

NUMERICAL METHOD FOR FEASIBLE AND APPROXIMATELY OPTIMAL SOLUTIONS OF MULTI-MARGINAL OPTIMAL TRANSPORT BEYOND DISCRETE MEASURES

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ABSTRACT. We propose a numerical algorithm for the computation of multi-marginal optimal transport (MMOT) problems involving general measures that are not necessarily discrete. By developing a relaxation scheme in which marginal constraints are replaced by finitely many linear constraints and by proving a specifically tailored duality result for this setting, we approximate the MMOT problem by a linear semi-infinite optimization problem. Moreover, we are able to recover a feasible and approximately optimal solution of the MMOT problem, and its sub-optimality can be controlled to be arbitrarily close to 0 under mild conditions. The developed relaxation scheme leads to a numerical algorithm which can compute a feasible approximate optimizer of the MMOT problem whose theoretical sub-optimality can be chosen to be arbitrarily small. Besides the approximate optimizer, the algorithm is also able to compute both an upper bound and a lower bound on the optimal value of the MMOT problem. The difference between the computed bounds provides an explicit upper bound on the sub-optimality of the computed approximate optimizer. Through a numerical example, we demonstrate that the proposed algorithm is capable of computing a high-quality solution of an MMOT problem involving as many as 50 marginals along with an explicit estimate of its sub-optimality that is much less conservative compared to the theoretical estimate.

1. INTRODUCTION

In this paper, we develop a numerical method for the computation of multi-marginal optimal transport (MMOT) problems. Given $N \in \mathbb{N}$ Borel probability measures μ_1, \dots, μ_N on Polish spaces $\mathcal{X}_1, \dots, \mathcal{X}_N$ and a cost function $f : \mathcal{X}_1 \times \dots \times \mathcal{X}_N \rightarrow \mathbb{R}$, the goal of the MMOT problem is to minimize the following quantity

$$\int_{\mathcal{X}_1 \times \dots \times \mathcal{X}_N} f(x_1, \dots, x_N) \mu(dx_1, \dots, dx_N)$$

over the set of joint probability measures μ on $\mathcal{X}_1 \times \dots \times \mathcal{X}_N$ with the given marginals μ_1, \dots, μ_N . This is an extension of the classical two-marginal (i.e., $N = 2$) optimal transport problem of Monge and Kantorovich, which has been thoroughly studied in the literature; see, e.g., [44, 49, 59, 60] as well as the recent survey by Benamou [6] and the references therein for applications of optimal transport and discussions about its computation. For various theoretical results in the general multi-marginal case (i.e., $N > 2$), we refer the reader to the duality results by Kellerer [41] and the survey by Pass [48] and the references therein.

The MMOT problem serves as the basis of other related problems such as the Wasserstein barycenter problem [2] and the martingale optimal transport problem [5]. The original MMOT problem and its various extensions have many modern theoretical and practical applications, including but not limited to: theoretical economics [13, 18, 31], density functional theory (DFT) in quantum mechanics [12, 15, 20, 21], computational fluid mechanics [7, 9], mathematical finance [5, 17, 23, 25, 29, 38, 40], statistics [53, 54], machine learning [51], tomographic image reconstruction [1], signal processing [30, 39], and operations research [16, 32, 33].

There exists a vast literature on the computational aspect of MMOT and related problems. Many such studies focus on the case where the marginals are discrete measures with finite support [3, 8, 50, 56], or where non-discrete marginals are replaced by their discrete approximations [14, 29, 36]. When all marginals have finite support, the MMOT problem corresponds to a linear programming problem typically involving a large number of decision variables. Moreover, when the marginals are non-discrete and after replacing the marginals with their discrete approximations, the optimal solutions of the linear

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programming problem and its dual are not feasible solutions of the original MMOT problem and its dual without discretization. This is a crucial shortcoming of discretization-based approaches since one is only able to obtain an infeasible solution of the MMOT problem that approximates the actual optimal solution, and the approximation error can only be controlled using theoretical estimates that can be over-conservative in practice.

There are approaches to solving MMOT and related problems which use regularization to speed up the computation. Most notably, Cuturi [22] proposed to use entropic regularization and the Sinkhorn algorithm for solving the optimal transport problem (i.e., when $N = 2$). See also [27, 47] for the theoretical properties of entropic regularization and the Sinkhorn algorithm. While most regularization-based approaches deal with discrete marginals, see, e.g., [9, 49, 56], there are also regularization-based approaches for solving MMOT problems with non-discrete marginals. These approaches involve solving an infinite-dimensional optimization problem by finite-dimensional parametrization such as deep neural network, see, e.g., [19, 23, 24, 26, 28, 29, 40]. A limitation of regularization-based approaches is that the regularization term introduces a bias (see, e.g., [6, Section 3.3]) which only goes to 0 asymptotically when the regularization term goes to 0. When the regularization term is close to 0, numerical instability may arise and complicate the computational procedure. See [49, Section 4.4] for a detailed discussion of this issue in the Sinkhorn algorithm and some of the remedies. Moreover, using deep neural networks to parametrize infinite-dimensional decision variables incurs various practical challenges when training the neural networks due to the non-convexity of the objective function, and thus the trained neural networks may represent optimal solutions of the MMOT problem poorly.

In this paper, we tackle the MMOT problem in its original form without any discretization or regularization. Our goal is to obtain feasible solutions of the MMOT problem and its dual as well as to control the difference between their corresponding objective values. This difference provides an upper bound on the sub-optimality of the pair of feasible solutions for the primal and the dual of the MMOT problem. Through this approach, we are able to take full advantage of the duality.

Our approach was inspired by the result of Breeden and Litzenberger [11] and its multi-dimensional extension by Talponen and Viitasaari [55], which can be roughly summarized as: under certain conditions, a probability measure μ on a measurable space (Ω, \mathcal{F}) can be completely characterized by the linear mapping $\mathcal{G} \ni g \mapsto \int_{\Omega} g d\mu \in \mathbb{R}$, where \mathcal{G} is an infinite class of real functions on Ω . This result inspired us to consider a relaxed-version of the MMOT problem shown in (MMOT_{relax}), in which the marginal constraints are replaced by a *finite* collection of properly chosen linear constraints. Therefore, instead of considering fixed marginals, we allow each marginal to be any probability measure satisfying the finitely many given linear constraints. This is related to the moment problem (see, e.g., [61]), and hence we refer to a set of probability measures satisfying a given collection of linear constraints as a *moment set*. The rigorous definition of *moment set* is presented in Definition 2.2.5. Subsequently, for any $\epsilon > 0$, an ϵ -optimal solution of (MMOT_{relax}) provides a lower bound on the optimal value of the MMOT problem.

Next, in order to recover a feasible solution of the MMOT problem from an approximately optimal solution of (MMOT_{relax}), we adopt an idea from the copula theory (see, e.g., [45, Chapter 5]). The idea is analogous to Sklar's theorem (see, e.g., [45, Equation (5.3) & Theorem 5.3]), which roughly states that: a multivariate distribution can be decomposed into its one-dimensional marginals and a copula which encodes all the dependence information; conversely, one can assemble a multivariate distribution from any given collection of one-dimensional marginals and a given copula. We extend this idea to probability measures on the product of general Polish spaces, and introduce a notion that we call *reassembly*. Intuitively, given a probability measure $\hat{\mu}$ on $\mathcal{X}_1 \times \cdots \times \mathcal{X}_N$ whose marginals are not necessarily equal to μ_1, \dots, μ_N , a *reassembly* of $\hat{\mu}$ with the marginals μ_1, \dots, μ_N is a probability measure on $\mathcal{X}_1 \times \cdots \times \mathcal{X}_N$ formed by *reassembling* the dependence structure of $\hat{\mu}$ and the marginals μ_1, \dots, μ_N . The mathematical details of *reassembly* and its existence are presented in Definition 2.2.2 and Lemma 2.2.3. Through the use of *reassembly*, we not only obtain a *feasible* solution of the MMOT problem, but also derive an upper bound on the sub-optimality of this feasible solution as shown in Theorem 2.2.8. Note that this approach produces a feasible solution of the MMOT problem even in the case where the given marginals are non-discrete. Moreover, through Lemma 3.1.1 and Proposition 3.1.2, we provide an explicit method to construct a *reassembly* under practically relevant conditions when the underlying spaces are Euclidean.

Now that we have obtained a lower bound on the optimal value of the MMOT problem through $(\text{MMOT}_{\text{relax}})$ and also an upper bound which is equal to the objective value of a *reassembly* measure, it remains to control the difference between these bounds. Following the results in Theorem 2.2.8, we aim to control the supremum Wasserstein distance between a marginal μ_i and any probability measure contained in a *moment set* around μ_i . In the case where $\mathcal{X}_1, \dots, \mathcal{X}_N$ are subsets of Euclidean spaces, we provide explicit methods to construct *moment sets* whose “sizes” in terms of the Wasserstein distance can be controlled to be arbitrarily close to 0. The details about these methods can be found in Definitions 3.2.2–3.2.4, Propositions 3.2.5–3.2.6, and Theorem 3.2.7. Combined with Theorem 2.2.8, this allows us to control the difference between the upper and lower bounds on the optimal value of the MMOT problem to be arbitrarily close to 0. Moreover, since this difference is also an upper bound on the sub-optimality of the feasible solution of the MMOT problem obtained via *reassembly*, we are able to control the sub-optimality of this feasible solution to be arbitrarily close to 0.

As a direct consequence of our results on controlling the Wasserstein “sizes” of *moment sets* in Theorem 3.2.7, we also obtain a non-asymptotic version of the results of Breeden and Litzenberger [11] and Talponen and Viitasaari [55]. This result is presented in Corollary 3.2.8 and its interpretation in the context of financial mathematics is discussed in Remark 3.2.9. In summary, Corollary 3.2.8 states that, given any $\epsilon > 0$, one can explicitly construct a finite collection of multi-asset financial derivatives such that the knowledge of their prices controls the model risk surrounding the risk-neutral pricing measure in terms of the Wasserstein distance to be at most ϵ .

Finally, the theoretical results in this paper enable us to develop a numerical algorithm for solving MMOT problems. We first show that the relaxed MMOT problem admits a dual which is a linear semi-infinite optimization problem given by $(\text{MMOT}_{\text{relax}}^*)$. This allows us to adopt well-established numerical methods for solving this type of problems. We provide sufficient conditions for the strong duality between the relaxed MMOT problem and its dual in Theorem 2.3.1 and Proposition 2.3.3. Then, we develop a cutting-plane algorithm for computing an approximately optimal solution of the linear semi-infinite optimization problem. Similar algorithms have been developed by Neufeld, Papapantoleon, and Xiang [46] for computing model-free upper and lower price bounds of multi-asset financial derivatives. The details and the theoretical properties of the proposed algorithm are presented and discussed in Algorithm 1, Remark 4.1.2, and Theorem 4.1.3. In summary, for any given $\epsilon > 0$, Algorithm 1 computes feasible solutions of $(\text{MMOT}_{\text{relax}})$ and its dual $(\text{MMOT}_{\text{relax}}^*)$ that are both ϵ -optimal. The feasible solution of $(\text{MMOT}_{\text{relax}}^*)$ is also a feasible solution of the dual of the MMOT problem since $(\text{MMOT}_{\text{relax}})$ is a relaxation of the MMOT problem. Subsequently, we combine Algorithm 1 and our theoretical results about *reassembly* and *moment sets* to develop Algorithm 2, which, for any given $\tilde{\epsilon} > 0$, can compute an $\tilde{\epsilon}$ -optimizer of a given MMOT problem. Moreover, it computes an upper and a lower bound on the optimal value of the MMOT problem. The details and the theoretical properties of Algorithm 2 are discussed in Remark 4.2.2 and Theorem 4.2.3. We showcase the performance of Algorithm 2 in a high-dimensional MMOT problem involving $N = 50$ marginals and discuss its practical advantages in Section 4.3.

Our main contributions are summarized as follows.

- (1) We develop a relaxation scheme for MMOT problems and provide sufficient conditions for the strong duality between a relaxed MMOT problem and its dual. The dual problem can be formulated as a linear semi-infinite optimization problem and numerically solved using an algorithm that we develop (i.e., Algorithm 1).
- (2) We introduce the notion of *reassembly*, which allows us to construct a feasible solution of the MMOT problem from an infeasible one, even when the given marginals are non-discrete. Combined with the proposed relaxation scheme, we are able to control the sub-optimality of the constructed feasible solution to be arbitrarily close to 0 under mild conditions.
- (3) We develop a numerical algorithm (i.e., Algorithm 2) which, for any given $\tilde{\epsilon} > 0$, is not only capable of computing an $\tilde{\epsilon}$ -optimizer of the MMOT problem but also capable of computing upper and lower bounds on its optimal value such that the difference between the bounds is at most $\tilde{\epsilon}$.
- (4) We perform a numerical experiment to demonstrate that the proposed algorithm can produce a high-quality solution in a large MMOT problem instance involving $N = 50$ marginals. Moreover, we showcase that the computed approximation errors are much less conservative compared to the theoretical estimates, which highlights a practical advantage of the proposed algorithm compared to existing methods.

The rest of this paper is organized as follows. Section 2.1 introduces the notations in the paper and the settings of the MMOT problem. In Section 2.2, we develop the notions of *reassembly* and *moment set*, and introduce the relaxation scheme to approximate the MMOT problem. Section 2.3 presents the duality results specifically tailored to the relaxed MMOT problem, which transforms it into a linear semi-infinite optimization problem. In Section 3.1, we demonstrate an explicit construction of a *reassembly* under some fairly general and practically relevant assumptions. In Section 3.2, we provide explicit constructions of *moment sets* on a Euclidean space and establish control on the “size” of the resulting *moment sets* in terms of the Wasserstein distance. Section 4.1 and Section 4.2 present numerical algorithms for approximately solving MMOT problems and their theoretical properties. Finally, Section 4.3 showcases the performance of the proposed numerical method in an example with $N = 50$ marginals and discusses some of its practical aspects. Section 5 contains the proofs of the theoretical results in this paper.

2. APPROXIMATION OF MULTI-MARGINAL OPTIMAL TRANSPORT

2.1. Settings. Throughout this paper, all vectors are assumed to be column vectors. We denote vectors and vector-valued functions by boldface symbols. In particular, for $n \in \mathbb{N}$, we denote by $\mathbf{0}_n$ the vector in \mathbb{R}^n with all entries equal to zero, i.e., $\mathbf{0}_n := \underbrace{(0, \dots, 0)}_{n \text{ times}}^\top$. We also use $\mathbf{0}$ when the dimension is

unambiguous. We denote by $\langle \cdot, \cdot \rangle$ the Euclidean dot product, i.e., $\langle \mathbf{x}, \mathbf{y} \rangle := \mathbf{x}^\top \mathbf{y}$. A subset of a Euclidean space is called a polyhedron or a polyhedral convex set if it is the intersection of finitely many closed half-spaces. In particular, a subset of a Euclidean space is called a polytope if it is a bounded polyhedron. For a subset A of a Euclidean space, let $\text{aff}(A)$, $\text{conv}(A)$, $\text{cone}(A)$ denote the affine hull, convex hull, and conic hull of A , respectively. Moreover, let $\text{cl}(A)$, $\text{int}(A)$, $\text{relint}(A)$, $\text{relbd}(A)$ denote the closure, interior, relative interior, and relative boundary of A , respectively.

For a Polish space $(\mathcal{Y}, d_{\mathcal{Y}})$ with its corresponding metric $d_{\mathcal{Y}}(\cdot, \cdot)$, let $\mathcal{B}(\mathcal{Y})$ denote the Borel subsets of \mathcal{Y} , let $\mathcal{P}(\mathcal{Y})$ denote the set of Borel probability measures on \mathcal{Y} , and let $\mathcal{P}_1(\mathcal{Y})$ denote the Wasserstein space of order 1 on \mathcal{Y} , which is given by

$$\mathcal{P}_1(\mathcal{Y}) := \left\{ \mu \in \mathcal{P}(\mathcal{Y}) : \exists \hat{y} \in \mathcal{Y} \text{ such that } \int_{\mathcal{Y}} d_{\mathcal{Y}}(\hat{y}, y) \mu(dy) < \infty \right\}. \quad (2.1)$$

We use $\Gamma(\cdot, \dots, \cdot)$ to denote the set of couplings of measures, i.e., the set of measures with fixed marginals, as detailed in the following definition.

Definition 2.1.1 (Coupling). For $m \in \mathbb{N}$ Polish spaces $(\mathcal{Y}_1, d_{\mathcal{Y}_1}), \dots, (\mathcal{Y}_m, d_{\mathcal{Y}_m})$ and probability measures $\nu_1 \in \mathcal{P}(\mathcal{Y}_1), \dots, \nu_m \in \mathcal{P}(\mathcal{Y}_m)$, let $\Gamma(\nu_1, \dots, \nu_m)$ denote the set of couplings of ν_1, \dots, ν_m , defined as

$$\Gamma(\nu_1, \dots, \nu_m) := \left\{ \gamma \in \mathcal{P}(\mathcal{Y}_1 \times \dots \times \mathcal{Y}_m) : \text{the marginal of } \gamma \text{ on } \mathcal{Y}_j \text{ is } \nu_j \text{ for } j = 1, \dots, m \right\}.$$

For any $\mu, \nu \in \mathcal{P}(\mathcal{Y})$, let $W_1(\mu, \nu)$ denote the Wasserstein metric of order 1 between μ and ν , which is given by

$$W_1(\mu, \nu) := \inf_{\gamma \in \Gamma(\mu, \nu)} \left\{ \int_{\mathcal{Y} \times \mathcal{Y}} d_{\mathcal{Y}}(x, y) \gamma(dx, dy) \right\}. \quad (2.2)$$

In particular, $W_1(\mu, \nu) < \infty$ if $\mu, \nu \in \mathcal{P}_1(\mathcal{X})$.

In the following, we consider $N \in \mathbb{N}$ Polish spaces $(\mathcal{X}_1, d_{\mathcal{X}_1}), \dots, (\mathcal{X}_N, d_{\mathcal{X}_N})$ with N associated probability measures μ_1, \dots, μ_N . This is detailed in the following assumption.

Assumption 2.1.2. $(\mathcal{X}_1, d_{\mathcal{X}_1}), \dots, (\mathcal{X}_N, d_{\mathcal{X}_N})$ are $N \in \mathbb{N}$ Polish spaces and $\mathcal{X} := \mathcal{X}_1 \times \dots \times \mathcal{X}_N$ is a Polish space equipped with the 1-product metric

$$d_{\mathcal{X}}((x_1, \dots, x_N), (y_1, \dots, y_N)) := \sum_{i=1}^N d_{\mathcal{X}_i}(x_i, y_i). \quad (2.3)$$

Moreover, we assume that $\mu_1 \in \mathcal{P}_1(\mathcal{X}_1), \dots, \mu_N \in \mathcal{P}_1(\mathcal{X}_N)$.

For $i = 1, \dots, N$, let $\pi_i : \mathcal{X} \rightarrow \mathcal{X}_i$ denote the projection function onto the i -th component. For $\mu \in \mathcal{P}(\mathcal{X})$ and $i = 1, \dots, N$, let $\mu \circ \pi_i^{-1}$ denote the push-forward of μ under π_i , which will also be referred to as the i -th marginal of μ .

Subsequently, let us first introduce the following technical assumptions about a cost function $f : \mathcal{X} \rightarrow \mathbb{R}$ in an MMOT problem.

Assumption 2.1.3. *In addition to Assumption 2.1.2, $f : \mathcal{X} \rightarrow \mathbb{R}$ is a cost function satisfying the following conditions.*

- (i) $f : \mathcal{X} \rightarrow \mathbb{R}$ is lower semi-continuous.
- (ii) There exist upper semi-continuous functions $h_i \in \mathcal{L}^1(\mathcal{X}_i, \mu_i)$ for $i = 1, \dots, N$ such that $\sum_{i=1}^N h_i \circ \pi_i(\mathbf{x}) \leq f(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{X}$.

Under Assumption 2.1.3, we study the following multi-marginal optimal transport problem:

$$\inf_{\mu \in \Gamma(\mu_1, \dots, \mu_N)} \left\{ \int_{\mathcal{X}} f \, d\mu \right\}. \quad (\text{MMOT})$$

By a multi-marginal extension of [60, Theorem 4.1], an optimal coupling exists for (MMOT).

2.2. The approximation scheme. In this subsection, we develop a relaxation scheme to approximate (MMOT) such that the approximation error can be controlled. The relaxation scheme depends crucially on two notions: (i) the *reassembly* of a measure and (ii) *moment sets*. Before we define the notion of *reassembly*, let us first recall the following gluing lemma from [59].

