determinant maximization. Below, we show inapproximability of MOT with such log-determinant costs. Note that for technical reasons we upper-bound the cost at 0 to avoid unbounded costs for tuples with null determinant:

$$C_{j_1, \ldots, j_k} = \min(0, -\log |\det(x_{j_1}, \ldots, x_{j_k})|).$$

(6.2)

Proposition 6.2 (Approximation hardness of MOT with log-determinant cost). Assuming $NP \neq BPP$, then there is no poly$(n,k,C_{\max}/\varepsilon)$ time algorithm that given $x_1, \ldots, x_n \in \mathbb{R}^k$ approximates $MOT_C$ to $\varepsilon$ additive accuracy for the cost $C$ in (6.2).

Proof. Let $x_1, \ldots, x_n \in \mathbb{Z}^k$ have poly$(n,k)$ bits each. It is known to be NP-hard to approximate $\min_{j_1, \ldots, j_k} -\log |\det(x_{j_1}, \ldots, x_{j_k})|$ to within additive error 0.0001 [36, Theorem 3.2]. Since $x_1, \ldots, x_n$ span $\mathbb{R}^k$ without loss of generality, this is equivalent to approximating $\min_{j_1, \ldots, j_k} C_{j_1, \ldots, j_k}$ to within additive error 0.0001. But by Theorem 3.2, given access to $MOT_C$ computations with additive accuracy $C_{\max}/\text{poly}(n,k)$, we can approximate $\text{MIN}_C(0) = \min_{j_1, \ldots, j_k} C_{j_1, \ldots, j_k}$ to within additive error 0.0001 in $\text{poly}(n,k)$ randomized time since $C_{\max}$ is of poly$(n,k)$ size here. Hence, assuming $BPP \neq NP$ there is no $\text{poly}(n,k,C_{\max}/\varepsilon)$-time algorithm that solves $MOT_C$ to accuracy $\varepsilon$. \hfill \square

6.2 Supermodular cost

We now consider MOT problems given by discrete functions that are either submodular or supermodular (see, e.g., [20] for definitions). Specifically, consider an MOT problem with $n=2$ and a cost $C : \{0,1\}^k \to \mathbb{R}$ that is submodular or supermodular.\footnote{Here, we index the marginals of the cost tensor $C$ with the ground set $\{0,1\}$, instead of $\{1,2\}$ as we would in the rest of the paper, to match the notational convention for supermodular/submodular functions.} Since $\{0,1\}^k$ corresponds to the power set of $[k]$, the cost $C$ can be equivalently viewed as a set function on subsets $S \subseteq [k]$. The MOT problem is of the form

$$\min_{P \in M(\text{Ber}(x_1), \ldots, \text{Ber}(x_k))} \mathbb{E}_{S \sim P} C(S)$$

(6.3)

where $x_1, \ldots, x_k \in [0,1]$ dictate the marginals $\mu_1, \ldots, \mu_k$, and $\text{Ber}(p)$ denotes a Bernoulli distribution taking value 1 with probability $p$. In words, (6.3) is an optimization problem over distributions $P$ on subsets of $[k]$, where the linear cost is the expected value of $C$ with respect to $P$.

We prove a dichotomy for MOT problems with these costs: MOT is polynomial-time solvable for general submodular costs, but is intractable for general supermodular costs. This aligns with our message that repulsive structure is a source of intractability in MOT, since submodular costs are a prototypical example of “attractive” costs, whereas supermodular costs are often used to model “repulsive” costs (see, e.g., [11, 33]).

Proposition 6.3. Consider a function $C : \{0,1\}^k \to \mathbb{R}$ given through oracle access for evaluation, and marginal probabilities $x_1, \ldots, x_k \in [0,1]$.
If $C$ is supermodular, then, assuming $P \neq NP$, there is no poly$(k)$-time algorithm for $MOT_C$. Moreover, assuming $NP \neq BPP$, there is no poly$(k, C_{\text{max}}/\varepsilon)$-time algorithm for computing an $\varepsilon$-approximation.

If $C$ is submodular, then $MOT_C$ is solvable in poly$(k)$ time.