Lemma 2.2.1 (Gluing lemma [59, Lemma 7.6]). *Suppose that ν_1, ν_2, ν_3 are three probability measures on three Polish spaces $(\mathcal{Y}_1, d_{\mathcal{Y}_1})$, $(\mathcal{Y}_2, d_{\mathcal{Y}_2})$, $(\mathcal{Y}_3, d_{\mathcal{Y}_3})$, respectively, and suppose that $\gamma_{12} \in \Gamma(\nu_1, \nu_2)$, $\gamma_{23} \in \Gamma(\nu_2, \nu_3)$. Then there exists a probability measure $\gamma \in \mathcal{P}(\mathcal{Y}_1 \times \mathcal{Y}_2 \times \mathcal{Y}_3)$ with marginals γ_{12} on $\mathcal{Y}_1 \times \mathcal{Y}_2$ and γ_{23} on $\mathcal{Y}_2 \times \mathcal{Y}_3$.*

Now, let us consider $\mu_1 \in \mathcal{P}_1(\mathcal{X}_1), \dots, \mu_N \in \mathcal{P}_1(\mathcal{X}_N)$ as in Assumption 2.1.2. Using the gluing lemma, from any coupling of $\hat{\mu}_1 \in \mathcal{P}_1(\mathcal{X}_1), \dots, \hat{\mu}_N \in \mathcal{P}_1(\mathcal{X}_N)$ one can *reassemble* a coupling of μ_1, \dots, μ_N . This is detailed in Definition 2.2.2 and Lemma 2.2.3 below. In the following, let $\bar{\mathcal{X}}_i := \mathcal{X}_i$ denote a copy of \mathcal{X}_i in order to differentiate \mathcal{X}_i and its copy.

Definition 2.2.2 (Reassembly). *Let Assumption 2.1.2 hold and let μ_1, \dots, μ_N be defined as in Assumption 2.1.2. For $\hat{\mu} \in \mathcal{P}_1(\mathcal{X})$, let its marginals on $\mathcal{X}_1, \dots, \mathcal{X}_N$ be denoted by $\hat{\mu}_1, \dots, \hat{\mu}_N$, respectively. $\tilde{\mu} \in \Gamma(\mu_1, \dots, \mu_N) \subset \mathcal{P}_1(\mathcal{X})$ is called a *reassembly* of $\hat{\mu}$ with marginals μ_1, \dots, μ_N if there exists $\gamma \in \mathcal{P}(\mathcal{X}_1 \times \dots \times \mathcal{X}_N \times \bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N)$ which satisfies the following conditions.*

- (i) *The marginal of γ on $\mathcal{X}_1 \times \dots \times \mathcal{X}_N$ is $\hat{\mu}$.*
- (ii) *For $i = 1, \dots, N$, the marginal γ on $\mathcal{X}_i \times \bar{\mathcal{X}}_i$, denoted by γ_i , is an optimal coupling of $\hat{\mu}_i$ and μ_i under the cost function $d_{\mathcal{X}_i}$, i.e., $\gamma_i \in \Gamma(\hat{\mu}_i, \mu_i)$ satisfies*

$$\int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} d_{\mathcal{X}_i}(x, y) \gamma_i(dx, dy) = W_1(\hat{\mu}_i, \mu_i).$$

- (iii) *The marginal of γ on $\bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N$ is $\tilde{\mu}$.*

Let $R(\hat{\mu}; \mu_1, \dots, \mu_N) \subset \Gamma(\mu_1, \dots, \mu_N)$ denote the set of reassemblies of $\hat{\mu}$ with marginals μ_1, \dots, μ_N .

Lemma 2.2.3 shows that $R(\hat{\mu}; \mu_1, \dots, \mu_N) \subset \Gamma(\mu_1, \dots, \mu_N) \subset \mathcal{P}_1(\mathcal{X})$ is non-empty.

Lemma 2.2.3 (Existence of reassembly). *Let Assumption 2.1.2 hold. Let μ_1, \dots, μ_N be defined as in Assumption 2.1.2 and let $\hat{\mu} \in \mathcal{P}_1(\mathcal{X})$. Then, there exists a reassembly $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$ with marginals μ_1, \dots, μ_N .*

Proof of Lemma 2.2.3. See Section 5.1. □

Remark 2.2.4. *In general, explicit construction of a reassembly $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$ is highly non-trivial due to the difficulty in explicitly constructing an optimal coupling between two arbitrarily probability measures. Nonetheless, such construction is possible under specific assumptions, as we will show in Section 3.1.*

Next, for a Polish space $(\mathcal{Y}, d_{\mathcal{Y}})$, let us consider convex subsets of $\mathcal{P}_1(\mathcal{Y})$ that are known as *moment sets*, see, e.g., [61]. They are formally defined as follows.

Definition 2.2.5 (Moment set). *Let $(\mathcal{Y}, d_{\mathcal{Y}})$ be a Polish space. For a collection \mathcal{G} of real-valued Borel measurable functions on \mathcal{Y} , let $\mathcal{P}_1(\mathcal{Y}; \mathcal{G}) := \{\mu \in \mathcal{P}_1(\mathcal{Y}) : \mathcal{G} \subseteq \mathcal{L}^1(\mathcal{Y}, \mu)\}$. Let $\overset{\mathcal{G}}{\sim}$ be defined as the following equivalence relation on $\mathcal{P}_1(\mathcal{Y}; \mathcal{G})$: for all $\mu, \nu \in \mathcal{P}_1(\mathcal{Y}; \mathcal{G})$,*

$$\mu \overset{\mathcal{G}}{\sim} \nu \iff \forall g \in \mathcal{G}, \int_{\mathcal{Y}} g d\mu = \int_{\mathcal{Y}} g d\nu. \quad (2.4)$$

For every $\mu \in \mathcal{P}_1(\mathcal{Y}; \mathcal{G})$, let $[\mu]_{\mathcal{G}} := \{\nu \in \mathcal{P}_1(\mathcal{Y}; \mathcal{G}) : \nu \overset{\mathcal{G}}{\sim} \mu\}$ be the equivalence class of μ under $\overset{\mathcal{G}}{\sim}$. We call $[\mu]_{\mathcal{G}}$ the *moment set centered at μ characterized by \mathcal{G}* . In addition, let $\overline{W}_{1, \mu}([\mu]_{\mathcal{G}})$ denote the supremum W_1 -metric between μ and members of $[\mu]_{\mathcal{G}}$, i.e.,

$$\overline{W}_{1, \mu}([\mu]_{\mathcal{G}}) := \sup_{\nu \in [\mu]_{\mathcal{G}}} \{W_1(\mu, \nu)\}. \quad (2.5)$$

Furthermore, for $m \in \mathbb{N}$ Polish spaces $(\mathcal{Y}_1, d_{\mathcal{Y}_1}), \dots, (\mathcal{Y}_m, d_{\mathcal{Y}_m})$, collections $\mathcal{G}_1, \dots, \mathcal{G}_m$ of real-valued Borel measurable functions on $\mathcal{Y}_1, \dots, \mathcal{Y}_m$, and $\nu_1 \in \mathcal{P}_1(\mathcal{Y}_1; \mathcal{G}_1), \dots, \nu_m \in \mathcal{P}_1(\mathcal{Y}_m; \mathcal{G}_m)$, we slightly abuse the notation and define $\Gamma([\nu_1]_{\mathcal{G}_1}, \dots, [\nu_m]_{\mathcal{G}_m})$ as follows:

$$\Gamma([\nu_1]_{\mathcal{G}_1}, \dots, [\nu_m]_{\mathcal{G}_m}) := \left\{ \gamma \in \Gamma(\eta_1, \dots, \eta_m) : \eta_j \in [\nu_j]_{\mathcal{G}_j} \forall 1 \leq j \leq m \right\}. \quad (2.6)$$

Let for a set of functions \mathcal{G} , let $\text{span}_1(\mathcal{G})$ denote the set of finite linear combinations of functions in \mathcal{G} plus a constant intercept, i.e., $\text{span}_1(\mathcal{G}) := \left\{ y_0 + \sum_{j=1}^k y_j g_j : k \in \mathbb{N}_0, y_0, y_1, \dots, y_k \in \mathbb{R}, (g_j)_{j=1:k} \subseteq \mathcal{G} \right\}$. By the definition of $\overset{\mathcal{G}}{\sim}$ in (2.4), it holds that if $\nu \in [\mu]_{\mathcal{G}}$, then $\int_{\mathcal{Y}} g d\mu = \int_{\mathcal{Y}} g d\nu$ for all $g \in \text{span}_1(\mathcal{G})$. In particular, we have $\mu \overset{\mathcal{G}}{\sim} \nu$ if and only if $\mu \overset{\text{span}_1(\mathcal{G})}{\sim} \nu$, and

$$[\mu]_{\mathcal{G}} = [\mu]_{\text{span}_1(\mathcal{G})}. \quad (2.7)$$

Now, for given marginals $\mu_1 \in \mathcal{P}_1(\mathcal{X}_1), \dots, \mu_N \in \mathcal{P}_1(\mathcal{X}_N)$ and cost function $f : \mathcal{X} \rightarrow \mathbb{R}$ satisfying Assumption 2.1.3, as well as N collections of functions $\mathcal{G}_1 \subseteq \mathcal{L}^1(\mathcal{X}_1, \mu_1), \dots, \mathcal{G}_N \subseteq \mathcal{L}^1(\mathcal{X}_N, \mu_N)$, we aim to solve the following relaxation of (MMOT):

$$\inf_{\mu \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})} \left\{ \int_{\mathcal{X}} f d\mu \right\}. \quad (\text{MMOT}_{\text{relax}})$$

Remark 2.2.6. *In general, the infimum in $(\text{MMOT}_{\text{relax}})$ is not necessarily attained. This is demonstrated by the following examples, where we let $N = 1$, $\mathcal{X} = \mathcal{X}_1 = \mathbb{R}_+$, and thus $\Gamma([\mu_1]_{\mathcal{G}_1}) = [\mu_1]_{\mathcal{G}_1}$. In the first example the set $[\mu_1]_{\mathcal{G}_1}$ lacks tightness, and in the second example the set $[\mu_1]_{\mathcal{G}_1}$ is tight but lacks weak closedness.*

- *Example 1: let $f(x) = \frac{2}{x+2}$, let $\mathcal{G}_1 = \{g\}$ where $g(x) = \frac{1}{x+1}$, and let $\mu_1 \in \mathcal{P}_1(\mathbb{R}_+)$ be any probability measure such that $\int_{\mathbb{R}_+} g d\mu_1 = \frac{1}{2}$. In this case, $\int_{\mathbb{R}_+} f d\nu > \frac{1}{2}$ for any $\nu \in [\mu_1]_{\mathcal{G}_1}$. However, if we let $\nu_n = \frac{n-1}{2n} \delta_0 + \frac{n+1}{2n} \delta_n$ for all $n \in \mathbb{N}$ (δ_n denotes the Dirac measure at n), then $\nu_n \in [\mu_1]_{\mathcal{G}_1}$ for all $n \in \mathbb{N}$, but $\lim_{n \rightarrow \infty} \int_{\mathbb{R}_+} f d\nu_n = \frac{1}{2}$. Hence, the infimum in $(\text{MMOT}_{\text{relax}})$ is not attained. We remark that the sequence $(\nu_n)_{n \in \mathbb{N}}$ does not converge weakly to any probability measure.*
- *Example 2: let $f(x) = \min\{x, 1\}$, let $\mathcal{G}_1 = \{g\}$ where $g(x) = x$, and let $\mu_1 \in \mathcal{P}_1(\mathbb{R}_+)$ be any probability measure such that $\int_{\mathbb{R}_+} g d\mu_1 = 1$. In this case, the only $\nu \in \mathcal{P}_1(\mathbb{R}_+)$ that satisfies $\int_{\mathbb{R}_+} f d\nu = 0$ is $\delta_0 \notin [\mu_1]_{\mathcal{G}_1}$. Hence, $\int_{\mathbb{R}_+} f d\nu > 0$ for any $\nu \in [\mu_1]_{\mathcal{G}_1}$. However, if we let $\nu_n = \frac{n-1}{n} \delta_0 + \frac{1}{n} \delta_n$ for all $n \in \mathbb{N}$, then $\nu_n \in [\mu_1]_{\mathcal{G}_1}$ for all $n \in \mathbb{N}$, but $\lim_{n \rightarrow \infty} \int_{\mathbb{R}_+} f d\nu_n = 0$. Hence, the infimum in $(\text{MMOT}_{\text{relax}})$ is not attained. Observe that here the sequence $(\nu_n)_{n \in \mathbb{N}}$ converges weakly to δ_0 , which is not in $[\mu_1]_{\mathcal{G}_1}$.*

To control the relaxation error of $(\text{MMOT}_{\text{relax}})$, we need to introduce additional assumptions on the cost function f and the marginals μ_1, \dots, μ_N besides Assumption 2.1.3. Since these assumptions depend on additional terms that affect the relaxation error, let us define the set $\mathcal{A}(L_f, D, \underline{f}_1, \bar{f}_1, \dots, \underline{f}_N, \bar{f}_N)$ as follows.

Definition 2.2.7. *Let Assumption 2.1.3 hold. For $L_f > 0$, $D \in \mathcal{B}(\mathcal{X})$, and Borel measurable functions $\underline{f}_i : \mathcal{X}_i \rightarrow \mathbb{R}$, $\bar{f}_i : \mathcal{X}_i \rightarrow \mathbb{R}$ with $\underline{f}_i \leq \bar{f}_i$ for $i = 1, \dots, N$, we say that $(\mu_1, \dots, \mu_N, f) \in \mathcal{A}(L_f, D, \underline{f}_1, \bar{f}_1, \dots, \underline{f}_N, \bar{f}_N)$ if the following conditions hold.*

- (i) $f : \mathcal{X} \rightarrow \mathbb{R}$ restricted to D is L_f -Lipschitz continuous.
- (ii) For $i = 1, \dots, N$, \underline{f}_i and \bar{f}_i are μ_i -integrable, and for all $\mathbf{x} \in \mathcal{X}$,

$$\sum_{i=1}^N \underline{f}_i \circ \pi_i(\mathbf{x}) \leq f(\mathbf{x}) \mathbb{1}_{\mathcal{X} \setminus D}(\mathbf{x}) \leq \sum_{i=1}^N \bar{f}_i \circ \pi_i(\mathbf{x}). \quad (2.8)$$

Theorem 2.2.8 below is the main result of this subsection. It states that an approximate optimizer of $(\text{MMOT}_{\text{relax}})$ can be reassembled into an approximate optimizer of (MMOT) , and that $(\text{MMOT}_{\text{relax}})$ gives a lower bound on (MMOT) where the quality of the bound depends on $L_f, D, \underline{f}_1, \bar{f}_1, \dots, \underline{f}_N, \bar{f}_N$ and $\mathcal{G}_1, \dots, \mathcal{G}_N$.

Theorem 2.2.8 (Approximation of multi-marginal optimal transport). *Let Assumption 2.1.3 hold and let $\mathcal{G}_i \subseteq \mathcal{L}^1(\mathcal{X}_i, \mu_i)$ for $i = 1, \dots, N$. Moreover, let $L_f > 0$, $D \in \mathcal{B}(\mathcal{X})$, let $(\underline{f}_i : \mathcal{X}_i \rightarrow \mathbb{R})_{i=1:N}, (\bar{f}_i : \mathcal{X}_i \rightarrow \mathbb{R})_{i=1:N}$ be Borel measurable functions such that $\underline{f}_i \in \text{span}_1(\mathcal{G}_i)$ and $\underline{f}_i \leq \bar{f}_i$ for $i = 1, \dots, N$, and*

$$(\mu_1, \dots, \mu_N, f) \in \mathcal{A}(L_f, D, \underline{f}_1, \bar{f}_1, \dots, \underline{f}_N, \bar{f}_N).$$

Furthermore, suppose that there exist $(\hat{x}_1, \dots, \hat{x}_N) \in D$, $h_1 \in \text{span}_1(\mathcal{G}_1), \dots, h_N \in \text{span}_1(\mathcal{G}_N)$ such that $d_{\mathcal{X}_i}(\hat{x}_i, \cdot) \leq h_i(\cdot)$ for $i = 1, \dots, N$. Then, the following statements hold.

- (i) Let $\hat{\mu}_i \in [\mu_i]_{\mathcal{G}_i}$ for $i = 1, \dots, N$. Then, for every $\hat{\mu} \in \Gamma(\hat{\mu}_1, \dots, \hat{\mu}_N)$ and every $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$, the following inequality holds:

$$\int_{\mathcal{X}} f \, d\tilde{\mu} - \int_{\mathcal{X}} f \, d\hat{\mu} \leq \sum_{i=1}^N \left(L_f W_1(\mu_i, \hat{\mu}_i) + \int_{\mathcal{X}_i} \bar{f}_i - \underline{f}_i \, d\hat{\mu}_i \right).$$

- (ii) The infimum in $(\text{MMOT}_{\text{relax}})$ is not equal to $-\infty$.

- (iii) For $i = 1, \dots, N$, $\bar{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i}) < \infty$.

- (iv) Let $\epsilon > 0$ and let $\tilde{\epsilon} := \epsilon + \sum_{i=1}^N \left(L_f \bar{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i}) + \int_{\mathcal{X}_i} \bar{f}_i - \underline{f}_i \, d\mu_i \right)$. Suppose that $\hat{\mu}$ is an ϵ -optimal solution of $(\text{MMOT}_{\text{relax}})$, i.e.,

$$\int_{\mathcal{X}} f \, d\hat{\mu} \leq \inf_{\mu \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} + \epsilon. \quad (2.9)$$

Then, every $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$ is an $\tilde{\epsilon}$ -optimal solution of (MMOT) , i.e.,

$$\int_{\mathcal{X}} f \, d\tilde{\mu} \leq \inf_{\mu \in \Gamma(\mu_1, \dots, \mu_N)} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} + \tilde{\epsilon}.$$

- (v) The following inequalities hold:

$$\begin{aligned} 0 &\leq \inf_{\mu \in \Gamma(\mu_1, \dots, \mu_N)} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} - \inf_{\mu \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} \\ &\leq \sum_{i=1}^N \left(L_f \bar{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i}) + \int_{\mathcal{X}_i} \bar{f}_i - \underline{f}_i \, d\mu_i \right) < \infty. \end{aligned} \quad (2.10)$$

Proof of Theorem 2.2.8. See Section 5.1. □

A special case of Theorem 2.2.8 is when f is L_f -Lipschitz continuous on \mathcal{X} for some $L_f > 0$. In this case, $(\mu_1, \dots, \mu_N, f) \in \mathcal{A}(L_f, \mathcal{X}, 0, 0, \dots, 0, 0)$ and the error terms in Theorem 2.2.8 can be simplified. The corresponding results for this case are shown in the following corollary.

Corollary 2.2.9. *Let Assumption 2.1.3 hold and let $\mathcal{G}_i \subseteq \mathcal{L}^1(\mathcal{X}_i, \mu_i)$ for $i = 1, \dots, N$. Moreover, suppose that there exist $L_f > 0$ such that f is L_f -Lipschitz continuous on \mathcal{X} . Furthermore, suppose that there exist $(\hat{x}_1, \dots, \hat{x}_N) \in \mathcal{X}$, $h_1 \in \text{span}_1(\mathcal{G}_1)$, \dots , $h_N \in \text{span}_1(\mathcal{G}_N)$ such that $d_{\mathcal{X}_i}(\hat{x}_i, \cdot) \leq h_i(\cdot)$ for $i = 1, \dots, N$. Then, the following statements hold.*

- (i) *Let $\hat{\mu}_i \in [\mu_i]_{\mathcal{G}_i}$ for $i = 1, \dots, N$. Then, for every $\hat{\mu} \in \Gamma(\hat{\mu}_1, \dots, \hat{\mu}_N)$ and every $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$, the following inequality holds:*

$$\int_{\mathcal{X}} f \, d\tilde{\mu} - \int_{\mathcal{X}} f \, d\hat{\mu} \leq \sum_{i=1}^N L_f W_1(\mu_i, \hat{\mu}_i).$$

- (ii) *The infimum in $(\text{MMOT}_{\text{relax}})$ is not equal to $-\infty$.*

- (iii) *For $i = 1, \dots, N$, $\overline{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i}) < \infty$.*

- (iv) *Let $\epsilon > 0$ and let $\tilde{\epsilon} := \epsilon + \sum_{i=1}^N L_f \overline{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i})$. Suppose that $\hat{\mu}$ is an ϵ -optimal solution of $(\text{MMOT}_{\text{relax}})$, i.e.,*

$$\int_{\mathcal{X}} f \, d\hat{\mu} \leq \inf_{\mu \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} + \epsilon.$$

Then, every $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$ is an $\tilde{\epsilon}$ -optimal solution of (MMOT) , i.e.,

$$\int_{\mathcal{X}} f \, d\tilde{\mu} \leq \inf_{\mu \in \Gamma(\mu_1, \dots, \mu_N)} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} + \tilde{\epsilon}.$$

- (v) *The following inequalities hold:*

$$0 \leq \inf_{\mu \in \Gamma(\mu_1, \dots, \mu_N)} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} - \inf_{\mu \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} \leq \sum_{i=1}^N L_f \overline{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i}) < \infty.$$

Theorem 2.2.8(iv) and Theorem 2.2.8(v) show that if one can find an ϵ -optimal solution $\hat{\mu}$ of $(\text{MMOT}_{\text{relax}})$ and construct a reassembly $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$, one will then obtain

$$\int_{\mathcal{X}} f \, d\hat{\mu} - \epsilon \leq \inf_{\mu \in \Gamma(\mu_1, \dots, \mu_N)} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} \leq \int_{\mathcal{X}} f \, d\tilde{\mu}$$

with $\int_{\mathcal{X}} f \, d\tilde{\mu} - (\int_{\mathcal{X}} f \, d\hat{\mu} - \epsilon) \leq \epsilon + \sum_{i=1}^N \left(L_f \overline{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i}) + \int_{\mathcal{X}_i} \bar{f}_i - \underline{f}_i \, d\mu_i \right)$, i.e., lower and upper bounds on (MMOT) such that the difference between the lower and upper bounds is controlled.

An observation from Theorem 2.2.8 is that if one can find increasingly better choices of L_f , D , \underline{f}_1 , $\bar{f}_1, \dots, \underline{f}_N, \bar{f}_N$, and $\mathcal{G}_1, \dots, \mathcal{G}_N$ such that $\sum_{i=1}^N \left(L_f \overline{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i}) + \int_{\mathcal{X}_i} \bar{f}_i - \underline{f}_i \, d\mu_i \right)$ shrinks to 0, then one can obtain an optimizer of (MMOT) in the limit. This is detailed in the next theorem. We will discuss how one can control $\sum_{i=1}^N \left(L_f \overline{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i}) + \int_{\mathcal{X}_i} \bar{f}_i - \underline{f}_i \, d\mu_i \right)$ to be arbitrarily close to 0 in Section 3.2.

Theorem 2.2.10 (Optimizers of multi-marginal optimal transport). *Let Assumption 2.1.3 hold and let $(L_f^{(l)}, D^{(l)}, \underline{f}_1^{(l)}, \bar{f}_1^{(l)}, \dots, \underline{f}_N^{(l)}, \bar{f}_N^{(l)}, \mathcal{G}_1^{(l)}, \dots, \mathcal{G}_N^{(l)})_{l \in \mathbb{N}}$ be such that:*

- (i) *for each $l \in \mathbb{N}$, $(\mu_1, \dots, \mu_N, f) \in \mathcal{A}(L_f^{(l)}, D^{(l)}, \underline{f}_1^{(l)}, \bar{f}_1^{(l)}, \dots, \underline{f}_N^{(l)}, \bar{f}_N^{(l)})$;*
(ii) *for each $l \in \mathbb{N}$ and for $i = 1, \dots, N$, $\underline{f}_i^{(l)} \in \text{span}_1(\mathcal{G}_i^{(l)}) \subseteq \mathcal{L}^1(\mathcal{X}_i, \mu_i)$;*
(iii) *for each $l \in \mathbb{N}$, there exist $(\hat{x}_1, \dots, \hat{x}_N) \in D^{(l)}$, $h_1 \in \text{span}_1(\mathcal{G}_1^{(l)})$, \dots , $h_N \in \text{span}_1(\mathcal{G}_N^{(l)})$ such that $d_{\mathcal{X}_i}(\hat{x}_i, \cdot) \leq h_i(\cdot)$ for $i = 1, \dots, N$;*
(iv) $\lim_{l \rightarrow \infty} \sum_{i=1}^N \left(L_f^{(l)} \overline{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i^{(l)}}) + \int_{\mathcal{X}_i} \bar{f}_i^{(l)} - \underline{f}_i^{(l)} \, d\mu_i \right) = 0$.

Let $(\epsilon^{(l)})_{l \in \mathbb{N}}$ be a sequence of positive real numbers such that $\lim_{l \rightarrow \infty} \epsilon^{(l)} = 0$. For each $l \in \mathbb{N}$, let $\hat{\mu}^{(l)}$ be an $\epsilon^{(l)}$ -optimal solution of $\inf_{\mu \in \Gamma([\mu_1]_{\mathcal{G}_1^{(l)}}, \dots, [\mu_N]_{\mathcal{G}_N^{(l)}})} \left\{ \int_{\mathcal{X}} f \, d\mu \right\}$, i.e.,

$$\int_{\mathcal{X}} f \, d\hat{\mu}^{(l)} \leq \inf_{\mu \in \Gamma([\mu_1]_{\mathcal{G}_1^{(l)}}, \dots, [\mu_N]_{\mathcal{G}_N^{(l)}})} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} + \epsilon^{(l)}, \quad (2.11)$$

and let $\tilde{\mu}^{(l)} \in R(\hat{\mu}^{(l)}; \mu_1, \dots, \mu_N)$ be a reassembly of $\hat{\mu}^{(l)}$ with marginals μ_1, \dots, μ_N . Then, $(\tilde{\mu}^{(l)})_{l \in \mathbb{N}}$ has at least one accumulation point in $(\mathcal{P}_1(\mathcal{X}), W_1)$ and every accumulation point is an optimizer of (MMOT).

Proof of Theorem 2.2.10. See Section 5.1. □

2.3. Duality results. In Section 2.2, we derived a relaxation of (MMOT) given by (MMOT_{relax}). This subsection is dedicated to the analysis of the dual optimization problem of (MMOT_{relax}), which is a linear semi-infinite programming (LSIP) problem. This LSIP formulation allows the use of state-of-the-art numerical algorithms to efficiently solve some instances of the MMOT problem.

Let Assumption 2.1.3 hold, let the moment set $[\mu_i]_{\mathcal{G}_i}$ be characterized by finitely many functions $\mathcal{G}_i := \{g_{i,1}, \dots, g_{i,m_i}\} \subset \mathcal{L}^1(\mathcal{X}_i, \mu_i)$ with $m_i \in \mathbb{N}$, for $i = 1, \dots, N$, and let $m := \sum_{i=1}^N m_i$. For notational simplicity, let $\mathbf{g} : \mathcal{X} \rightarrow \mathbb{R}^m$ be the vector-valued function given by

$$(x_1, \dots, x_N) \mapsto \mathbf{g}(x_1, \dots, x_N) = \left(g_{1,1}(x_1), \dots, g_{1,m_1}(x_1), \dots, g_{N,1}(x_N), \dots, g_{N,m_N}(x_N) \right)^\top. \quad (2.12)$$

For every $\mathbf{y} = (y_{1,1}, \dots, y_{1,m_1}, \dots, y_{N,1}, \dots, y_{N,m_N})^\top \in \mathbb{R}^m$, let $\langle \mathbf{y}, \mathbf{g} \rangle : \mathcal{X} \rightarrow \mathbb{R}$ denote the function given by

$$(x_1, \dots, x_N) \mapsto \langle \mathbf{y}, \mathbf{g}(x_1, \dots, x_N) \rangle := \sum_{i=1}^N \sum_{j=1}^{m_i} y_{i,j} g_{i,j}(x_i).$$

Moreover, let

$$\mathbf{v} := \left(\int_{\mathcal{X}_1} g_{1,1} \, d\mu_1, \dots, \int_{\mathcal{X}_1} g_{1,m_1} \, d\mu_1, \dots, \int_{\mathcal{X}_N} g_{N,1} \, d\mu_N, \dots, \int_{\mathcal{X}_N} g_{N,m_N} \, d\mu_N \right)^\top \in \mathbb{R}^m. \quad (2.13)$$

Then, the dual optimization problem of (MMOT_{relax}) is an LSIP problem given by

$$\begin{aligned} & \underset{y_0, \mathbf{y}}{\text{maximize}} && y_0 + \langle \mathbf{y}, \mathbf{v} \rangle \\ & \text{subject to} && y_0 + \langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle \leq f(\mathbf{x}) \quad \forall \mathbf{x} \in \mathcal{X}, \\ & && y_0 \in \mathbb{R}, \mathbf{y} \in \mathbb{R}^m. \end{aligned} \quad (\text{MMOT}_{\text{relax}}^*)$$

Following the strong duality results in the theory of linear semi-infinite optimization (see, e.g., [35]), we can derive the following strong duality tailored to (MMOT_{relax}) and (MMOT_{relax}^{*}).

Theorem 2.3.1 (Strong duality). *Let Assumption 2.1.3 hold. Let $\mathcal{G}_i = \{g_{i,1}, \dots, g_{i,m_i}\} \subset \mathcal{L}^1(\mathcal{X}_i, \mu_i)$ where $m_i \in \mathbb{N}$, for $i = 1, \dots, N$, let $m := \sum_{i=1}^N m_i$, and let $\mathbf{g}(\cdot)$ and \mathbf{v} be given as in (2.12) and (2.13). Then,*

(i) *the following weak duality between (MMOT_{relax}^{*}) and (MMOT_{relax}) holds:*

$$\sup_{y_0 \in \mathbb{R}, \mathbf{y} \in \mathbb{R}^m} \left\{ y_0 + \langle \mathbf{y}, \mathbf{v} \rangle : y_0 + \langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle \leq f(\mathbf{x}) \quad \forall \mathbf{x} \in \mathcal{X} \right\} \leq \inf_{\mu \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})} \left\{ \int_{\mathcal{X}} f \, d\mu \right\}. \quad (2.14)$$

Moreover, suppose that the left-hand side of (2.14) is not¹ $-\infty$. Let the sets $K \subseteq \mathbb{R}^m$ and $C \subset \mathbb{R}^{m+2}$ be defined as follows:

$$K := \text{conv} \left(\{ \mathbf{g}(\mathbf{x}) : \mathbf{x} \in \mathcal{X} \} \right), \quad (2.15)$$

$$C := \text{cone} \left(\{ (1, \mathbf{g}(\mathbf{x})^\top, f(\mathbf{x}))^\top : \mathbf{x} \in \mathcal{X} \} \right), \quad (2.16)$$

¹that is, the corresponding maximization problem is feasible.

and let the conditions (SD1), (SD2), and (SD3) be defined as follows:

(SD1) $v \in \text{relint}(K)$;

(SD2) $v \in \text{int}(K)$;

(SD3) C is closed.

Then, the following statements hold.

(ii) If either (SD1) or (SD3) holds, then the following strong duality between $(\text{MMOT}_{\text{relax}}^*)$ and $(\text{MMOT}_{\text{relax}})$ holds:

$$\sup_{y_0 \in \mathbb{R}, \mathbf{y} \in \mathbb{R}^m} \left\{ y_0 + \langle \mathbf{y}, \mathbf{v} \rangle : y_0 + \langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle \leq f(\mathbf{x}) \quad \forall \mathbf{x} \in \mathcal{X} \right\} = \inf_{\mu \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})} \left\{ \int_{\mathcal{X}} f \, d\mu \right\}. \quad (2.17)$$

(iii) If (SD1) holds, then the set of optimizers of $(\text{MMOT}_{\text{relax}}^*)$ is non-empty.

(iv) If (SD2) holds, then the set of optimizers of $(\text{MMOT}_{\text{relax}}^*)$ is bounded.

Proof of Theorem 2.3.1. See Section 5.2. □

Remark 2.3.2. One can guarantee that the LSIP problem $(\text{MMOT}_{\text{relax}}^*)$ has a non-empty feasible set (and thus the left-hand side of (2.14) is not $-\infty$) under fairly general assumptions. For example, under the assumptions of Theorem 2.2.8, the LSIP problem $(\text{MMOT}_{\text{relax}}^*)$ has a feasible solution by (5.4) in the proof of Theorem 2.2.8(ii) (see Section 5.1).

The next proposition presents sufficient conditions under which the conditions (SD1), (SD2), and (SD3) in Theorem 2.3.1 hold.

Proposition 2.3.3. Let Assumption 2.1.3 hold. For $i = 1, \dots, N$, let $\mathcal{G}_i = \{g_{i,1}, \dots, g_{i,m_i}\} \subset \mathcal{L}^1(\mathcal{X}_i, \mu_i)$ where $m_i \in \mathbb{N}$. Let $m := \sum_{i=1}^N m_i$. Then, the following statements hold.

- (i) For $i = 1, \dots, N$, suppose that² $\text{supp}(\mu_i) = \mathcal{X}_i$ and \mathcal{G}_i contains only continuous functions. Then, the condition (SD1) in Theorem 2.3.1 holds.
- (ii) For $i = 1, \dots, N$, let $\mathcal{X}_i \ni x \mapsto \mathbf{g}_i(x) := (g_{i,1}(x), \dots, g_{i,m_i}(x))^T \in \mathbb{R}^{m_i}$. Suppose that in addition to the assumptions in statement (i), for $i = 1, \dots, N$, there exist $m_i + 1$ points $x_{i,1}, \dots, x_{i,m_i+1} \in \mathcal{X}_i$ such that the points $\mathbf{g}_i(x_{i,1}), \dots, \mathbf{g}_i(x_{i,m_i+1}) \in \mathbb{R}^{m_i}$ are affinely independent. Then, the condition (SD2) in Theorem 2.3.1 holds.
- (iii) For $i = 1, \dots, N$, suppose that \mathcal{X}_i is compact, \mathcal{G}_i contains only continuous functions, and f is continuous. Then, the condition (SD3) in Theorem 2.3.1 holds.

Proof of Proposition 2.3.3. See Section 5.2. □

3. EXPLICIT CONSTRUCTION OF REASSEMBLIES AND MOMENT SETS

In Section 2, we have developed the theoretical machinery to approximate a multi-marginal optimal transport problems (MMOT) by a relaxed problem $(\text{MMOT}_{\text{relax}})$ via *reassembly* and *moment sets*, as well as the dual formulation of the resulting problem into an LSIP problem $(\text{MMOT}_{\text{relax}}^*)$. In this section, we address the following practical questions from Section 2.

- For given $\hat{\mu} \in \mathcal{P}_1(\mathcal{X})$, $\mu_1 \in \mathcal{P}_1(\mathcal{X}_1), \dots, \mu_N \in \mathcal{P}_1(\mathcal{X}_N)$, how can one construct a reassembly of $\hat{\mu}$ with the marginals μ_1, \dots, μ_N , i.e., $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$? This is discussed in Section 3.1.
- For a Polish space $(\mathcal{Y}, d_{\mathcal{Y}})$ and a given $\mu \in \mathcal{P}_1(\mathcal{Y})$, how can one construct a finite set $\mathcal{G} \subset \mathcal{L}^1(\mathcal{Y}, \mu)$ containing only continuous functions (see Proposition 2.3.3) to control $\overline{W}_{1,\mu}([\mu]_{\mathcal{G}})$? This is discussed in Section 3.2.

Specifically, in Section 3.1, we construct a reassembly in the *semi-discrete* case, i.e., when $\hat{\mu}$ is a finitely supported discrete measure and μ_1, \dots, μ_N are absolutely continuous with respect to the Lebesgue measure on a Euclidean space, by adapting existing results from the field of computational geometry. In Section 3.2, we show that when \mathcal{Y} is a closed subset of a Euclidean space, one can explicitly construct finitely many continuous functions $\mathcal{G} \subset \mathcal{L}^1(\mathcal{Y}, \mu)$ for a given $\mu \in \mathcal{P}_1(\mathcal{Y})$ such that $\overline{W}_{1,\mu}([\mu]_{\mathcal{G}})$ can be controlled to be arbitrarily close to 0. Moreover, when \mathcal{Y} is a compact subset of a Euclidean space, we prove a stronger result, which states that one can explicitly construct finitely many continuous functions \mathcal{G} on \mathcal{Y} such that the supremum W_1 “diameter” among all moment sets

² $\text{supp}(\mu_i)$ denotes the support of μ_i

$\{[\mu]_{\mathcal{G}} : \mu \in \mathcal{P}_1(\mathcal{X})\}$, i.e., $\sup \{W_1(\mu, \nu) : \mu \overset{\mathcal{G}}{\approx} \nu\}$, can be uniformly controlled to be arbitrarily close to 0.

3.1. Reassembly in the semi-discrete case via Laguerre diagrams. In this subsection, let us consider the case where for $i = 1, \dots, N$, \mathcal{X}_i is a closed subset of a Euclidean space \mathbb{R}^{m_i} for some $m_i \in \mathbb{N}$. We characterize reassembly in the *semi-discrete* setting, that is, when $\hat{\mu} \in \mathcal{P}_1(\mathcal{X})$ is a finitely supported measure and for $i = 1, \dots, N$, $\mu_i \in \mathcal{P}_1(\mathcal{X}_i)$ is absolutely continuous with respect to the Lebesgue measure on \mathbb{R}^{m_i} . Optimal couplings in the *semi-discrete* setting have been previously studied in the field of computational geometry; see, e.g., [4, 34, 42, 43] and [49, Chapter 5] for related discussions. However, these studies only focus on optimal couplings under the *squared* Euclidean distance, which is not directly applicable to our setting since we are interested in finding an optimal coupling where the cost function is a general norm on the underlying space. Therefore, in Proposition 3.1.2, we provide results about optimal couplings and reassembly under the assumption that the cost function is induced by a norm under which the closed unit ball is strictly convex.

Before presenting the construction, let us first introduce the following lemma which states that we only need to consider the special case where $\mathcal{X}_i = \mathbb{R}^{m_i}$ for $i = 1, \dots, N$ without loss of generality.

Lemma 3.1.1. *Let Assumption 2.1.2 hold. Suppose that for $i = 1, \dots, N$, $m_i \in \mathbb{N}$, $\mathcal{X}_i \subseteq \mathbb{R}^{m_i}$ is closed, and $d_{\mathcal{X}_i}$ is induced by a norm $\|\cdot\|$ on \mathbb{R}^{m_i} . Let $m := \sum_{i=1}^N m_i$. For $i = 1, \dots, N$, let \mathbb{R}^{m_i} be equipped with the metric induced by the norm $\|\cdot\|$ and let $\mu_i^\dagger \in \mathcal{P}_1(\mathbb{R}^{m_i})$ be defined by $\mu_i^\dagger(E) := \mu_i(E \cap \mathcal{X}_i)$ for all $E \in \mathcal{B}(\mathbb{R}^{m_i})$. Similarly, for any $\mu \in \mathcal{P}_1(\mathcal{X})$, let $\mu^\dagger \in \mathcal{P}_1(\mathbb{R}^m)$ be defined by $\mu^\dagger(E) := \mu(E \cap \mathcal{X})$ for all $E \in \mathcal{B}(\mathbb{R}^m)$. Then, for any $\hat{\mu}, \tilde{\mu} \in \mathcal{P}_1(\mathcal{X})$, $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$ if and only if $\tilde{\mu}^\dagger \in R(\hat{\mu}^\dagger; \mu_1^\dagger, \dots, \mu_N^\dagger)$.*

Proof of Lemma 3.1.1. See Section 5.3. □

By Lemma 3.1.1, to construct a reassembly when \mathcal{X}_i is a closed subset of \mathbb{R}^{m_i} for $i = 1, \dots, N$, one can first extend $\hat{\mu} \in \mathcal{P}_1(\mathcal{X})$, $\mu_1 \in \mathcal{P}_1(\mathcal{X}_1), \dots, \mu_N \in \mathcal{P}_1(\mathcal{X}_N)$ to $\hat{\mu}^\dagger \in \mathcal{P}_1(\mathbb{R}^m)$ (where $m := \sum_{i=1}^N m_i$), $\mu_1^\dagger \in \mathcal{P}_1(\mathbb{R}^{m_1}), \dots, \mu_N^\dagger \in \mathcal{P}_1(\mathbb{R}^{m_N})$ and construct a reassembly $\tilde{\mu}^\dagger \in R(\hat{\mu}^\dagger; \mu_1^\dagger, \dots, \mu_N^\dagger)$. This can be done via the construction in Proposition 3.1.2 below under some additional assumptions. Subsequently, one can define $\tilde{\mu} \in \mathcal{P}_1(\mathcal{X})$ by $\tilde{\mu}(E) := \tilde{\mu}^\dagger(E)$ for all $E \in \mathcal{B}(\mathcal{X})$ and get $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$.