**Proof.** To show the intractability of computing the $MOT_C$ problem (6.3) with supermodular costs, consider the case in which $C$ is the supermodular function encoding the NP-hard MAX-CUT problem for a graph on $k$ vertices (refer to e.g., [18]). In this case, $C$ is integer-valued, so MAX-CUT reduces to approximating $\text{MIN}_C(0) = \min_{S \subseteq \{0,1\}^k} C(S)$ to within, say, $\pm 0.49$ additive error. Thus, $\text{MIN}_C(0)$ is hard to approximate to $\pm 0.49$ error. Theorem 3.1 reduces computing $\text{MIN}_C(0)$ to exactly computing $\text{MOT}_C$, hence exact computation of $\text{MOT}_C$ is also NP-hard. Furthermore, Theorem 3.2 uses a randomized algorithm to reduce computing $\text{MIN}_C(0) \pm 0.49$ to $1/poly(k)$-approximating $\text{MOT}_C$, since the range of $C$ is bounded by $C_{\text{max}} \in k^2$. Therefore, if $NP \neq BPP$, then there is no poly$(k, C_{\text{max}}/\varepsilon)$-time algorithm for $\varepsilon$-approximation of $\text{MOT}_C$.

On the other hand, if $C$ is submodular, then the problem is tractable. The proof hinges on the observation that the $MOT_C$ problem (6.3) with marginals $\mu_i = \text{Ber}(x_i)$ is equivalent to the LP characterization of evaluating the convex envelope $F : [0,1]^k \to \mathbb{R}$ of $C$ at the point $x = (x_1, \ldots, x_k)$ [23, §10.1]. If $C$ is submodular, then $F$ can be evaluated in $O(k)$ evaluations of $C$ and $O(k \log k)$ additional processing time by leveraging the equivalence of $F$ to the Lovász extension of $C$ [23, §10.1].

**6.3 Application to Density Functional Theory**

A popular application of MOT is to formulate a relaxation of the Density Functional Theory problem (DFT) from quantum chemistry. We refer the reader to [15] for an introduction of the MOT formulation of DFT, and sketch the simplest case below. In the simplest version of the MOT relaxation, we are given $k$ electron clouds in space, and the objective is to couple the electron clouds in a way that minimizes the expected potential energy of the electron configuration. Suppose the electron clouds are given as distributions $\mu_1, \ldots, \mu_k$ supported on $x_1, \ldots, x_n \in \mathbb{R}^3$; again, for convenience of notation, we think of $\mu_1, \ldots, \mu_k$ as distributions in the simplex $\Delta_n$, and write $[\mu_i]_{j}$ to mean the mass of $\mu_i$ on $x_j$. Then, the MOT relaxation of DFT is to compute a minimum-cost coupling of $\mu_1, \ldots, \mu_k$, with cost given by the Coulomb potential

$$C_{j_1, \ldots, j_k} = \sum_{1 \leq i < j \leq k} \frac{1}{\|x_{j_i} - x_{j_j}\|_2}. \quad (6.4)$$

This is a repulsive cost that encourages tuples $(j_1, \ldots, j_n) \in [n]^k$ such that $x_{j_1}, \ldots, x_{j_n}$ are spread as far as possible, since the Coulomb potential decreases as two electrons move farther apart. Despite significant algorithmic interest, provable polynomial-time algorithms have not yet been found. We conjecture that in fact solving MOT with the Coulomb potential is NP-hard.

**Conjecture 6.4.** Assuming $P \neq NP$, there is no poly$(n, k)$-time algorithm solving $MOT_C$ with the Coulomb potential cost (6.4).

In this section, we make progress towards the conjecture by proving hardness of DFT with the related Coulomb-Buckingham potential, which is similar to the Coulomb potential, but has extra energy terms that grow as $1/r^6$ and $\exp(-\Theta(r))$. The Coulomb-Buckingham potential is popular for modeling the structures of ionic crystals [1], and is defined for two particles at distance $r$ with
then there is no \( \text{poly} \) 3.2, it suffices to show that computing \( \text{min} \) exactly computing \( \text{MIN} \) \( \text{poly} \) for the proof, we show

\[ C \]

\[ \text{(Hardness of DFT with Coulomb-Buckingham potential)} \]