Proposition 3.1.2 (Reassembly in the semi-discrete case). *Let Assumption 2.1.2 hold. Suppose that for $i = 1, \dots, N$, $\mathcal{X}_i = \mathbb{R}^{m_i}$ for $m_i \in \mathbb{N}$ and that $d_{\mathcal{X}_i}$ is induced by a norm $\|\cdot\|$ on \mathbb{R}^{m_i} under which the closed unit ball $\{\mathbf{x} \in \mathbb{R}^{m_i} : \|\mathbf{x}\| \leq 1\}$ is a strictly convex set³. Moreover, suppose that for $i = 1, \dots, N$, $\mu_i \in \mathcal{P}_1(\mathcal{X}_i)$ is absolutely continuous with respect to the Lebesgue measure on \mathbb{R}^{m_i} . Let $\hat{\mu} \in \mathcal{P}_1(\mathcal{X})$ be a finitely supported measure with marginals $\hat{\mu}_1, \dots, \hat{\mu}_N$. For $i = 1, \dots, N$, let $\hat{\mu}_i$ be represented as $\hat{\mu}_i = \sum_{j=1}^{J_i} \alpha_{i,j} \delta_{\mathbf{x}_{i,j}}$ for $J_i \in \mathbb{N}$ distinct points $(\mathbf{x}_{i,j})_{j=1:J_i} \subset \mathcal{X}_i$, and positive real numbers $(\alpha_{i,j})_{j=1:J_i}$ such that $\sum_{j=1}^{J_i} \alpha_{i,j} = 1$. Then, the following statements hold.*

(i) For $i = 1, \dots, N$, there exist $(\phi_{i,j}^*)_{j=1:J_i} \subset \mathbb{R}$ that solve the following concave maximization problem:

$$\sup_{\phi_{i,1}, \dots, \phi_{i,J_i} \in \mathbb{R}} \left\{ \sum_{j=1}^{J_i} \phi_{i,j} \alpha_{i,j} - \int_{\mathbb{R}^{m_i}} \max_{1 \leq j \leq J_i} \{ \phi_{i,j} - d_{\mathcal{X}_i}(\mathbf{x}_{i,j}, \mathbf{z}) \} \mu_i(d\mathbf{z}) \right\}. \quad (3.1)$$

(ii) For $i = 1, \dots, N$, let $(\phi_{i,j}^*)_{j=1:J_i} \subset \mathbb{R}$ solve the problem (3.1). For $i = 1, \dots, N$, $j = 1, \dots, J_i$, let

$$V_{i,j} := \left\{ \mathbf{z} \in \mathbb{R}^{m_i} : \phi_{i,j}^* - d_{\mathcal{X}_i}(\mathbf{x}_{i,j}, \mathbf{z}) = \max_{1 \leq k \leq J_i} \{ \phi_{i,k}^* - d_{\mathcal{X}_i}(\mathbf{x}_{i,k}, \mathbf{z}) \} \right\}. \quad (3.2)$$

Then, $\mu_i(V_{i,j}) = \alpha_{i,j}$.

³for example, under the p -norm, this condition is satisfied for all $1 < p < \infty$ (by the Minkowski inequality), but fails when $p = 1$ or $p = \infty$.

(iii) Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space and let $(X_1, \dots, X_N) : \Omega \rightarrow \mathcal{X}$ be a random vector with law $\hat{\mu}$. Let the sets $(V_{i,j})_{j=1:J_i, i=1:N}$ be given by (3.2). For $i = 1, \dots, N$, let $Y_i : \Omega \rightarrow \mathcal{X}_i$ be a random vector such that the distribution of Y_i conditional on X_i is specified as follows:

$$\mathbb{P}[Y_i \in E | X_i = \mathbf{x}_{i,j}] = \frac{\mu_i(E \cap V_{i,j})}{\mu_i(V_{i,j})} \quad \forall E \in \mathcal{B}(\mathcal{X}_i) \forall 1 \leq j \leq J_i. \quad (3.3)$$

Let $\tilde{\mu}$ be the law of (Y_1, \dots, Y_N) . Then, $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$.

Proof of Proposition 3.1.2. See Section 5.3. □

Remark 3.1.3. We would like to remark that the assumption that $\hat{\mu}$ has finite support in the statement of Proposition 3.1.2 is relevant in practice, since the numerical method that we use to solve (MMOT_{relax}) in Section 4.1 returns an approximate optimizer of (MMOT_{relax}) that has a finite support (see Algorithm 1 and Theorem 4.1.3).

3.2. Construction of moment sets on a Euclidean space. In this subsection, we consider the case where \mathcal{Y} is a closed subset of a Euclidean space and $\mu \in \mathcal{P}_1(\mathcal{Y})$. We discuss the problem of constructing a finite collection of continuous functions $\mathcal{G} \subset \mathcal{L}^1(\mathcal{Y}, \mu)$ that characterizes a moment set $[\mu]_{\mathcal{H}}$ such that $\overline{W}_{1,\mu}([\mu]_{\mathcal{G}})$ can be controlled. Let us first recall the notions of faces, extreme points, and extreme directions of convex sets from [52, Section 18].

Definition 3.2.1 (Faces, extreme points, and extreme directions of convex sets, see [52, Section 18]). Let $m \in \mathbb{N}$. A convex subset C' of a convex set $C \subseteq \mathbb{R}^m$ is called a *face* of C if for all $0 < \lambda < 1$ and all $\mathbf{x}_1, \mathbf{x}_2 \in C$,

$$\lambda \mathbf{x}_1 + (1 - \lambda) \mathbf{x}_2 \in C' \implies \mathbf{x}_1 \in C', \mathbf{x}_2 \in C'.$$

In particular, every face of a polyhedron is also a polyhedron by [52, Theorem 19.1]. A point \mathbf{x} in a convex set $C \subseteq \mathbb{R}^m$ is called an *extreme point* of C if it is a face of C . A vector $\mathbf{z} \in \mathbb{R}^m$ is called an *extreme direction* of a convex set $C \subseteq \mathbb{R}^m$ if there exists $\mathbf{x} \in C$ such that $\{\mathbf{x} + \lambda \mathbf{z} : \lambda \geq 0\}$ is a face of C .

Let us now introduce the following notions of polyhedral cover and interpolation function basis.

Definition 3.2.2 (Polyhedral cover). Let $m \in \mathbb{N}$, let \mathbb{R}^m be equipped with a norm $\|\cdot\|$, and let $\mathcal{Y} \subseteq \mathbb{R}^m$. A collection \mathfrak{C} of subsets of \mathbb{R}^m is called a *polyhedral cover* of \mathcal{Y} if:

- (i) $|\mathfrak{C}| < \infty$ and every $C \in \mathfrak{C}$ is a polyhedron which has at least one extreme point;
- (ii) $\bigcup_{C \in \mathfrak{C}} C \supseteq \mathcal{Y}$;
- (iii) if $C_1, C_2 \in \mathfrak{C}$ and $C_1 \cap C_2 \neq \emptyset$, then $C_1 \cap C_2$ is a face of both C_1 and C_2 .

For a polyhedron $C \subset \mathbb{R}^m$ that has at least one extreme point, let $V(C) \subset \mathbb{R}^m$ denote the finite set of extreme points of C and let $D(C) \subset \mathbb{R}^m$ denote the finite (possibly empty) set of extreme directions of C . Let $\mathfrak{F}(\mathfrak{C}) := \{F \subset \mathbb{R}^m : F \text{ is a non-empty face of } C, C \in \mathfrak{C}\}$ denote the collection of non-empty faces in the polyhedral cover \mathfrak{C} (note that every $F \in \mathfrak{F}(\mathfrak{C})$ is also a polyhedron), let $V(\mathfrak{C}) := \bigcup_{C \in \mathfrak{C}} V(C)$ denote the set of extreme points in the polyhedral cover, and let $D(\mathfrak{C}) := \bigcup_{C \in \mathfrak{C}} D(C)$ denote the (possibly empty) set of extreme directions in the polyhedral cover. Note that if $F \subseteq C$ is a face of some $C \in \mathfrak{C}$, then $V(F) \subseteq V(C)$ and $D(F) \subseteq D(C)$. Let $\eta(\mathfrak{C})$ denote the mesh size of a polyhedral cover \mathfrak{C} given by

$$\eta(\mathfrak{C}) := \max_{C \in \mathfrak{C}} \max_{\mathbf{v}, \mathbf{v}' \in V(C)} \{\|\mathbf{v} - \mathbf{v}'\|\}. \quad (3.4)$$

Definition 3.2.3 (Simplicial cover). Let $m \in \mathbb{N}$, let \mathbb{R}^m be equipped with a norm $\|\cdot\|$, and let $\mathcal{Y} \subseteq \mathbb{R}^m$ be bounded. A collection \mathfrak{C} of subsets of \mathbb{R}^m is called a *simplicial cover* of \mathcal{Y} if \mathfrak{C} is a polyhedral cover of \mathcal{Y} and every $C \in \mathfrak{C}$ is an m -simplex (i.e., the convex hull of $m + 1$ affinely independent points).

Definition 3.2.4 (Interpolation function basis). Let $m \in \mathbb{N}$, let \mathbb{R}^m be equipped with a norm $\|\cdot\|$, and let $\mathcal{Y} \subseteq \mathbb{R}^m$. Let \mathfrak{C} be a polyhedral cover of \mathcal{Y} . A set of real-valued functions \mathcal{G} on $\bigcup_{C \in \mathfrak{C}} C$ is called an *interpolation function basis* associated with \mathfrak{C} if there exist continuous functions $\{g_{\mathbf{v}} : \mathbf{v} \in V(\mathfrak{C})\} \subset \text{span}_1(\mathcal{G})$ and $\{\bar{g}_{\mathbf{u}} : \mathbf{u} \in D(\mathfrak{C})\} \subset \text{span}_1(\mathcal{G})$ with the properties (IFB1)–(IFB6) below.

(IFB1) For every $\mathbf{v} \in V(\mathfrak{C})$ and every $\mathbf{x} \in \bigcup_{C \in \mathfrak{C}} C$, $g_{\mathbf{v}}(\mathbf{x}) \geq 0$.

- (IFB2) For every pair of $\mathbf{v}, \mathbf{v}' \in V(\mathfrak{C})$, $g_{\mathbf{v}}(\mathbf{v}') = \mathbb{1}_{\{\mathbf{v}=\mathbf{v}'\}}$.
- (IFB3) For every $F \in \mathfrak{F}(\mathfrak{C})$ and every $\mathbf{x} \in F$, $\sum_{\mathbf{v} \in V(F)} g_{\mathbf{v}}(\mathbf{x}) = 1$.
- (IFB4) For every $F \in \mathfrak{F}(\mathfrak{C})$, every $\mathbf{x} \in F$, and every $\mathbf{v} \in V(\mathfrak{C}) \setminus V(F)$, $g_{\mathbf{v}}(\mathbf{x}) = 0$.
- (IFB5) For every $\mathbf{u} \in D(\mathfrak{C})$ and every $\mathbf{x} \in \bigcup_{C \in \mathfrak{C}} C$, $\bar{g}_{\mathbf{u}}(\mathbf{x}) \geq 0$.
- (IFB6) For every $F \in \mathfrak{F}(\mathfrak{C})$ such that $D(F) \neq \emptyset$ and every $\mathbf{x} \in F$,

$$\min_{\mathbf{y} \in \text{conv}(V(F))} \{\|\mathbf{x} - \mathbf{y}\|\} \leq \sum_{\mathbf{u} \in D(F)} \bar{g}_{\mathbf{u}}(\mathbf{x}).$$

The definition of interpolation function basis can be interpreted as follows. Let us consider a polyhedral cover \mathfrak{C} of \mathcal{Y} and its associated interpolation function basis \mathcal{G} . By the property (IFB1), each member of $\{g_{\mathbf{v}} : \mathbf{v} \in V(\mathfrak{C})\} \subset \text{span}_1(\mathcal{G})$ is a non-negative basis function associated with an extreme point $\mathbf{v} \in V(\mathfrak{C})$. By the property (IFB2), the functions $\{g_{\mathbf{v}} : \mathbf{v} \in V(\mathfrak{C})\}$ are “orthogonal” in the sense that the function $g_{\mathbf{v}}(\cdot)$ is only “in charge of” a single extreme point \mathbf{v} , and $g_{\mathbf{v}}(\mathbf{v}') = 0$ for all $\mathbf{v}' \in V(\mathfrak{C}) \setminus \{\mathbf{v}\}$. The property (IFB3) requires that the functions $\{g_{\mathbf{v}} : \mathbf{v} \in V(\mathfrak{C})\}$ interpolate “nicely” on each face $F \in \mathfrak{F}(\mathfrak{C})$, in the sense that for each face $F \in \mathfrak{F}(\mathfrak{C})$, the function $\mathbf{x} \mapsto \sum_{\mathbf{v} \in V(F)} g_{\mathbf{v}}(\mathbf{x})$ is constant on F . The property (IFB4) requires $g_{\mathbf{v}}(\cdot)$ to be “local” to \mathbf{v} , in the sense that it can only be non-zero in the faces “adjacent to” the extreme point \mathbf{v} , i.e., $\{F \in \mathfrak{F}(\mathfrak{C}) : \mathbf{v} \in V(F)\}$. Similar to $\{g_{\mathbf{v}} : \mathbf{v} \in V(\mathfrak{C})\}$, by the property (IFB5), each member of $\{\bar{g}_{\mathbf{u}} : \mathbf{u} \in D(\mathfrak{C})\} \subset \text{span}_1(\mathcal{G})$ is a non-negative basis function associated with an extreme direction $\mathbf{u} \in D(\mathfrak{C})$. As required by the property (IFB6), for an unbounded face $F \in \mathfrak{F}(\mathfrak{C})$ with $D(F) \neq \emptyset$, the functions $\{\bar{g}_{\mathbf{u}} : \mathbf{u} \in D(F)\}$ control the distance traveled when transporting a point $\mathbf{x} \in F$ to the bounded set $\text{conv}(V(F))$. Informally speaking, the functions $\{\bar{g}_{\mathbf{u}} : \mathbf{u} \in D(\mathfrak{C})\}$ are used to control the rate at which probability mass can “escape to infinity” in each possible direction $\mathbf{u} \in D(\mathfrak{C})$.

Now, let us demonstrate an explicit construction of a simplicial cover. Let $m \in \mathbb{N}$ and let \mathbb{R}^m be equipped with a norm $\|\cdot\|$. For a bounded set $\mathcal{Y} \subseteq \mathbb{R}^m$ and for any $\epsilon > 0$, a simplicial cover \mathfrak{C} of \mathcal{Y} with mesh size $\eta(\mathfrak{C}) < \epsilon$ can be constructed via the following process.

- Step 1: let C_0 be an m -simplex such that $C_0 \supseteq \mathcal{Y}$, and let $\mathfrak{C} \leftarrow \{C_0\}$.
- Step 2: repeat the following steps until $\eta(\mathfrak{C}) < \epsilon$.
 - Step 2a: Find a longest edge $E_{\mathbf{v}, \mathbf{w}}$ in $\mathfrak{F}(\mathfrak{C})$, where an edge $E_{\mathbf{v}, \mathbf{w}} := \{\lambda \mathbf{v} + (1 - \lambda) \mathbf{w} : 0 \leq \lambda \leq 1\}$ is a line segment between two extreme points $\mathbf{v}, \mathbf{w} \in V(C)$ for some $C \in \mathfrak{C}$.
 - Step 2b: For every $C \in \mathfrak{C}$ which has $E_{\mathbf{v}, \mathbf{w}}$ as a face, bisect the simplex C at the midpoint of the edge $E_{\mathbf{v}, \mathbf{w}}$, i.e.,

$$\mathfrak{C} \leftarrow (\mathfrak{C} \setminus C) \cup \left\{ \text{conv}\left([V(C) \setminus \{\mathbf{v}\}] \cup \left\{\frac{\mathbf{v}+\mathbf{w}}{2}\right\}\right), \text{conv}\left([V(C) \setminus \{\mathbf{w}\}] \cup \left\{\frac{\mathbf{v}+\mathbf{w}}{2}\right\}\right) \right\}.$$

Indeed, since there are always only finitely many edges in a simplicial cover, this construction process will terminate and the resulting \mathfrak{C} is a simplicial cover of \mathcal{Y} with mesh size $\eta(\mathfrak{C}) < \epsilon$. Proposition 3.2.5 shows how one can construct an interpolation function basis associated with a given simplicial cover.

Proposition 3.2.5 (Interpolation function basis associated with a simplicial cover). *Let $m \in \mathbb{N}$, let \mathbb{R}^m be equipped with a norm $\|\cdot\|$, and let $\mathcal{Y} \subseteq \mathbb{R}^m$ be bounded. Let \mathfrak{C} be a simplicial cover of \mathcal{Y} . Then, the following statements hold.*

- (i) The sets in $\{\text{relint}(F) : F \in \mathfrak{F}(\mathfrak{C})\}$ are pairwise disjoint and $\bigcup_{F \in \mathfrak{F}(\mathfrak{C})} \text{relint}(F) = \bigcup_{C \in \mathfrak{C}} C$.
- (ii) For every fixed face $F \in \mathfrak{F}(\mathfrak{C})$, every $\mathbf{x} \in \text{relint}(F)$ can be uniquely represented as $\mathbf{x} = \sum_{\mathbf{w} \in V(F)} \lambda_{F, \mathbf{w}}(\mathbf{x}) \mathbf{w}$ where $\sum_{\mathbf{w} \in V(F)} \lambda_{F, \mathbf{w}}(\mathbf{x}) = 1$ and $\lambda_{F, \mathbf{w}}(\mathbf{x}) > 0$ for all $\mathbf{w} \in V(F)$.
- (iii) For every $\mathbf{v} \in V(\mathfrak{C})$, let $g_{\mathbf{v}} : \bigcup_{C \in \mathfrak{C}} C \rightarrow \mathbb{R}$ be defined as follows⁴:

$$g_{\mathbf{v}}(\mathbf{x}) := \sum_{\mathbf{w} \in V(F)} \lambda_{F, \mathbf{w}}(\mathbf{x}) \mathbb{1}_{\{\mathbf{w}=\mathbf{v}\}} \quad \forall \mathbf{x} \in \text{relint}(F), \quad (3.5)$$

where $\mathbf{x} = \sum_{\mathbf{w} \in V(F)} \lambda_{F, \mathbf{w}}(\mathbf{x}) \mathbf{w}$ as in statement (ii) and $F \in \mathfrak{F}(\mathfrak{C})$. Then, $\{g_{\mathbf{v}} : \mathbf{v} \in V(\mathfrak{C})\}$ is an interpolation function basis associated with \mathfrak{C} .

Proof of Proposition 3.2.5. See Section 5.4. □

⁴Note that $g_{\mathbf{v}}(\mathbf{x})$ is well-defined for every $\mathbf{x} \in \bigcup_{C \in \mathfrak{C}} C$ by statement (i).

Proposition 3.2.6 (Interpolation function basis associated with hyperrectangles). *Let $m \in \mathbb{N}$ and let \mathbb{R}^m be equipped with a norm $\|\cdot\|$. For $i = 1, \dots, m$, let $n_i \in \mathbb{N}$, $\beta_i > 0$, $\underline{\kappa}_i \in \mathbb{R}$, and let $\kappa_{i,j} := \underline{\kappa}_i + j\beta_i$ for $j = 0, \dots, n_i$. Moreover, for $i = 1, \dots, m$, let $\mathcal{I}_i := \{(-\infty, \kappa_{i,0}], [\kappa_{i,0}, \kappa_{i,1}], \dots, [\kappa_{i,n_i-1}, \kappa_{i,n_i}], [\kappa_{i,n_i}, \infty)\}$, and let \mathfrak{C} and \mathcal{G} be defined as follows:*

$$\begin{aligned} \mathfrak{C} &:= \{I_1 \times \dots \times I_m : I_i \in \mathcal{I}_i \forall 1 \leq i \leq m\}, \\ \mathcal{G} &:= \left\{ \mathbb{R}^m \ni (x_1, \dots, x_m)^\top \mapsto \left(\max_{i \in L} \{\beta_i^{-1} (x_i - \kappa_{i,j_i})^+\} \right)^+ \in \mathbb{R} : \right. \\ &\quad \left. 0 \leq j_i \leq n_i \forall i \in L, L \subseteq \{1, \dots, m\} \right\} \\ &\cup \{ \mathbb{R}^m \ni (x_1, \dots, x_m)^\top \mapsto x_i \in \mathbb{R} : 1 \leq i \leq m \}. \end{aligned} \quad (3.6)$$

Then, \mathfrak{C} is a polyhedral cover of \mathbb{R}^m (and so also of any $\mathcal{Y} \subseteq \mathbb{R}^m$) and \mathcal{G} is an interpolation function basis associated with \mathfrak{C} .

Proof of Proposition 3.2.6. See Section 5.4. □

Given a polyhedral cover \mathfrak{C} of a closed set $\mathcal{Y} \subseteq \mathbb{R}^m$ and its associated interpolation function basis \mathcal{G} , the following theorem establishes an upper bound on $W_1(\mu, \nu)$ for all $\mu, \nu \in \mathcal{P}_1(\mathcal{Y}; \mathcal{G})$ satisfying $\mu \stackrel{\mathcal{G}}{\sim} \nu$.

Theorem 3.2.7 (Moment set on a closed subset of a Euclidean space). *Let $m \in \mathbb{N}$, let $\|\cdot\|$ be a norm on \mathbb{R}^m , let $\mathcal{Y} \subseteq \mathbb{R}^m$ be closed, and let $d_{\mathcal{Y}}$ be the metric on \mathcal{Y} induced by $\|\cdot\|$. Let \mathfrak{C} be a polyhedral cover of \mathcal{Y} with mesh size $\eta(\mathfrak{C})$ and let \mathcal{G} be an interpolation function basis associated with \mathfrak{C} . Moreover, let $\{g_{\mathbf{v}} : \mathbf{v} \in V(\mathfrak{C})\} \subset \text{span}_1(\mathcal{G})$ and $\{\bar{g}_{\mathbf{u}} : \mathbf{u} \in D(\mathfrak{C})\} \subset \text{span}_1(\mathcal{G})$ be the functions that satisfy the properties (IFB1)–(IFB6) in Definition 3.2.4. Then, for any $\mu, \nu \in \mathcal{P}_1(\mathcal{Y}; \mathcal{G})$,*

$$\mu \stackrel{\mathcal{G}}{\sim} \nu \implies W_1(\mu, \nu) \leq 2 \left(\eta(\mathfrak{C}) + \sum_{\mathbf{u} \in D(\mathfrak{C})} \int_{\mathcal{Y}} \bar{g}_{\mathbf{u}} d\mu \right).$$

In particular, if \mathfrak{C} contains only bounded sets, then

$$\mu \stackrel{\mathcal{G}}{\sim} \nu \implies W_1(\mu, \nu) \leq 2\eta(\mathfrak{C}).$$

Proof of Theorem 3.2.7. See Section 5.4. □

The following corollary is a consequence of Theorem 3.2.7 and Proposition 3.2.6 which has a natural interpretation in the context of mathematical finance, as discussed in Remark 3.2.9.

Corollary 3.2.8. *Let $m \in \mathbb{N}$, $\mathcal{Y} = \mathbb{R}^m$, and let $d_{\mathcal{Y}}$ be the metric induced by a norm $\|\cdot\|$ on \mathbb{R}^m . Let $\mu \in \mathcal{P}_1(\mathcal{Y})$ and let $\mu_i \in \mathcal{P}_1(\mathbb{R})$ denote the i -th marginal of μ for $i = 1, \dots, m$. Let $\beta > 0$. For $i = 1, \dots, m$, let $n_i \in \mathbb{N}$, $\underline{\kappa}_i \in \mathbb{R}$, and let $\kappa_{i,j} := \underline{\kappa}_i + j\beta$ for $j = 0, \dots, n_i$. Moreover, let \mathcal{G} be a finite collection of functions given by*

$$\begin{aligned} \mathcal{G} &:= \left\{ \mathbb{R}^m \ni (x_1, \dots, x_m)^\top \mapsto \left(\max_{i \in L} \{(x_i - \kappa_{i,j_i})^+\} \right)^+ \in \mathbb{R} : \right. \\ &\quad \left. 0 \leq j_i \leq n_i \forall i \in L, L \subseteq \{1, \dots, m\} \right\} \\ &\cup \{ \mathbb{R}^m \ni (x_1, \dots, x_m)^\top \mapsto x_i \in \mathbb{R} : 1 \leq i \leq m \}. \end{aligned} \quad (3.7)$$

Then,

$$\overline{W}_{1,\mu}([\mu]_{\mathcal{G}}) := \sup_{\nu \in [\mu]_{\mathcal{G}}} \{W_1(\mu, \nu)\} \leq 2\theta \left(m\beta + \sum_{i=1}^m \int_{\mathbb{R}} (\kappa_{i,0} - x_i)^+ + (x_i - \kappa_{i,n_i})^+ \mu_i(dx_i) \right), \quad (3.8)$$

where $\theta \geq 1$ is a constant such that $\|\mathbf{x}\| \leq \theta \|\mathbf{x}\|_1$ for all $\mathbf{x} \in \mathbb{R}^m$. In particular, for any $\epsilon > 0$, there exist $\beta > 0$, $(n_i)_{i=1:m} \subset \mathbb{N}$, and $(\underline{\kappa}_i)_{i=1:m} \subset \mathbb{R}$ such that $\overline{W}_{1,\mu}([\mu]_{\mathcal{G}}) \leq \epsilon$.

Proof of Corollary 3.2.8. See Section 5.4. □

Remark 3.2.9 (Financial interpretation of Corollary 3.2.8). *Corollary 3.2.8 has a natural interpretation in mathematical finance. Consider a financial market where $m \in \mathbb{N}$ risky assets are traded. Let $\mathcal{Y} \subseteq \mathbb{R}^m$ (typically $\mathcal{Y} = \mathbb{R}_+^m$) be a closed set that corresponds to the possible prices of these assets at a fixed future time, called the maturity. Then, for $i = 1, \dots, m$, the function*

$$\mathcal{Y} \ni (x_1, \dots, x_m)^\top \mapsto x_i \in \mathbb{R}$$

corresponds to the payoff at maturity when investing into a single unit of asset i . Moreover, for any non-empty set $L \subseteq \{1, \dots, m\}$ and any $(\kappa_i)_{i \in L} \subset \mathbb{R}$, the function

$$\mathcal{Y} \ni (x_1, \dots, x_m)^\top \mapsto \left(\max_{i \in L} \{ (x_i - \kappa_i)^+ \} \right)^+ \in \mathbb{R}$$

corresponds to the payoff of a best-of-call option (a type of financial derivative) written on the assets in the set L with strike prices $(\kappa_i)_{i \in L}$. Let us consider $\mu \in \mathcal{P}_1(\mathcal{Y})$ as a risk-neutral pricing measure for this financial market, and let \mathcal{G} be defined by (3.7). Then, the set $[\mu]_{\mathcal{G}}$ corresponds to the set of risk-neutral pricing measures that produce the same forward prices (for each of the assets) as well as the same prices of best-of-call options written on any non-empty subset L of the assets with strikes $\{\kappa_i + j\beta : 0 \leq j \leq n_i, i \in L\}$. $\bar{W}_{1,\mu}([\mu]_{\mathcal{G}})$ is thus an upper bound for the model risk in terms of the W_1 -metric when we only assume the knowledge of forward prices and the aforementioned best-of-call option prices. Corollary 3.2.8 states that, for any $\epsilon > 0$, one can select finitely many best-of-call options to control the model risk such that $\bar{W}_{1,\mu}([\mu]_{\mathcal{G}}) \leq \epsilon$. This is related to the classical result of Breeden and Litzenberger [11], which states that: for $\mu \in \mathcal{P}_1(\mathbb{R})$ that is absolutely continuous with respect to the Lebesgue measure, if the function

$$\mathbb{R} \ni \kappa \mapsto \int_{\mathbb{R}} (x - \kappa)^+ \mu(dx)$$

is twice continuously differentiable, then it uniquely characterizes the density of μ . Talponen and Vitasaari [55] later generalized this result to the multi-dimensional case. Theorem 2.1 of [55] states that: for $\mu \in \mathcal{P}_1(\mathbb{R}_+^m)$ that is absolutely continuous with respect to the Lebesgue measure, the density of μ is uniquely characterized by the function

$$\mathbb{R}_+^m \ni (\kappa_1, \dots, \kappa_m) \mapsto \int_{\mathbb{R}_+^m} \left(\max_{1 \leq i \leq m} \{ (x_i - \kappa_i)^+ \} \right)^+ \mu(dx_1, \dots, dx_m) \in \mathbb{R}.$$

Corollary 3.2.8 can therefore be seen as a non-asymptotic generalization of [55, Theorem 2.1].

4. NUMERICAL METHODS

In this section, we discuss the numerical methods for solving the LSIP problem ($\text{MMOT}_{\text{relax}}^*$). Specifically, we apply the so-called cutting-plane discretization method (see, e.g., [35, Conceptual Algorithm 11.4.1]). The idea of the cutting-plane discretization method is to replace the semi-infinite constraint in an LSIP problem by a finite subcollection of constraints, which relaxes the LSIP problem by a linear programming (LP) problem. Subsequently, one iteratively adds more constraints to the existing subcollection until the approximation error falls below a pre-specified tolerance threshold. The addition of constraints can be thought of as introducing “cuts” to restrict the feasible set of the LP relaxation of the LSIP problem. However, in order to prove the convergence of this method, it is crucial to show the boundedness of the superlevel sets of the initial LP relaxation. By [35, Corollary 9.3.1], the existence of such a relaxation is equivalent to the boundedness of the set of optimizers of ($\text{MMOT}_{\text{relax}}^*$). Hence, in Section 4.1, we establish this boundedness condition for ($\text{MMOT}_{\text{relax}}^*$) when the underlying spaces are compact subsets of Euclidean spaces. Then, we provide a cutting-plane discretization algorithm (i.e., Algorithm 1) for solving ($\text{MMOT}_{\text{relax}}^*$), which, for any $\epsilon > 0$, can provide an ϵ -optimal solution. Subsequently, in Section 4.2, we provide an algorithm (i.e., Algorithm 2) such that for any $\tilde{\epsilon} > 0$, it is able to compute an $\tilde{\epsilon}$ -optimal solution of (MMOT) based on Algorithm 1. Moreover, it computes both an upper bound and a lower bound on (MMOT) that are at most $\tilde{\epsilon}$ apart. Finally, in Section 4.3, we demonstrate the numerical performance of the developed algorithms in an MMOT problem involving $N = 50$ marginals.

Algorithm 1: Cutting-plane discretization algorithm for solving (MMOT*_{relax})

Input: $(\mathcal{X}_i)_{i=1:N}$, m , $f(\cdot)$, $g(\cdot)$, v , $\mathcal{X}^{\dagger(0)} \subset \mathcal{X}$, $\epsilon > 0$
Output: $\text{MMOT}_{\text{relax}}^{\text{UB}}$, $\text{MMOT}_{\text{relax}}^{\text{LB}}$, \hat{y}_0 , \hat{y} , $\hat{\mu}$

- 1 $r \leftarrow 0$.
- 2 **while true do**
- 3 Solve the LP problem:

$$\phi^{(r)} \leftarrow \max_{y_0 \in \mathbb{R}, \mathbf{y} \in \mathbb{R}^m} \left\{ y_0 + \langle \mathbf{y}, v \rangle : y_0 + \langle \mathbf{y}, g(x) \rangle \leq f(x) \forall x \in \mathcal{X}^{\dagger(r)} \right\}$$
, denote the computed optimizer as $(y_0^{(r)}, \mathbf{y}^{(r)})$, and denote the corresponding dual optimizer as $(\mu_x^{(r)})_{x \in \mathcal{X}^{\dagger(r)}}$.
- 4 Solve the global maximization problem $s^{(r)} \leftarrow \max_{x \in \mathcal{X}} \left\{ y_0^{(r)} + \langle \mathbf{y}^{(r)}, g(x) \rangle - f(x) \right\}$ and denote the computed optimizer as x^* .
- 5 **if** $s^{(r)} \leq \epsilon$ **then**
- 6 Skip to Line 10.
- 7 Let $\mathcal{X}^* \subset \mathcal{X}$ be a finite set such that $x^* \in \mathcal{X}^*$.
- 8 $\mathcal{X}^{\dagger(r+1)} \leftarrow \mathcal{X}^{\dagger(r)} \cup \mathcal{X}^*$.
- 9 $r \leftarrow r + 1$.

10 $\text{MMOT}_{\text{relax}}^{\text{UB}} \leftarrow \phi^{(r)}$, $\text{MMOT}_{\text{relax}}^{\text{LB}} \leftarrow \phi^{(r)} - s^{(r)}$.

11 $\hat{y}_0 \leftarrow y_0^{(r)} - s^{(r)}$, $\hat{y} \leftarrow \mathbf{y}^{(r)}$.

12 $\hat{\mu} \leftarrow \sum_{x \in \mathcal{X}^{\dagger(r)}} \mu_x^{(r)} \delta_x$.

13 **return** $\text{MMOT}_{\text{relax}}^{\text{UB}}$, $\text{MMOT}_{\text{relax}}^{\text{LB}}$, \hat{y}_0 , \hat{y} , $\hat{\mu}$.

4.1. Cutting-plane discretization algorithm for solving (MMOT*_{relax}). The following proposition establishes the boundedness condition for the optimizers of (MMOT*_{relax}) under some mild assumptions when $\mathcal{X}_1, \dots, \mathcal{X}_N$ are compact subsets of Euclidean spaces.

Proposition 4.1.1 (Boundedness of the optimizers of (MMOT*_{relax})). *Let Assumption 2.1.3 hold. Assume that for $i = 1, \dots, N$, \mathcal{X}_i is a compact subset of a Euclidean space and $d_{\mathcal{X}_i}$ is a metric on \mathcal{X}_i induced by a norm $\|\cdot\|$. Let \mathcal{C}_i be a polyhedral cover of \mathcal{X}_i such that $\bigcup_{C \in \mathcal{C}_i} C = \mathcal{X}_i$, and let continuous real-valued functions $\{g_{i,t} : t \in V(\mathcal{C}_i)\}$ on \mathcal{X}_i satisfy the properties (IFB1)–(IFB4) with respect to \mathcal{C}_i as well as $\int_{\mathcal{X}_i} g_{i,t} d\mu_i > 0$ for all $t \in V(\mathcal{C}_i)$. Let $m_i := |V(\mathcal{C}_i)| - 1$ and enumerate $V(\mathcal{C}_i)$ arbitrarily by $V(\mathcal{C}_i) = \{t_{i,0}, t_{i,1}, \dots, t_{i,m_i}\}$. Let $g_{i,j} := g_{i,t_{i,j}}$ for $j = 0, 1, \dots, m_i$ and let $\mathcal{G}_i := \{g_{i,1}, \dots, g_{i,m_i}\}$. Moreover, let $g(\cdot)$ and v be given as in (2.12) and (2.13). Then, the set of optimizers of the LSIP problem (MMOT*_{relax}) is bounded.*

Proof of Proposition 4.1.1. See Section 5.5. □

Algorithm 1 provides a concrete implementation of the cutting-plane discretization method. Remark 4.1.2 explains the assumptions and details of Algorithm 1. The properties of Algorithm 1 are detailed in Theorem 4.1.3.

Remark 4.1.2 (Details of Algorithm 1). *Algorithm 1 is inspired by the Conceptual Algorithm 11.4.1 in [35]. In addition to Assumption 2.1.3, we assume that the conditions (CPD1) and (CPD2) below hold.*

(CPD1) *For $i = 1, \dots, N$, \mathcal{X}_i is a compact subset of a Euclidean space equipped with a norm-induced metric, \mathcal{C}_i is a polyhedral cover of \mathcal{X}_i such that $\bigcup_{C \in \mathcal{C}_i} C = \mathcal{X}_i$, $\{g_{i,t} : t \in V(\mathcal{C}_i)\}$ is a set of continuous real-valued functions on \mathcal{X}_i satisfying the properties (IFB1)–(IFB4) with respect to \mathcal{C}_i , $m_i := |V(\mathcal{C}_i)| - 1$, $g_{i,j} := g_{i,t_{i,j}}$ for $j = 0, 1, \dots, m_i$, where $\{t_{i,0}, t_{i,1}, \dots, t_{i,m_i}\}$ is an arbitrary enumeration of $V(\mathcal{C}_i)$, $\mathcal{G}_i := \{g_{i,1}, \dots, g_{i,m_i}\}$.*

(CPD2) *For $i = 1, \dots, N$, $j = 0, 1, \dots, m_i$, $\int_{\mathcal{X}_i} g_{i,j} d\mu_i > 0$.*

Below is a list explaining the inputs to Algorithm 1.

- $(\mathcal{X}_i)_{i=1:N}$ are compact sets that satisfy (CPD1).
- $m := \sum_{i=1}^N m_i$.

- $f : \mathcal{X} \rightarrow \mathbb{R}$ is the cost function in Assumption 2.1.3.
- $\mathbf{g}(\cdot)$ and \mathbf{v} are defined in (2.12) and (2.13).
- $\mathcal{X}^{\dagger(0)} \subset \mathcal{X}$ is a finite set such that the LP problem:

$$\max_{y_0 \in \mathbb{R}, \mathbf{y} \in \mathbb{R}^m} \left\{ y_0 + \langle \mathbf{y}, \mathbf{v} \rangle : y_0 + \langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle \leq f(\mathbf{x}) \quad \forall \mathbf{x} \in \mathcal{X}^{\dagger(0)} \right\}$$

has bounded superlevel sets. The existence of such $\mathcal{X}^{\dagger(0)}$ is shown in Theorem 4.1.3(i).

- $\epsilon > 0$ is a pre-specified numerical tolerance value (see Theorem 4.1.3).

The list below provides further explanations of some lines in Algorithm 1.

- Line 3 solves an LP relaxation of $(\text{MMOT}_{\text{relax}}^*)$ where the semi-infinite constraint is replaced by finitely many constraints each corresponding to an element of $\mathcal{X}^{\dagger(r)}$. When solving the LP relaxation in Line 3 by the dual simplex algorithm (see, e.g., [57, Chapter 6.4]) or the interior point algorithm (see, e.g., [57, Chapter 18]), one can obtain the corresponding optimizer of the dual LP problem from the output of these algorithms.
- Line 7 allows more than one constraints to be generated in each iteration. \mathcal{X}^* can be thought of as a set of approximate optimizers of the global maximization problem in Line 4.
- Line 10 provides an upper bound $\text{MMOT}_{\text{relax}}^{\text{UB}}$ and a lower bound $\text{MMOT}_{\text{relax}}^{\text{LB}}$ on the optimal value of $(\text{MMOT}_{\text{relax}}^*)$ as shown in Theorem 4.1.3(iii).
- Line 11 constructs an ϵ -optimal solution of $(\text{MMOT}_{\text{relax}}^*)$ as shown in Theorem 4.1.3(iv).
- Line 12 constructs an ϵ -optimal solution of $(\text{MMOT}_{\text{relax}})$ which is a discrete measure with finite support in $\mathcal{X}^{\dagger(r)}$ as shown in Theorem 4.1.3(v).

Theorem 4.1.3 (Properties of Algorithm 1). *Let Assumption 2.1.3 hold and assume that the conditions (CPD1) and (CPD2) in Remark 4.1.2 hold. Then,*

- (i) *there exists a finite set $\mathcal{X}^{\dagger(0)} \subset \mathcal{X}$ such that the LP problem:*

$$\max_{y_0 \in \mathbb{R}, \mathbf{y} \in \mathbb{R}^m} \left\{ y_0 + \langle \mathbf{y}, \mathbf{v} \rangle : y_0 + \langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle \leq f(\mathbf{x}) \quad \forall \mathbf{x} \in \mathcal{X}^{\dagger(0)} \right\}$$

has bounded superlevel sets.

Moreover, assume that all inputs of Algorithm 1 are set according to Remark 4.1.2. Then, the following statements hold.

- (ii) *Algorithm 1 terminates after finitely many iterations.*
 (iii) $\text{MMOT}_{\text{relax}}^{\text{LB}} \leq (\text{MMOT}_{\text{relax}}^*) \leq \text{MMOT}_{\text{relax}}^{\text{UB}}$ where $\text{MMOT}_{\text{relax}}^{\text{UB}} - \text{MMOT}_{\text{relax}}^{\text{LB}} \leq \epsilon$.
 (iv) $(\hat{y}_0, \hat{\mathbf{y}})$ is an ϵ -optimal solution of $(\text{MMOT}_{\text{relax}}^*)$ and $\hat{y}_0 + \langle \hat{\mathbf{y}}, \mathbf{v} \rangle = \text{MMOT}_{\text{relax}}^{\text{LB}}$.
 (v) $\hat{\mu}$ is an ϵ -optimal solution of $(\text{MMOT}_{\text{relax}})$ and $\int_{\mathcal{X}} f \, d\hat{\mu} = \text{MMOT}_{\text{relax}}^{\text{UB}}$.