Proposition 6.5

Assuming \( \text{P} \neq \text{NP} \), then there is no \( \text{poly}(n,k) \)-time algorithm that, given positions \( x_1, \ldots, x_n \in \mathbb{R}^3 \), charges \( q_1, \ldots, q_n \in \{-1, +1\} \), parameters \( A_{\pm 1}, B_{\pm 1}, C_{\pm 1}, M > 0 \), and marginals \( \mu_1, \ldots, \mu_k \in \Delta_n \), solves \( \text{MOT}_C \) with cost \( C \) given by (6.5).

\[ C_{j_1, \ldots, j_k} = \begin{cases} M, & \sum_{i \in [k]} q_{j_i} 
eq 0, \\ \sum_{i \in [k]} q_{j_i} = 0. & \end{cases} \]

Proposition 6.6 (Approximation hardness of DFT with Coulomb-Buckingham potential). If

\[ \text{NP} \notin \text{BPP} \], there is no \( \text{poly}(n,k,C_{\max}/\epsilon) \)-time algorithm computing an \( \epsilon \)-additive approximation to \( \text{MOT}_C \), where \( C \) is as in Proposition 6.5.

The proof of Proposition 6.6 is identical to the proof of Proposition 6.5 once we show that the \( \text{MIN}_C(0) \) problem is hard to solve approximately. While [1, Theorem 5] only shows hardness of exactly computing \( \text{MIN}_C(0) \), a slightly more careful analysis extends this hardness to approximate computation; details are deferred to the appendix.

7 Neccesity of dual weights

This section fleshes out the details for Remark 1.5. Namely, in §4, §5, and §6, we showed that \( \text{MOT}_C \) was hard to compute for some family of costs \( C \) by proving that \( \text{MIN}_C(0) \) was hard to compute. Here, we show that such arguments do not use the full power of Theorems 3.1 and 3.2: we construct a family of cost tensors \( C \) for which \( \text{MOT}_C \) is \( \text{NP} \)-hard to compute yet \( \text{MIN}_C(0) \) is polynomial-time computable.

The cost family is as follows: given a 2-SAT formula \( \phi : \{0,1\}^k \to \{0,1\} \), define

\[ C_{j_1, \ldots, j_k} = -\phi(j_1, \ldots, j_k). \]


Proposition 7.1. Given a 2-SAT formula $\phi$, it is \textsf{NP}-hard to solve $\text{MOT}_C$ for the cost \eqref{eq:7.1}. However, $\text{MIN}_C(0)$ can be computed in polynomial time.

Proof. Observe that $\text{MIN}_C(0) = \min_{j_1,\ldots,j_k} C_{j_1,\ldots,j_k} = -\max_{j_1,\ldots,j_k} \phi(j_1,\ldots,j_k)$ is the satisfiability problem for $\phi$, which can be solved in polynomial-time since $\phi$ is a 2-SAT formula \cite{24}.

On the other hand, let $p = (p_1,\ldots,p_k) \in \mathbb{R}^{2^k}$ be given by $p_1 = p_2 = \cdots = p_k = (0, -1/(2k)) \in \mathbb{R}^2$. Then $\text{MIN}_C(p) = \min_{j_1,\ldots,j_k} \phi(j_1,\ldots,j_k) - \sum_{i=1}^k [p_i]_{j_i} = -\max_{j_1,\ldots,j_k} \phi(j_1,\ldots,j_k) - \|\vec{j}\|/(2k)$ solves the problem of finding the minimum weight of a satisfying assignment to $\phi$. This problem is \textsf{NP}-hard \cite{24}, hence $\text{MIN}_C(p)$ is \textsf{NP}-hard. Therefore $\text{MOT}_C$ is \textsf{NP}-hard by Theorem 3.1. \hfill \Box

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References

[1] D. Adamson, A. Deligiakos, V. V. Gusev, and I. Potapov. On the hardness of energy minimisation for crystal structure prediction. In International Conference on Current Trends in Theory and Practice of Informatics, pages 587–596. Springer, 2020.

[2] J. M. Altschuler and E. Boix-Adserà. Polynomial-time algorithms for Multimarginal Optimal Transport problems with decomposability structure. \textit{arXiv pre-print arXiv:2008.03006}, 2020.

[3] J. M. Altschuler and E. Boix-Adserà. Wasserstein barycenters can be computed in polynomial time in fixed dimension. \textit{arXiv pre-print arXiv:2006.08012}, 2020.