Proof of Theorem 4.1.3. See Section 5.5. □

4.2. Algorithm for solving (MMOT). Before introducing the algorithm for solving (MMOT), we establish the following lemma in order to extend the domain of the cost function f to a (possibly) larger set. This helps to take care of the case where $\mathcal{X}_1, \dots, \mathcal{X}_N$ cannot be expressed as finite union of polyhedrons. In this case, in order to apply Algorithm 1, one has to first extend \mathcal{X}_i to $\tilde{\mathcal{X}}_i := \bigcup_{C \in \mathfrak{C}_i} C$ for $i = 1, \dots, N$, where \mathfrak{C}_i is a polyhedral cover of \mathcal{X}_i , and then extend $f : \mathcal{X} \rightarrow \mathbb{R}$ to $\tilde{f} : (\times_{i=1}^N \tilde{\mathcal{X}}_i) \rightarrow \mathbb{R}$.

Lemma 4.2.1. *Let $(\mathcal{Y}, d_{\mathcal{Y}})$ be a Polish space and let $D \subseteq \tilde{D} \subseteq \mathcal{Y}$. Let $f : D \rightarrow \mathbb{R}$ be an L_f -Lipschitz continuous function for $L_f > 0$ and let $\tilde{f} : \tilde{D} \rightarrow \mathbb{R}$ be defined as*

$$\tilde{f}(x) := \inf_{x' \in D} \{ f(x') + L_f d_{\mathcal{Y}}(x, x') \}.$$

Then, \tilde{f} is L_f -Lipschitz continuous and $\tilde{f}(x) = f(x)$ for all $x \in D$.

Proof of Lemma 4.2.1. See Section 5.6. □

The concrete procedure for computing an $\tilde{\epsilon}$ -optimal solution of (MMOT) is detailed in Algorithm 2. Remark 4.2.2 explains the assumptions and details of Algorithm 2. The properties of Algorithm 2 are detailed in Theorem 4.2.3.

Algorithm 2: Procedure for solving (MMOT)

-
- Input:** $(\mathcal{X}_i)_{i=1:N}$, $(\mu_i)_{i=1:N}$, $f(\cdot)$, L_f , $\tilde{\epsilon} > 0$
Output: MMOT^{UB} , MMOT^{LB} , $\tilde{\mu}$
- 1 Choose $\epsilon \in (0, \tilde{\epsilon})$.
 - 2 **for** $i = 1, \dots, N$ **do**
 - 3 Construct a polyhedral cover \mathfrak{C}_i of \mathcal{X}_i containing only bounded sets such that $\eta(\mathfrak{C}_i) \leq \frac{\tilde{\epsilon} - \epsilon}{2NL_f}$.
 - 4 $\tilde{\mathcal{X}}_i \leftarrow \bigcup_{C \in \mathfrak{C}_i} C$.
 - 5 Construct a set of continuous real-valued functions $\{g_{i,t} : t \in V(\mathfrak{C}_i)\}$ on $\tilde{\mathcal{X}}_i$ satisfying the properties (IFB1)–(IFB4) with respect to \mathfrak{C}_i .
 - 6 $m_i \leftarrow |V(\mathfrak{C}_i)| - 1$, $g_{i,j} \leftarrow g_{i,t_{i,j}}$ for $j = 0, 1, \dots, m_i$, where $\{t_{i,0}, t_{i,1}, \dots, t_{i,m_i}\}$ is an arbitrary enumeration of $V(\mathfrak{C}_i)$, $\mathcal{G}_i \leftarrow \{g_{i,1}, \dots, g_{i,m_i}\}$.
 - 7 $\tilde{\mathcal{X}} \leftarrow \times_{i=1}^N \tilde{\mathcal{X}}_i$. Let $\tilde{f} : \tilde{\mathcal{X}} \rightarrow \mathbb{R}$ be an L_f -Lipschitz continuous function such that $\tilde{f}(x) = f(x)$ for all $x \in \mathcal{X}$ (e.g., by the construction in Lemma 4.2.1).
 - 8 $m \leftarrow \sum_{i=1}^N m_i$. Let $\mathbf{g}(\cdot)$ and \mathbf{v} be defined by (2.12) and (2.13).
 - 9 Construct a finite set $\mathcal{X}^{\dagger(0)} \subset \tilde{\mathcal{X}}$ such that the LP problem $\max_{y_0 \in \mathbb{R}, \mathbf{y} \in \mathbb{R}^m} \{y_0 + \langle \mathbf{y}, \mathbf{v} \rangle : y_0 + \langle \mathbf{y}, \mathbf{g}(x) \rangle \leq \tilde{f}(x) \forall x \in \mathcal{X}^{\dagger(0)}\}$ has bounded superlevel sets.
 - 10 $(\text{MMOT}_{\text{relax}}^{\text{UB}}, \text{MMOT}_{\text{relax}}^{\text{LB}}, \hat{y}_0, \hat{\mathbf{y}}, \hat{\mu}) \leftarrow$ the outputs of Algorithm 1 with inputs $((\tilde{\mathcal{X}}_i)_{i=1:N}, m, \tilde{f}(\cdot), \mathbf{g}(\cdot), \mathbf{v}, \mathcal{X}^{\dagger(0)}, \epsilon)$.
 - 11 For $i = 1, \dots, N$, let $\mu_i^\dagger \in \mathcal{P}_1(\tilde{\mathcal{X}}_i)$ be defined by $\mu_i^\dagger(E) := \mu_i(E \cap \mathcal{X}_i)$ for all $E \in \mathcal{B}(\tilde{\mathcal{X}}_i)$.
 - 12 Let $\tilde{\mu}^\dagger \in R(\hat{\mu}; \mu_1^\dagger, \dots, \mu_N^\dagger) \subset \mathcal{P}_1(\tilde{\mathcal{X}})$. Let $\tilde{\mu} \in \mathcal{P}_1(\mathcal{X})$ be defined by $\tilde{\mu}(E) := \tilde{\mu}^\dagger(E)$ for all $E \in \mathcal{B}(\mathcal{X})$.
 - 13 $\text{MMOT}^{\text{LB}} \leftarrow \text{MMOT}_{\text{relax}}^{\text{LB}}$, $\text{MMOT}^{\text{UB}} \leftarrow \int_{\mathcal{X}} f \, d\tilde{\mu}$.
 - 14 **return** MMOT^{UB} , MMOT^{LB} , $\tilde{\mu}$.
-

Remark 4.2.2 (Details of Algorithm 2). *In addition to Assumption 2.1.3, we make the following assumptions about the inputs of Algorithm 2.*

- (A1) For $i = 1, \dots, N$, \mathcal{X}_i is a compact subset of a Euclidean space equipped with a norm-induced metric.
- (A2) For $i = 1, \dots, N$, $(g_{i,j})_{j=0:m_i}$ constructed and defined in Line 6 satisfies the condition (CPD2) in Remark 4.1.2 with respect to μ_i . For example, this condition is satisfied if \mathfrak{C}_i is a simplicial cover of \mathcal{X}_i satisfying $\text{int}(C \cap \mathcal{X}_i) \neq \emptyset$ for all $C \in \mathfrak{C}_i$, $\{g_{i,t} : t \in V(\mathfrak{C}_i)\}$ is the interpolation function basis associated with \mathfrak{C}_i defined in Proposition 3.2.5, and $\text{supp}(\mu_i) = \mathcal{X}_i$.
- (A3) f is L_f -Lipschitz continuous.
- (A4) $\tilde{\epsilon} > 0$ is arbitrary.

The list below provides further explanations of some lines in Algorithm 2.

- Under the assumption (A1), it is possible to construct a polyhedral cover \mathfrak{C}_i in Line 3 satisfying $\eta(\mathfrak{C}_i) \leq \frac{\tilde{\epsilon} - \epsilon}{2NL_f}$ as well as its associated interpolation function basis $\{g_{i,t} : t \in V(\mathfrak{C}_i)\}$ in Line 5, for example by the approach with a simplicial cover described in Proposition 3.2.5. This is formally stated in Theorem 4.2.3(i).
- In Line 7, $f : \mathcal{X} \rightarrow \mathbb{R}$ is extended to $\tilde{f} : \tilde{\mathcal{X}} \rightarrow \mathbb{R}$ defined on a (possibly) larger compact set $\tilde{\mathcal{X}}$ such that \tilde{f} coincides with f on \mathcal{X} and remains L_f -Lipschitz continuous. For example, this can be done via the construction in Lemma 4.2.1.
- Line 9 constructs a finite set $\mathcal{X}^{\dagger(0)}$ which is then used as input to Algorithm 1 in Line 10. This is possible due to the assumption (A2) as well as Theorem 4.1.3(i). This is formally stated in Theorem 4.2.3(ii).

Theorem 4.2.3 (Properties of Algorithm 2). *Let Assumption 2.1.3 as well as the conditions (A1)–(A4) in Remark 4.2.2 hold. Then, the following statements hold.*

- (i) *For $i = 1, \dots, N$, there exists a polyhedral cover \mathfrak{C}_i of \mathcal{X}_i containing only bounded sets such that $\eta(\mathfrak{C}_i) \leq \frac{\tilde{\epsilon} - \epsilon}{2NL_f}$. Moreover, there exists a set of continuous real-valued functions $\{g_{i,t} : t \in V(\mathfrak{C}_i)\}$ on $\tilde{\mathcal{X}}_i$ which satisfies the properties (IFB1)–(IFB4) with respect to \mathfrak{C}_i .*
- (ii) *There exists a finite set $\mathcal{X}^{\dagger(0)} \subset \mathcal{X}$ such that the LP problem*

$$\max_{y_0 \in \mathbb{R}, \mathbf{y} \in \mathbb{R}^m} \left\{ y_0 + \langle \mathbf{y}, \mathbf{v} \rangle : y_0 + \langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle \leq \tilde{f}(\mathbf{x}) \quad \forall \mathbf{x} \in \mathcal{X}^{\dagger(0)} \right\}$$

has bounded superlevel sets.

- (iii) $\text{MMOT}^{\text{LB}} \leq (\text{MMOT}) \leq \text{MMOT}^{\text{UB}}$ where $\text{MMOT}^{\text{UB}} - \text{MMOT}^{\text{LB}} \leq \tilde{\epsilon}$.
- (iv) $\tilde{\mu}$ is an $\hat{\epsilon}$ -optimal solution of (MMOT), where $\hat{\epsilon} := \text{MMOT}^{\text{UB}} - \text{MMOT}^{\text{LB}} \leq \tilde{\epsilon}$.

Proof of Theorem 4.2.3. See Section 5.6. □

Remark 4.2.4. *Since $\tilde{\epsilon} > 0$ is arbitrary, Theorem 4.2.3(iii) guarantees that the upper bound MMOT^{UB} and the lower bound MMOT^{LB} returned by Algorithm 2 can be arbitrarily close to each other. Moreover, the difference between the upper and lower bounds, i.e., $\hat{\epsilon} := \text{MMOT}^{\text{UB}} - \text{MMOT}^{\text{LB}}$, which measures the sub-optimality of the approximate optimizer $\tilde{\mu}$ of (MMOT) returned by Algorithm 2, is in practice even smaller than the pre-specified theoretical upper bound $\tilde{\epsilon}$; see also Figure 4.1.*

4.3. A numerical example. In this subsection, we showcase Algorithm 1 and Algorithm 2 in a high-dimensional numerical example. In the example, we let $N = 50$ and let $\mathcal{X}_i := [\underline{\kappa}_i, \bar{\kappa}_i]$, where $\underline{\kappa}_i = -10$ and $\bar{\kappa}_i = 10$ for $i = 1, \dots, N$. Hence, $\mathcal{X} := \times_{i=1}^N \mathcal{X}_i \subset \mathbb{R}^N$ is an N -cell. Moreover, we consider a cost function $f : \mathcal{X} \rightarrow \mathbb{R}$ which is given by:

$$f(\mathbf{x}) := \left(\sum_{k=1}^2 |\langle \mathbf{s}_k^+, \mathbf{x} \rangle - t_k^+| \right) - \left(\sum_{k=1}^2 |\langle \mathbf{s}_k^-, \mathbf{x} \rangle - t_k^-| \right), \quad (4.1)$$

where $\mathbf{s}_1^+, \mathbf{s}_2^+, \mathbf{s}_1^-, \mathbf{s}_2^-$ are uniformly randomly generated from the unit sphere in \mathbb{R}^N , and $t_1^+, t_2^+, t_1^-, t_2^-$ are randomly generated real constants. Notice that f is neither convex nor concave, and that $f(\mathbf{x})$ cannot be separated into a sum of functions involving disjoint components of \mathbf{x} (otherwise (MMOT) can be decomposed into independent sub-problems). We chose this f in order to demonstrate the performance of Algorithm 1 and Algorithm 2 in a high-dimensional setting. For $i = 1, \dots, N$, we let the marginal $\mu_i \in \mathcal{P}(\mathcal{X}_i)$ be a mixture of three equally weighted distributions in which each mixture component is a normal distribution with randomly generated parameters that is truncated to the interval $[\underline{\kappa}_i, \bar{\kappa}_i]$.

In order to approximately solve (MMOT), we first construct a simplicial cover $\mathfrak{C}_i = \{[\kappa_{i,0}, \kappa_{i,1}], \dots, [\kappa_{i,m_i-1}, \kappa_{i,m_i}]\}$ where $m_i \in \mathbb{N}$ and $\underline{\kappa}_i =: \kappa_{i,0} < \kappa_{i,1} < \dots < \kappa_{i,m_i} := \bar{\kappa}_i$ for $i = 1, \dots, N$. Subsequently, we construct an interpolation function basis \mathcal{G}_i associated with the simplicial cover \mathfrak{C}_i via the method described in Proposition 3.2.5 for $i = 1, \dots, N$. Specifically, we have $\mathcal{G}_i := \{g_{i,1}, \dots, g_{i,m_i}\}$ where

$$\begin{aligned} [\underline{\kappa}_i, \bar{\kappa}_i] \ni x_i \mapsto g_{i,j}(x_i) &:= \frac{(x_i - \kappa_{i,j-1})^+}{\kappa_{i,j} - \kappa_{i,j-1}} \wedge \frac{(\kappa_{i,j+1} - x_i)^+}{\kappa_{i,j+1} - \kappa_{i,j}} \quad \text{for } j = 1, \dots, m_i - 1, \\ [\underline{\kappa}_i, \bar{\kappa}_i] \ni x_i \mapsto g_{i,m_i}(x_i) &:= \frac{(x_i - \kappa_{i,m_i-1})^+}{\kappa_{i,m_i} - \kappa_{i,m_i-1}}. \end{aligned} \quad (4.2)$$

Notice that the function $[\underline{\kappa}_i, \bar{\kappa}_i] \ni x_i \mapsto \frac{(\kappa_{i,1} - x_i)^+}{\kappa_{i,1} - \kappa_{i,0}} \in \mathbb{R}$ has been excluded from \mathcal{G}_i in order to guarantee the boundedness of the set of optimizers of (MMOT_{relax}^{*}) (see Proposition 4.1.1). In particular, for any given $(y_{i,j})_{j=1:m_i} \subset \mathbb{R}$, the function $[\underline{\kappa}_i, \bar{\kappa}_i] \ni x_i \mapsto l_i(x_i) := \sum_{j=1}^{m_i} y_{i,j} g_{i,j}(x_i) \in \mathbb{R}$ is continuous and piece-wise affine on the intervals $[\kappa_{i,0}, \kappa_{i,1}], \dots, [\kappa_{i,m_i-1}, \kappa_{i,m_i}]$, and it satisfies $l_i(\kappa_{i,0}) = 0$ and $l_i(\kappa_{i,j}) = y_{i,j}$ for $j = 1, \dots, m_i$. Due to this property, we refer to $(m_i + 1)$ as the number of knots in dimension i . When solving (MMOT_{relax}^{*}) under this setting, the global optimization problem in Line 4 of Algorithm 1 can be formulated into a mixed-integer linear programming problem and solved using state-of-the-art solvers such as Gurobi [37]. The details of this formulation are discussed in Appendix A.

In the experiment, rather than fixing the value of $\tilde{\epsilon}$ and then constructing $(\mathfrak{C}_i)_{i=1:N}$ and $(\mathcal{G}_i)_{i=1:N}$ as described in Line 3 of Algorithm 2, we fix $\epsilon = 0.0001$, let $m_1 = \dots = m_N$, and vary m_i between 4 and

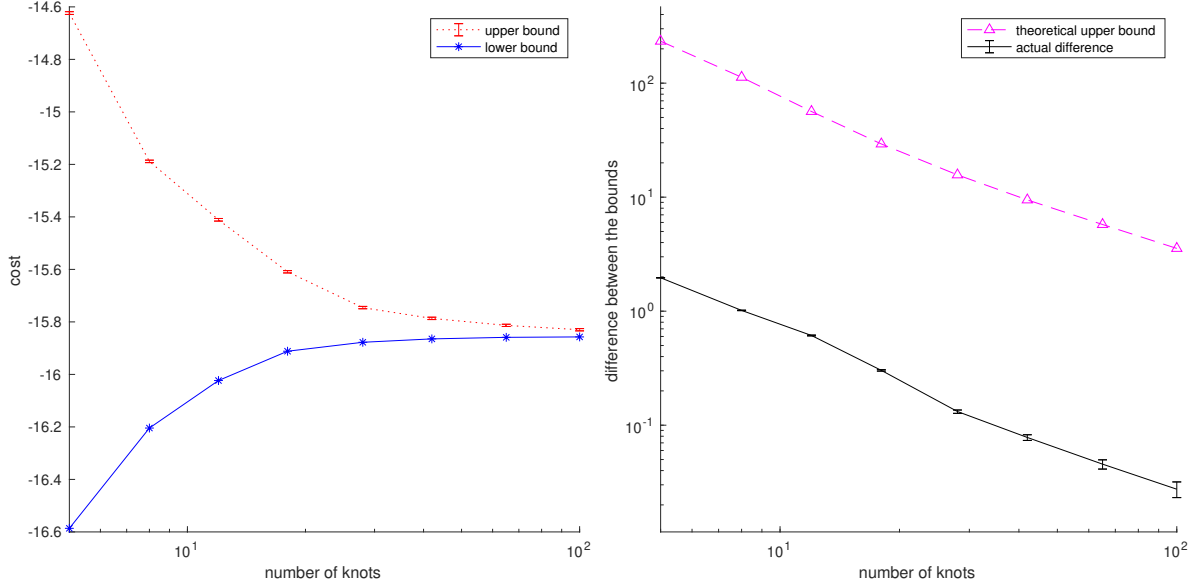


FIGURE 4.1. Results from the numerical example. *Left*: upper and lower bounds on (MMOT) resulted from Algorithm 2 (i.e., MMOT^{UB} and MMOT^{LB}) plotted against the number of knots in each dimension (i.e., $m_i + 1$). The error bars around the upper bounds mark the 95% Monte Carlo error bounds. *Right*: theoretical upper bounds on $\text{MMOT}^{\text{UB}} - \text{MMOT}^{\text{LB}}$ versus the actual differences resulted from computation. The error bars around the actual gaps mark the 95% Monte Carlo error bounds.

99. For each value of m_i , the corresponding simplicial cover \mathcal{C}_i is iteratively constructed using a greedy procedure, where, in each iteration, we first define $\mathcal{G}_i := \{g_{i,1}, \dots, g_{i,m_i}\}$ by (4.2) and then bisect one of the existing intervals $[\kappa_{i,0}, \kappa_{i,1}], \dots, [\kappa_{i,m_i-1}, \kappa_{i,m_i}]$ in order to achieve the maximum reduction in an upper bound on $\overline{W}_{1,\mu_i}([\mu_i]_{\mathcal{G}_i})$. Subsequently, for each value of m_i , we use Lines 7–14 of Algorithm 2 to compute the corresponding values of MMOT^{LB} and MMOT^{UB} .

Since $\mathcal{X}_1, \dots, \mathcal{X}_N$ are all one-dimensional, the reassembly step $\tilde{\mu}^\dagger \in R(\hat{\mu}; \mu_1^\dagger, \dots, \mu_N^\dagger) \subset \mathcal{P}_1(\tilde{\mathcal{X}})$ is performed by applying the Sklar’s theorem from the copula theory (see, e.g., [45, Equation (5.3) & Theorem 5.3]). The computation of MMOT^{UB} in Line 13 of Algorithm 2 is done via Monte Carlo integration using 10^6 independent samples. The Monte Carlo step is repeated 1000 times in order to construct the Monte Carlo error bounds (see Figure 4.1 below). The code used in this work is available on GitHub⁵.