[4] E. Anderes, S. Borgwardt, and J. Miller. Discrete Wasserstein barycenters: Optimal transport for discrete data. \textit{Mathematical Methods of Operations Research}, 84(2):389–409, 2016.

[5] A. Belloni, T. Liang, H. Narayanan, and A. Rakhlin. Escaping the local minima via simulated annealing: optimization of approximately convex functions. In \textit{Conference on Learning Theory}, pages 240–265, 2015.

[6] J.-D. Benamou, G. Carlier, M. Cuturi, L. Nenna, and G. Peyré. Iterative Bregman projections for regularized transportation problems. \textit{SIAM Journal on Scientific Computing}, 37(2):A1111–A1138, 2015.

[7] J.-D. Benamou, G. Carlier, S. Di Marino, and L. Nenna. An entropy minimization approach to second-order variational mean-field games. \textit{arXiv preprint arXiv:1807.09078}, 2018.

[8] J.-D. Benamou, G. Carlier, and L. Nenna. A numerical method to solve multi-marginal optimal transport problems with Coulomb cost. In \textit{Splitting Methods in Communication, Imaging, Science, and Engineering}, pages 577–601. Springer, 2016.

[9] J.-D. Benamou, G. Carlier, and L. Nenna. Generalized incompressible flows, multi-marginal transport and Sinkhorn algorithm. \textit{Numerische Mathematik}, 142(1):33–54, 2019.

[10] S. Borgwardt and S. Patterson. On the computational complexity of finding a sparse Wasserstein barycenter. \textit{arXiv preprint arXiv:1910.07568}, 2019.

[11] A. Borodin, H. C. Lee, and Y. Ye. Max-sum diversification, monotone submodular functions and dynamic updates. In Symposium on Principles of Database Systems, pages 155–166, 2012.

[12] G. Buttazzo, L. De Pascale, and P. Gori-Giorgi. Optimal-transport formulation of electronic density-functional theory. \textit{Physical Review A}, 85(6):062502, 2012.

[13] G. Carlier and B. Nazaret. Optimal transportation for the determinant. \textit{ESAIM: Control, Optimisation and Calculus of Variations}, 14(4):678–698, 2008.
[14] G. Carlier, A. Oberman, and E. Oudet. Numerical methods for matching for teams and Wasserstein barycenters. *ESAIM: Mathematical Modelling and Numerical Analysis*, 49(6):1621–1642, 2015.

[15] C. Cotar, G. Friesecke, and C. Klüppelberg. Density functional theory and optimal transportation with Coulomb cost. *Communications on Pure and Applied Mathematics*, 66(4):548–599, 2013.

[16] J. A. De Loera and E. D. Kim. Combinatorics and geometry of transportation polytopes: an update. *Discrete geometry and algebraic combinatorics*, 625:37–76, 2014.

[17] S. Di Marino, A. Gerolin, and L. Nenna. Optimal transportation theory with repulsive costs. *Topological optimization and optimal transport*, 17:204–256, 2017.

[18] U. Feige, V. S. Mirrokni, and J. Vondrák. Maximizing non-monotone submodular functions. *SIAM Journal on Computing*, 40(4):1133–1153, 2011.

[19] S. Friedland. Tensor optimal transport, distance between sets of measures and tensor scaling. *arXiv pre-print arXiv:2005.00945*, 2020.

[20] S. Fujishige. *Submodular functions and optimization*. Elsevier, 2005.

[21] M. R. Garey and D. S. Johnson. *Computers and intractability*, volume 174.

[22] M. Grötschel, L. Lovász, and A. Schrijver. The ellipsoid method and its consequences in combinatorial optimization. *Combinatorica*, 1(2):169–197, 1981.

[23] M. Grötschel, L. Lovász, and A. Schrijver. *Geometric algorithms and combinatorial optimization*, volume 2. Springer Science & Business Media, 2012.

[24] D. Gusfield and L. Pitt. A bounded approximation for the minimum cost 2-SAT problem. *Algorithmica*, 8(1-6):103–117, 1992.

[25] I. Haasler, A. Ringh, Y. Chen, and J. Karlsson. Multi-marginal optimal transport and Schrödinger bridges on trees. *arXiv preprint arXiv:2004.06909*, 2020.