The results in this experiment are shown in Figure 4.1. The left panel of Figure 4.1 shows the values of MMOT^{LB} and MMOT^{UB} as the number of knots increases from 5 to 100. Since MMOT^{UB} was approximated by Monte Carlo integration, we have plotted the 95% Monte Carlo error bounds around the estimated values of MMOT^{UB} . It can be observed that both MMOT^{LB} and MMOT^{UB} improved drastically when the number of knots increased from 5 to 18. After that, when more knots were added, the improvements in MMOT^{LB} and MMOT^{UB} both shrunk. When 100 knots were used, the difference between MMOT^{UB} and MMOT^{LB} was around 0.027. This shows that with 100 knots the approximate optimizer $\tilde{\mu}$ of (MMOT) returned by Algorithm 2 was close to being optimal. The right panel of Figure 4.1 compares the differences between MMOT^{UB} and MMOT^{LB} computed by Algorithm 2 with their theoretical upper bounds. These theoretical upper bounds on the gaps were computed based on (4.1) and upper bounds on $\overline{W}_{1,\mu_i}([\mu_i]_{\mathcal{G}_i})$ for $i = 1, \dots, N$. One can observe that the actual differences are about two orders of magnitude smaller than their theoretical upper bounds. This shows that despite our theoretical analysis of Algorithm 2 in Theorem 4.2.3 requiring $\eta(\mathcal{C}_i) \leq \frac{\tilde{\epsilon} - \epsilon}{2NL_f}$ for $i = 1, \dots, N$ in order to guarantee $\text{MMOT}^{\text{UB}} - \text{MMOT}^{\text{LB}} \leq \tilde{\epsilon}$, the actual difference between MMOT^{UB} and MMOT^{LB} is likely much smaller than $\tilde{\epsilon}$ in practice. This also means that one may use much fewer knots in practice than what the theoretical analysis suggests.

⁵<https://github.com/qikunxiang/MultiMarginalOptimalTransport>

5. PROOF OF THEORETICAL RESULTS

5.1. Proof of results in Section 2.2.

Proof of Lemma 2.2.3. Let $\hat{\mu}_1, \dots, \hat{\mu}_N$ denote the marginals of $\hat{\mu}$ on $\mathcal{X}_1, \dots, \mathcal{X}_N$, respectively. Since $\hat{\mu} \in \mathcal{P}_1(\mathcal{X})$, we have $\hat{\mu}_i \in \mathcal{P}_1(\mathcal{X}_i)$ for $i = 1, \dots, N$ by (2.3). Moreover, the existence of an optimal coupling γ_i of $\hat{\mu}_i$ and μ_i under the cost function $d_{\mathcal{X}_i}$ follows from [60, Theorem 4.1], $d_{\mathcal{X}_i} \geq 0$, and the continuity of $d_{\mathcal{X}_i}$. The existence of a probability measure $\gamma \in \mathcal{P}(\mathcal{X}_1 \times \dots \times \mathcal{X}_N \times \bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N)$ that satisfies the conditions in Definition 2.2.2 follows from the following inductive argument that repeatedly applies Lemma 2.2.1. Specifically, one first applies Lemma 2.2.1 with $\mathcal{Y}_1 := \mathcal{X}_2 \times \dots \times \mathcal{X}_N$, $\mathcal{Y}_2 := \mathcal{X}_1$, $\mathcal{Y}_3 := \bar{\mathcal{X}}_1$ to “glue together” $\hat{\mu}$ and γ_1 and obtain $\gamma^{(1)} \in \mathcal{P}(\mathcal{X}_1 \times \dots \times \mathcal{X}_N \times \bar{\mathcal{X}}_1)$. Subsequently, for $i = 2, \dots, N$, one applies Lemma 2.2.1 with $\mathcal{Y}_1 := \left(\times_{j=1, \dots, N, j \neq i} \mathcal{X}_j \right) \times \left(\times_{k=1, \dots, i-1} \bar{\mathcal{X}}_k \right)$, $\mathcal{Y}_2 := \mathcal{X}_i$, $\mathcal{Y}_3 := \bar{\mathcal{X}}_i$ to “glue together” $\gamma^{(i-1)}$ and γ_i and obtain $\gamma^{(i)} \in \mathcal{P}(\mathcal{X}_1 \times \dots \times \mathcal{X}_N \times \bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_i)$. One may check that $\gamma^{(N)}$ satisfies all the required properties of γ and thus letting $\gamma := \gamma^{(N)}$ completes the construction. Finally, one may check that the marginal $\tilde{\mu}$ of γ on $\bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N$ satisfies $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$. \square

Proof of Theorem 2.2.8. To prove statement (i), let us split the left-hand side of the inequality into two parts:

$$\int_{\mathcal{X}} f d\tilde{\mu} - \int_{\mathcal{X}} f d\hat{\mu} = \left(\int_D f d\tilde{\mu} - \int_D f d\hat{\mu} \right) + \left(\int_{\mathcal{X} \setminus D} f d\tilde{\mu} - \int_{\mathcal{X} \setminus D} f d\hat{\mu} \right) \quad (5.1)$$

and control them separately. By the assumption that $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$ and Definition 2.2.2, there exists a probability measure $\gamma \in \mathcal{P}(\mathcal{X}_1 \times \dots \times \mathcal{X}_N \times \bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N)$, such that the marginal of γ on $\mathcal{X}_1 \times \dots \times \mathcal{X}_N$ is $\hat{\mu}$, the marginal $\gamma_i \in \Gamma(\hat{\mu}_i, \mu_i)$ of γ on $\mathcal{X}_i \times \bar{\mathcal{X}}_i$ satisfies $\int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} d_{\mathcal{X}_i}(x, y) \gamma_i(dx, dy) = W_1(\hat{\mu}_i, \mu_i)$ for $i = 1, \dots, N$, and the marginal of γ on $\bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N$ is $\tilde{\mu}$. Thus, we have by (2.3) that

$$\begin{aligned} \int_D f d\tilde{\mu} - \int_D f d\hat{\mu} &= \int_{D \times D} f(\bar{x}_1, \dots, \bar{x}_N) - f(x_1, \dots, x_N) \gamma(dx_1, \dots, dx_N, d\bar{x}_1, \dots, d\bar{x}_N) \\ &\leq \int_{D \times D} L_f d\mathcal{X}((x_1, \dots, x_N), (\bar{x}_1, \dots, \bar{x}_N)) \gamma(dx_1, \dots, dx_N, d\bar{x}_1, \dots, d\bar{x}_N) \\ &\leq \int_{\mathcal{X} \times \mathcal{X}} L_f d\mathcal{X}((x_1, \dots, x_N), (\bar{x}_1, \dots, \bar{x}_N)) \gamma(dx_1, \dots, dx_N, d\bar{x}_1, \dots, d\bar{x}_N) \\ &= L_f \int_{\mathcal{X} \times \mathcal{X}} \sum_{i=1}^N d_{\mathcal{X}_i}(x_i, \bar{x}_i) \gamma(dx_1, \dots, dx_N, d\bar{x}_1, \dots, d\bar{x}_N) \\ &= \sum_{i=1}^N L_f \int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} d_{\mathcal{X}_i}(x_i, \bar{x}_i) \gamma_i(dx_i, d\bar{x}_i) \\ &= \sum_{i=1}^N L_f W_1(\mu_i, \hat{\mu}_i). \end{aligned} \quad (5.2)$$

Moreover, by the assumption that $\hat{\mu}_i \in [\mu_i]_{\mathcal{G}_i}$ and $\underline{f}_i \in \text{span}_1(\mathcal{G}_i)$ for $i = 1, \dots, N$, we have

$$\begin{aligned} \int_{\mathcal{X} \setminus D} f d\tilde{\mu} - \int_{\mathcal{X} \setminus D} f d\hat{\mu} &\leq \int_{\mathcal{X}} \left(\sum_{i=1}^N \bar{f}_i \circ \pi_i \right) d\tilde{\mu} - \int_{\mathcal{X}} \left(\sum_{i=1}^N \underline{f}_i \circ \pi_i \right) d\hat{\mu} \\ &= \sum_{i=1}^N \left(\int_{\mathcal{X}_i} \bar{f}_i d\mu_i - \int_{\mathcal{X}_i} \underline{f}_i d\hat{\mu}_i \right) \\ &= \sum_{i=1}^N \int_{\mathcal{X}_i} \bar{f}_i - \underline{f}_i d\mu_i. \end{aligned} \quad (5.3)$$

Subsequently, combining (5.1), (5.2), and (5.3) proves statement (i).

To prove statement (ii), observe that for any $\mathbf{x} = (x_1, \dots, x_N) \in \mathcal{X}$, since $(\hat{x}_1, \dots, \hat{x}_N) \in D$, we obtain

$$\begin{aligned} f(\mathbf{x}) &= f(\mathbf{x})\mathbb{1}_D(\mathbf{x}) + f(\mathbf{x})\mathbb{1}_{\mathcal{X} \setminus D}(\mathbf{x}) \\ &\geq -|f(\hat{x}_1, \dots, \hat{x}_N)| - L_f \left(\sum_{i=1}^N d_{\mathcal{X}_i}(x_i, \hat{x}_i) \right) + \left(\sum_{i=1}^N \underline{f}_i(x_i) \right) \\ &\geq -|f(\hat{x}_1, \dots, \hat{x}_N)| - L_f \left(\sum_{i=1}^N h_i(x_i) \right) + \left(\sum_{i=1}^N \underline{f}_i(x_i) \right). \end{aligned} \quad (5.4)$$

Thus, for any $\hat{\mu} \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})$, we have

$$\begin{aligned} \int_{\mathcal{X}} f \, d\hat{\mu} &\geq -|f(\hat{x}_1, \dots, \hat{x}_N)| - L_f \left(\sum_{i=1}^N \int_{\mathcal{X}} h_i \circ \pi_i \, d\hat{\mu} \right) + \sum_{i=1}^N \int_{\mathcal{X}} \underline{f}_i \circ \pi_i \, d\hat{\mu} \\ &= -|f(\hat{x}_1, \dots, \hat{x}_N)| - L_f \left(\sum_{i=1}^N \int_{\mathcal{X}_i} h_i \, d\mu_i \right) + \sum_{i=1}^N \int_{\mathcal{X}_i} \underline{f}_i \, d\mu_i > -\infty, \end{aligned}$$

which does not depend on $\hat{\mu}$. This proves statement (ii).

To prove statement (iii), let us fix an arbitrary $i \in \{1, \dots, N\}$. For any $\nu_i \in [\mu_i]_{\mathcal{G}_i}$, it holds that

$$\begin{aligned} W_1(\mu_i, \nu_i) &\leq W_1(\mu_i, \delta_{\hat{x}_i}) + W_1(\nu_i, \delta_{\hat{x}_i}) \\ &= W_1(\mu_i, \delta_{\hat{x}_i}) + \int_{\mathcal{X}_i} d_{\mathcal{X}_i}(\hat{x}_i, x) \nu_i(dx) \\ &\leq W_1(\mu_i, \delta_{\hat{x}_i}) + \int_{\mathcal{X}_i} h_i(x) \nu_i(dx) \\ &= W_1(\mu_i, \delta_{\hat{x}_i}) + \int_{\mathcal{X}_i} h_i(x) \mu_i(dx) \\ &< \infty. \end{aligned}$$

Thus, $\overline{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i}) = \sup_{\nu_i \in [\mu_i]_{\mathcal{G}_i}} \{W_1(\mu_i, \nu_i)\} \leq W_1(\mu_i, \delta_{\hat{x}_i}) + \int_{\mathcal{X}} h_i(x) \mu_i(dx) < \infty$, which proves statement (iii).

Let us now prove statement (iv). For $i = 1, \dots, N$, let $\hat{\mu}_i \in \mathcal{P}_1(\mathcal{X}_i)$ denote the marginal of $\hat{\mu}$ on \mathcal{X}_i . We have $\hat{\mu}_i \in [\mu_i]_{\mathcal{G}_i}$ by the definition of $\Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})$. By statement (i), we have

$$\begin{aligned} \int_{\mathcal{X}} f \, d\tilde{\mu} - \int_{\mathcal{X}} f \, d\hat{\mu} &\leq \sum_{i=1}^N \left(L_f W_1(\mu_i, \hat{\mu}_i) + \int_{\mathcal{X}_i} \bar{f}_i - \underline{f}_i \, d\mu_i \right) \\ &\leq \sum_{i=1}^N \left(L_f \overline{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i}) + \int_{\mathcal{X}_i} \bar{f}_i - \underline{f}_i \, d\mu_i \right). \end{aligned} \quad (5.5)$$

Moreover, since by definition $\mu_i \in [\mu_i]_{\mathcal{G}_i}$ for $i = 1, \dots, N$, we have $\Gamma(\mu_1, \dots, \mu_N) \subseteq \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})$. Hence,

$$\inf_{\mu \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} \leq \inf_{\mu \in \Gamma(\mu_1, \dots, \mu_N)} \left\{ \int_{\mathcal{X}} f \, d\mu \right\}. \quad (5.6)$$

We then combine (5.5), (2.9), and (5.6) to finish the proof of statement (iv).

Finally, let us prove statement (v). The first inequality in (2.10) follows from (5.6). Moreover, for every $\hat{\mu} \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})$ and every $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N) \subset \Gamma(\mu_1, \dots, \mu_N)$, we have by (5.5) that

$$\begin{aligned} \inf_{\mu \in \Gamma(\mu_1, \dots, \mu_N)} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} - \int_{\mathcal{X}} f \, d\hat{\mu} &\leq \int_{\mathcal{X}} f \, d\tilde{\mu} - \int_{\mathcal{X}} f \, d\hat{\mu} \\ &\leq \sum_{i=1}^N \left(L_f \overline{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i}) + \int_{\mathcal{X}_i} \bar{f}_i - \underline{f}_i \, d\mu_i \right) < \infty. \end{aligned}$$

By taking the infimum over $\hat{\mu} \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})$ in the inequality above, we conclude that the second inequality in (2.10) holds. The proof is now complete. \square

Proof of Theorem 2.2.10. By a multi-marginal extension of [60, Lemma 4.4], one can show that $\Gamma(\mu_1, \dots, \mu_N)$ is weakly precompact. Hence, $(\tilde{\mu}^{(l)})_{l \in \mathbb{N}}$ has at least one weakly convergent subsequence. Now, assume without loss of generality that $\tilde{\mu}^{(l)}$ converges weakly to $\tilde{\mu}$ as $l \rightarrow \infty$, where $\tilde{\mu} \in \mathcal{P}(\mathcal{X})$. For $i = 1, \dots, N$ and for any bounded continuous function $h : \mathcal{X}_i \rightarrow \mathbb{R}$, we have

$$\int_{\mathcal{X}} h \circ \pi_i d\tilde{\mu} = \lim_{l \rightarrow \infty} \int_{\mathcal{X}} h \circ \pi_i d\tilde{\mu}^{(l)} = \int_{\mathcal{X}_i} h d\mu_i.$$

Thus, $\tilde{\mu} \in \Gamma(\mu_1, \dots, \mu_N)$. Moreover, for any $\hat{x} = (\hat{x}_1, \dots, \hat{x}_N) \in \mathcal{X}$, we have

$$\lim_{l \rightarrow \infty} \int_{\mathcal{X}} d_{\mathcal{X}}(\hat{x}, x) \tilde{\mu}^{(l)}(dx) = \sum_{i=1}^N \int_{\mathcal{X}_i} d_{\mathcal{X}_i}(\hat{x}_i, x) \mu_i(dx) = \int_{\mathcal{X}} d_{\mathcal{X}}(\hat{x}, x) \tilde{\mu}(dx).$$

Therefore, we have by [60, Definition 6.8] and [60, Theorem 6.9] that $\tilde{\mu}^{(l)} \rightarrow \tilde{\mu}$ in $(\mathcal{P}_1(\mathcal{X}), W_1)$ as $l \rightarrow \infty$. By (5.5), we have for every $l \in \mathbb{N}$ that

$$\int_{\mathcal{X}} f d\tilde{\mu}^{(l)} \leq \int_{\mathcal{X}} f d\hat{\mu}^{(l)} + \sum_{i=1}^N \left(L_f^{(l)} \overline{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i^{(l)}}) + \int_{\mathcal{X}_i} \bar{f}_i^{(l)} - \underline{f}_i^{(l)} d\mu_i \right).$$

Thus, for every $l \in \mathbb{N}$, we have by (2.11) and Theorem 2.2.8(iv) that

$$\inf_{\mu \in \Gamma(\mu_1, \dots, \mu_N)} \left\{ \int_{\mathcal{X}} f d\mu \right\} \geq \int_{\mathcal{X}} f d\tilde{\mu}^{(l)} - \left(\sum_{i=1}^N L_f^{(l)} \overline{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i^{(l)}}) + \int_{\mathcal{X}_i} \bar{f}_i^{(l)} - \underline{f}_i^{(l)} d\mu_i \right) - \epsilon^{(l)}.$$

Moreover, by Assumption 2.1.3 and a multi-marginal extension of [60, Lemma 4.3], we have $\liminf_{l \rightarrow \infty} \left\{ \int_{\mathcal{X}} f d\tilde{\mu}^{(l)} \right\} \geq \int_{\mathcal{X}} f d\tilde{\mu}$. Hence,

$$\begin{aligned} \int_{\mathcal{X}} f d\tilde{\mu} &\geq \inf_{\mu \in \Gamma(\mu_1, \dots, \mu_N)} \left\{ \int_{\mathcal{X}} f d\mu \right\} \\ &\geq \liminf_{l \rightarrow \infty} \left[\int_{\mathcal{X}} f d\tilde{\mu}^{(l)} - \left(\sum_{i=1}^N L_f^{(l)} \overline{W}_{1, \mu_i}([\mu_i]_{\mathcal{G}_i^{(l)}}) + \int_{\mathcal{X}_i} \bar{f}_i^{(l)} - \underline{f}_i^{(l)} d\mu_i \right) - \epsilon^{(l)} \right] \\ &\geq \int_{\mathcal{X}} f d\tilde{\mu}. \end{aligned}$$

This shows that $\tilde{\mu}$ is an optimizer of (MMOT). The proof is now complete. \square

5.2. Proof of results in Section 2.3.

Proof of Theorem 2.3.1. For any $y_0 \in \mathbb{R}$ and $\mathbf{y} \in \mathbb{R}^m$ such that $y_0 + \langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle \leq f(\mathbf{x}) \forall \mathbf{x} \in \mathcal{X}$, and any $\mu \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})$, it holds that

$$y_0 + \langle \mathbf{y}, \mathbf{v} \rangle = \int_{\mathcal{X}} y_0 + \langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle \mu(d\mathbf{x}) \leq \int_{\mathcal{X}} f(\mathbf{x}) \mu(d\mathbf{x}). \quad (5.7)$$

Taking the supremum over all such $y_0 \in \mathbb{R}$ and $\mathbf{y} \in \mathbb{R}^m$ and taking the infimum over all $\mu \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})$ yields the weak duality (2.14). This proves statement (i).

Now, to establish the strong duality, we assume that the left-hand side of (2.14) is not $-\infty$. We first show that $\mathbf{v} \in \text{cl}(K)$. Suppose, for the sake of contradiction, that $\mathbf{v} \notin \text{cl}(K)$. Then, due to strong separation (see, e.g., [52, Corollary 11.4.2]), there exist $\mathbf{y} \in \mathbb{R}^m$ and $\alpha > 0$ such that $\langle \mathbf{y}, \mathbf{w} \rangle - \langle \mathbf{y}, \mathbf{v} \rangle \geq \alpha$ for all $\mathbf{w} \in \text{cl}(K)$. In particular, we have $\langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle - \langle \mathbf{y}, \mathbf{v} \rangle \geq \alpha$ for all $\mathbf{x} \in \mathcal{X}$. However, this implies that for any $\mu \in \Gamma(\mu_1, \dots, \mu_N)$, we have

$$0 = \langle \mathbf{y}, \mathbf{v} \rangle - \langle \mathbf{y}, \mathbf{v} \rangle = \int_{\mathcal{X}} \langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle - \langle \mathbf{y}, \mathbf{v} \rangle \mu(d\mathbf{x}) \geq \alpha > 0,$$

which is a contradiction. This shows that $\mathbf{v} \in \text{cl}(K)$.