[26] R. M. Karp. Reducibility among combinatorial problems. In *Complexity of computer computations*, pages 85–103. Springer, 1972.

[27] T. Lin, N. Ho, M. Cuturi, and M. I. Jordan. On the complexity of approximating multimarginal optimal transport. *arXiv preprint arXiv:1910.00152*, 2019.

[28] L. Nenna. *Numerical methods for multi-marginal optimal transportation*. PhD thesis, 2016.

[29] C. H. Papadimitriou. The largest subdeterminant of a matrix. *Bulletin of the Greek Mathematical Society*, 25(25):95–105, 1984.

[30] C. H. Papadimitriou and T. Roughgarden. Computing correlated equilibria in multi-player games. *Journal of the ACM (JACM)*, 55(3):1–29, 2008.

[31] B. Pass. Multi-marginal optimal transport: theory and applications. *ESAIM: Mathematical Modelling and Numerical Analysis*, 49(6):1771–1790, 2015.

[32] G. Peyré and M. Cuturi. Computational optimal transport. *Foundations and Trends in Machine Learning*, 2017.

[33] A. Prasad, S. Jegelka, and D. Batra. Submodular meets structured: Finding diverse subsets in exponentially-large structured item sets. In *Advances in Neural Information Processing Systems*, pages 2645–2653, 2014.

[34] A. Risteski and Y. Li. Algorithms and matching lower bounds for approximately-convex optimization. In *Advances in Neural Information Processing Systems*, pages 4745–4753, 2016.
A Proof of Proposition 6.6

Proof of Proposition 6.6. By Theorem 3.2, it suffices to prove that approximating $\text{MIN}_C(0)$ up to $\leq C_{\text{max}}/\text{poly}(n,k)$ additive error is NP-hard. By the reasoning in the proof of Proposition 6.5, it suffices to prove that

$$\min \left\{ \frac{1}{2} \sum_{j \in S, j' \in S \setminus \{j\}} U(\|x_j - x_{j'}\|_2, q_j, q_{j'}) : S \subset [n], |S| = k, \sum_{j \in S} q_j = 0 \right\} \quad (A.1)$$

is NP-hard to $C_{\text{max}}/\text{poly}(n,k)$-approximate. We modify the proof of [1, Theorem 5] to prove this. Note that for the parameters $A_{\pm}, B_{\pm}, C_{\pm}$ chosen in Lemma 1 of [1, Theorem 5], we have $C_{\text{max}} = \text{poly}(n,k)$, and also the inequalities (1)-(3) of [1] are met with a small polynomial gap of at least $1/n^{10}$ in the sense that for large enough $n$,

$$\frac{A_+}{e^{B_+} n} - \frac{C_+}{n^6} + \frac{1}{n} + \frac{A_-}{e^{B_-} \sqrt{1+n^2}} - \frac{C_-}{(1+n^2)^3} - \frac{1}{\sqrt{1+n^2}} \geq \left| \frac{A_-}{e^{B_-}} - C_- - 1 \right| + 1/n^{10}$$

and

$$\frac{A_+}{e^{B_+} r} - \frac{C_+}{r^6} + \frac{1}{r} + \frac{A_-}{e^{B_-} \sqrt{1+r^2}} - \frac{C_-}{(1+r^2)^3} - \frac{1}{\sqrt{1+r^2}} \leq \left| \frac{A_-}{e^{B_-}} - C_- - 1 \right| - 1/n^{10}, \quad r \geq \sqrt{2n}$$

and

$$\frac{A_+}{e^{B_+} r} - \frac{C_+}{r^6} + \frac{1}{r} + \frac{A_-}{e^{B_-} \sqrt{1+r^2}} - \frac{C_-}{(1+r^2)^3} - \frac{1}{\sqrt{1+r^2}} > 1/n^{10}, \quad r \geq \sqrt{2n}. \quad \square$$

Tracing through the reasoning of Lemmas 2, 3, and 4 of [1], this gap implies that a $\pm 0.49/n^{10}$ approximation to the objective (A.1) suffices to determine whether or not the construction in [1, Theorem 5] encodes a graph with an independent set of size $k/2$. This proves NP-hardness of $C_{\text{max}}/\text{poly}(n,k)$ approximation for (A.1).