Next, to prove statement (ii), let us first suppose that the condition (SD1) holds, i.e., $\mathbf{v} \in \text{relint}(K)$. Let $U := \text{cone}\left(\left\{(1, \mathbf{g}(\mathbf{x})^\top)^\top : \mathbf{x} \in \mathcal{X}\right\}\right) = \text{cone}\left(\left\{(1, \mathbf{u}^\top)^\top : \mathbf{u} \in K\right\}\right) \subset \mathbb{R}^{m+1}$. By [52, Corollary 6.8.1], it holds that

$$\text{relint}(U) = \{(\lambda, \lambda \mathbf{u}^\top)^\top : \lambda > 0, \mathbf{u} \in \text{relint}(K)\}. \quad (5.8)$$

Under the assumption that $\mathbf{v} \in \text{relint}(K)$, we have $(1, \mathbf{v}^\top)^\top \in \text{relint}(U)$, and thus by [35, Theorem 8.2] (see the fifth case in [35, Table 8.1]), with $M \leftarrow U$, $N \leftarrow C$, $K \leftarrow \text{cone}\left(C \cup \{(\mathbf{0}_{m+1}^\top, 1)^\top\}\right)$, $c \leftarrow (1, \mathbf{v}^\top)^\top$ in the notation of [35] (see also [35, p. 81 & p. 49]), the left-hand side of (2.14) coincides with the optimal value of the following problem:

$$\begin{aligned} & \underset{(\alpha_l, \mathbf{x}_l)}{\text{minimize}} && \sum_{l=1}^k \alpha_l f(\mathbf{x}_l) \\ & \text{subject to} && \sum_{l=1}^k \alpha_l = 1, \\ & && \sum_{l=1}^k \alpha_l \mathbf{g}(\mathbf{x}_l) = \mathbf{v}, \\ & && k \in \mathbb{N}, (\alpha_l)_{l=1:k} \subset \mathbb{R}_+, (\mathbf{x}_l)_{l=1:k} \subset \mathcal{X}. \end{aligned} \quad (5.9)$$

Notice that for any $(\alpha_l)_{l=1:k} \subset \mathbb{R}_+$, $(\mathbf{x}_l)_{l=1:k} \subset \mathcal{X}$ that is feasible for problem (5.9), it holds by (2.12) and (2.13) that $\hat{\mu} := \sum_{l=1}^k \alpha_l \delta_{\mathbf{x}_l}$ is a positive Borel measure which satisfies

$$\begin{aligned} \hat{\mu}(\mathcal{X}) &= \sum_{l=1}^k \alpha_l = 1, \\ \int_{\mathcal{X}} g_{i,j} \circ \pi_i \, d\hat{\mu} &= \sum_{l=1}^k \alpha_l g_{i,j} \circ \pi_i(\mathbf{x}_l) = \int_{\mathcal{X}_i} g_{i,j} \, d\mu_i \quad \forall 1 \leq j \leq m_i, \forall 1 \leq i \leq N. \end{aligned}$$

This shows that $\hat{\mu} \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})$. Moreover, since $\int_{\mathcal{X}} f \, d\hat{\mu} = \sum_{l=1}^k \alpha_l f(\mathbf{x}_l)$, it holds that $\inf_{\mu \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})} \left\{ \int_{\mathcal{X}} f \, d\mu \right\}$ is less than or equal to the optimal value of problem (5.9). Consequently, (2.17) holds.

In the following, we assume that $\mathbf{v} \notin \text{relint}(K)$ (i.e., the condition (SD1) does not hold). Then, while we have $(1, \mathbf{v}^\top)^\top \in \{1\} \times \text{cl}(K) \subset \text{cl}(U)$, we have by (5.8) that $(1, \mathbf{v}^\top)^\top \notin \text{relint}(U)$. Hence, $(1, \mathbf{v}^\top)^\top \in \text{relbd}(U)$. Now, suppose that the condition (SD3) holds, i.e., C is closed. By the assumption that the left-hand side of (2.14) is not $-\infty$, we have by [35, Theorem 4.5], again with $M \leftarrow U$, $N \leftarrow C$, $K \leftarrow \text{cone}\left(C \cup \{(\mathbf{0}_{m+1}^\top, 1)^\top\}\right)$, $c \leftarrow (1, \mathbf{v}^\top)^\top$ in the notation of [35], that $\text{cone}\left(C \cup \{(\mathbf{0}_{m+1}^\top, 1)^\top\}\right)$ is also closed. Thus, (2.17) follows from [35, Theorem 8.2] (see the sixth case in [35, Table 8.1]) and a similar argument as above. We have thus proved statement (ii). Moreover, note that statement (iii) follows directly from [35, Theorem 8.1(v)] since $(1, \mathbf{v}^\top)^\top \in \text{relint}(U)$ by (5.8).

Finally, if the condition (SD2) holds, then K has non-empty interior, and thus contains $m+1$ affinely independent points, say $\mathbf{g}(\mathbf{x}_1), \dots, \mathbf{g}(\mathbf{x}_{m+1})$ for some $\mathbf{x}_1, \dots, \mathbf{x}_{m+1} \in \mathcal{X}$. Consequently, $(0, \mathbf{0}_m^\top)^\top, (1, \mathbf{g}(\mathbf{x}_1)^\top)^\top, \dots, (1, \mathbf{g}(\mathbf{x}_{m+1})^\top)^\top \in U$ are $m+2$ affinely independent points in \mathbb{R}^{m+1} , which implies that $\text{aff}(U) = \mathbb{R}^{m+1}$ and $(1, \mathbf{v}^\top)^\top \in \text{relint}(U) = \text{int}(U)$. Statement (iv) then follows from [35, Theorem 8.1(vi)]. The proof is now complete. \square

Proof of Proposition 2.3.3. Let us first prove statement (i). Suppose, for the sake of contradiction, that $\mathbf{v} \notin \text{relint}(K)$. Since K is convex, by [52, Theorem 20.2], there exists a hyperplane

$$H := \{\mathbf{w} \in \mathbb{R}^m : \langle \mathbf{y}, \mathbf{w} \rangle = \alpha\},$$

where $\mathbf{y} = (y_{1,1}, \dots, y_{1,m_1}, \dots, y_{N,1}, \dots, y_{N,m_N}) \in \mathbb{R}^m$ with $\mathbf{y} \neq \mathbf{0}$ and $\alpha \in \mathbb{R}$, that separates K and $\{\mathbf{v}\}$ properly and that $K \not\subset H$. Suppose without loss of generality that \mathbf{v} is contained in the closed

half-space $\{\mathbf{w} \in \mathbb{R}^m : \langle \mathbf{y}, \mathbf{w} \rangle \leq \alpha\}$. Then, we have $\langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle \geq \alpha \geq \langle \mathbf{y}, \mathbf{v} \rangle$ for all $\mathbf{x} \in \mathcal{X}$. This implies that

$$\sum_{i=1}^N \sum_{j=1}^{m_i} y_{i,j} \left(g_{i,j}(x_i) - \int_{\mathcal{X}_i} g_{i,j} d\mu_i \right) \geq 0 \quad \forall x_1 \in \mathcal{X}_1, \dots, \forall x_N \in \mathcal{X}_N. \quad (5.10)$$

We claim that for each i satisfying $\sum_{j=1}^{m_i} y_{i,j} \left(g_{i,j}(x_i) - \int_{\mathcal{X}_i} g_{i,j} d\mu_i \right) \geq 0$ for all $x_i \in \mathcal{X}_i$, it holds that $\sum_{j=1}^{m_i} y_{i,j} \left(g_{i,j}(x_i) - \int_{\mathcal{X}_i} g_{i,j} d\mu_i \right) = 0$ for all $x_i \in \mathcal{X}_i$. If the claim holds, then we can conclude by (5.10) that $\sum_{i=1}^N \sum_{j=1}^{m_i} y_{i,j} \left(g_{i,j}(x_i) - \int_{\mathcal{X}_i} g_{i,j} d\mu_i \right) = 0$ for all $x_1 \in \mathcal{X}_1, \dots, x_N \in \mathcal{X}_N$.

Let us now prove the claim. Suppose, for the sake of contradiction, that for i satisfying $\sum_{j=1}^{m_i} y_{i,j} \left(g_{i,j}(x_i) - \int_{\mathcal{X}_i} g_{i,j} d\mu_i \right) \geq 0$ for all $x_i \in \mathcal{X}_i$, there exists $\hat{x}_i \in \mathcal{X}_i$ such that $\sum_{j=1}^{m_i} y_{i,j} \left(g_{i,j}(\hat{x}_i) - \int_{\mathcal{X}_i} g_{i,j} d\mu_i \right) = \beta > 0$. Then, by the continuity of $g_{i,1}, \dots, g_{i,m_i}$, there exists an open set $E \subset \mathcal{X}_i$ such that $\hat{x}_i \in E$ and

$$\sum_{j=1}^{m_i} y_{i,j} \left(g_{i,j}(x_i) - \int_{\mathcal{X}_i} g_{i,j} d\mu_i \right) > \frac{\beta}{2} \quad \forall x_i \in E.$$

By the assumption that $\text{supp}(\mu_i) = \mathcal{X}_i$, we have $\mu_i(E) > 0$. Thus,

$$\begin{aligned} 0 &= \int_{\mathcal{X}_i} \sum_{j=1}^{m_i} y_{i,j} \left(g_{i,j}(x_i) - \int_{\mathcal{X}_i} g_{i,j} d\mu_i \right) \mu_i(dx_i) \\ &\geq \int_E \sum_{j=1}^{m_i} y_{i,j} \left(g_{i,j}(x_i) - \int_{\mathcal{X}_i} g_{i,j} d\mu_i \right) \mu_i(dx_i) \\ &\geq \frac{\beta \mu_i(E)}{2} > 0, \end{aligned}$$

which is a contradiction. Hence, the claim holds.

Therefore, we have shown that indeed $\sum_{i=1}^N \sum_{j=1}^{m_i} y_{i,j} \left(g_{i,j}(x_i) - \int_{\mathcal{X}_i} g_{i,j} d\mu_i \right) = 0$ holds for all $x_1 \in \mathcal{X}_1, \dots, x_N \in \mathcal{X}_N$. This shows that $\langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle = \langle \mathbf{y}, \mathbf{v} \rangle = \alpha$ for all $\mathbf{x} \in \mathcal{X}$, which implies that $\langle \mathbf{y}, \mathbf{w} \rangle = \langle \mathbf{y}, \mathbf{v} \rangle = \alpha$ for all $\mathbf{w} \in K$. Thus, $K \subseteq H$, which contradicts $K \not\subseteq H$. The proof of statement (i) is now complete.

To prove statement (ii), let $K_i := \text{conv}(\{\mathbf{g}_i(x_i) : x_i \in \mathcal{X}_i\})$ for $i = 1, \dots, N$. It follows from (2.12) and (2.15) that $K = \times_{i=1}^N K_i$. Since K_i contains $\text{conv}(\{\mathbf{g}_i(x_{i,1}), \dots, \mathbf{g}_i(x_{i,m_i+1})\})$, which is an m_i -simplex, we have $\text{aff}(K_i) = \mathbb{R}^{m_i}$. Therefore, $\text{aff}(K) = \times_{i=1}^N \mathbb{R}^{m_i} = \mathbb{R}^m$ and $\text{relint}(K) = \text{int}(K)$. Consequently, statement (ii) follows from statement (i).

Finally, to prove statement (iii), notice that if \mathcal{X}_i is compact, \mathcal{G}_i contains only continuous functions for $i = 1, \dots, N$, and f is continuous, then the set $S := \{(1, \mathbf{g}(\mathbf{x})^\top, f(\mathbf{x}))^\top : \mathbf{x} \in \mathcal{X}\}$ is compact. By [52, Theorem 17.2], it holds that $\text{conv}(S)$ is also compact. Since $C := \text{cone}(S) = \text{cone}(\text{conv}(S))$ and $\mathbf{0} \notin \text{conv}(S)$, the condition (SD3) in Theorem 2.3.1 follows from [52, Corollary 9.6.1]. \square

5.3. Proof of results in Section 3.1.

Proof of Lemma 3.1.1. In this proof, we let $\widetilde{\mathbb{R}}^k := \mathbb{R}^k$ for $k \in \mathbb{N}$ in order to differentiate different copies of the same Euclidean space. Let us first suppose that $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$ for some $\hat{\mu}, \tilde{\mu} \in \mathcal{P}_1(\mathcal{X})$. For $i = 1, \dots, N$, let $\hat{\mu}_i$ denote the i -th marginal of $\hat{\mu}$ and let $\hat{\mu}_i^\dagger$ denote the i -th marginal of $\hat{\mu}^\dagger$. By Definition 2.2.2, $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$ implies that there exists $\gamma \in \mathcal{P}(\mathcal{X}_1 \times \dots \times \mathcal{X}_N \times \bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N)$ such that the marginal of γ on $\mathcal{X}_1 \times \dots \times \mathcal{X}_N$ is $\hat{\mu}$, the marginal of γ on $\bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N$ is $\tilde{\mu}$, and the marginal γ_i of γ on $\mathcal{X}_i \times \bar{\mathcal{X}}_i$ satisfies $\int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} d\mathcal{X}_i(\mathbf{x}, \mathbf{y}) \gamma_i(d\mathbf{x}, d\mathbf{y}) = W_1(\hat{\mu}_i, \mu_i)$ for $i = 1, \dots, N$. Let us define $\gamma^\dagger \in \mathcal{P}(\mathbb{R}^{m_1} \times \dots \times \mathbb{R}^{m_N} \times \widetilde{\mathbb{R}}^{m_1} \times \dots \times \widetilde{\mathbb{R}}^{m_N})$ by $\gamma^\dagger(E) := \gamma(E \cap (\mathcal{X}_1 \times \dots \times \mathcal{X}_N \times \bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N))$ for all $E \in \mathcal{B}(\mathbb{R}^{2m})$. Then, by construction, the marginal of γ^\dagger on $\mathbb{R}^{m_1} \times \dots \times \mathbb{R}^{m_N}$ is exactly $\hat{\mu}^\dagger$ and the marginal of γ^\dagger on $\widetilde{\mathbb{R}}^{m_1} \times \dots \times \widetilde{\mathbb{R}}^{m_N}$ is exactly $\tilde{\mu}^\dagger$. For $i = 1, \dots, N$, let us denote the marginal of

γ^\dagger on $\mathbb{R}^{m_i} \times \widetilde{\mathbb{R}}^{m_i}$ by γ_i^\dagger . By construction, for $i = 1, \dots, N$, $\gamma_i^\dagger(E) = \gamma_i(E)$ for all $E \in \mathcal{B}(\mathcal{X}_i \times \bar{\mathcal{X}}_i)$ and in particular $\gamma_i^\dagger(\mathcal{X}_i \times \bar{\mathcal{X}}_i) = 1$. Thus,

$$\begin{aligned} \int_{\mathbb{R}^{m_i} \times \widetilde{\mathbb{R}}^{m_i}} \|\mathbf{x} - \mathbf{y}\| \gamma_i^\dagger(d\mathbf{x}, d\mathbf{y}) &= \int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} \|\mathbf{x} - \mathbf{y}\| \gamma_i^\dagger(d\mathbf{x}, d\mathbf{y}) \\ &= \int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} d\mathcal{X}_i(\mathbf{x}, \mathbf{y}) \gamma_i(d\mathbf{x}, d\mathbf{y}) \\ &= W_1(\hat{\mu}_i, \mu_i). \end{aligned}$$

Moreover, for any $\theta_i^\dagger \in \Gamma(\hat{\mu}_i^\dagger, \mu_i^\dagger) \subset \mathcal{P}(\mathbb{R}^{m_i} \times \widetilde{\mathbb{R}}^{m_i})$, we have $\theta_i^\dagger((\mathbb{R}^{m_i} \times \widetilde{\mathbb{R}}^{m_i}) \setminus (\mathcal{X}_i \times \bar{\mathcal{X}}_i)) \leq \hat{\mu}_i^\dagger(\mathbb{R}^{m_i} \setminus \mathcal{X}_i) + \mu_i^\dagger(\widetilde{\mathbb{R}}^{m_i} \setminus \bar{\mathcal{X}}_i) = 0$ and thus $\theta_i^\dagger(\mathcal{X}_i \times \bar{\mathcal{X}}_i) = 1$. Let us define $\theta_i \in \mathcal{P}(\mathcal{X}_i \times \bar{\mathcal{X}}_i)$ by $\theta_i(E) := \theta_i^\dagger(E)$ for all $E \in \mathcal{B}(\mathcal{X}_i \times \bar{\mathcal{X}}_i)$. Then, since $\theta_i \in \Gamma(\hat{\mu}_i, \mu_i)$,

$$\begin{aligned} \int_{\mathbb{R}^{m_i} \times \widetilde{\mathbb{R}}^{m_i}} \|\mathbf{x} - \mathbf{y}\| \theta_i^\dagger(d\mathbf{x}, d\mathbf{y}) &= \int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} \|\mathbf{x} - \mathbf{y}\| \theta_i^\dagger(d\mathbf{x}, d\mathbf{y}) \\ &= \int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} d\mathcal{X}_i(\mathbf{x}, \mathbf{y}) \theta_i(d\mathbf{x}, d\mathbf{y}) \\ &\geq W_1(\hat{\mu}_i, \mu_i) \\ &= \int_{\mathbb{R}^{m_i} \times \widetilde{\mathbb{R}}^{m_i}} \|\mathbf{x} - \mathbf{y}\| \gamma_i^\dagger(d\mathbf{x}, d\mathbf{y}). \end{aligned}$$

This shows that γ_i^\dagger is an optimal coupling between $\hat{\mu}_i^\dagger$ and μ_i^\dagger under the cost function induced by the norm $\|\cdot\|$ on \mathbb{R}^{m_i} . Consequently, by Definition 2.2.2, it holds that $\tilde{\mu}^\dagger \in R(\hat{\mu}^\dagger; \mu_1^\dagger, \dots, \mu_N^\dagger)$.

Conversely, let us suppose that $\tilde{\mu}^\dagger \in R(\hat{\mu}^\dagger; \mu_1^\dagger, \dots, \mu_N^\dagger)$ for some $\hat{\mu}, \tilde{\mu} \in \mathcal{P}_1(\mathcal{X})$. Again, for $i = 1, \dots, N$, let $\hat{\mu}_i$ denote the i -th marginal of $\hat{\mu}$ and let $\hat{\mu}_i^\dagger$ denote the i -th marginal of $\hat{\mu}^\dagger$. By Definition 2.2.2, this implies that there exists $\gamma^\dagger \in \mathcal{P}(\mathbb{R}^{m_1} \times \dots \times \mathbb{R}^{m_N} \times \widetilde{\mathbb{R}}^{m_1} \times \dots \times \widetilde{\mathbb{R}}^{m_N})$ such that the marginal of γ^\dagger on $\mathbb{R}^{m_1} \times \dots \times \mathbb{R}^{m_N}$ is $\hat{\mu}^\dagger$, the marginal of γ^\dagger on $\widetilde{\mathbb{R}}^{m_1} \times \dots \times \widetilde{\mathbb{R}}^{m_N}$ is $\tilde{\mu}^\dagger$, and the marginal γ_i^\dagger of γ^\dagger on $\mathbb{R}^{m_i} \times \widetilde{\mathbb{R}}^{m_i}$ satisfies $\int_{\mathbb{R}^{m_i} \times \widetilde{\mathbb{R}}^{m_i}} \|\mathbf{x} - \mathbf{y}\| \gamma_i^\dagger(d\mathbf{x}, d\mathbf{y}) = W_1(\hat{\mu}_i^\dagger, \mu_i^\dagger)$ for $i = 1, \dots, N$. Since $\gamma^\dagger(\mathcal{X}_1 \times \dots \times \mathcal{X}_N \times \bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N) = 1$, let us define $\gamma \in \mathcal{P}(\mathcal{X}_1 \times \dots \times \mathcal{X}_N \times \bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N)$ by $\gamma(E) := \gamma^\dagger(E)$ for all $E \in \mathcal{B}(\mathcal{X}_1 \times \dots \times \mathcal{X}_N \times \bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N)$. Then, by construction, the marginal of γ on $\mathcal{X}_1 \times \dots \times \mathcal{X}_N$ is exactly $\hat{\mu}$ and the marginal of γ on $\bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N$ is exactly $\tilde{\mu}$. For $i = 1, \dots, N$, denote the marginal of γ on $\mathcal{X}_i \times \bar{\mathcal{X}}_i$ by γ_i . By construction, for $i = 1, \dots, N$, $\gamma_i(E) = \gamma_i^\dagger(E)$ for all $E \in \mathcal{B}(\mathcal{X}_i \times \bar{\mathcal{X}}_i)$. Thus,

$$\begin{aligned} \int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} d\mathcal{X}_i(\mathbf{x}, \mathbf{y}) \gamma_i(d\mathbf{x}, d\mathbf{y}) &= \int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} \|\mathbf{x} - \mathbf{y}\| \gamma_i^\dagger(d\mathbf{x}, d\mathbf{y}) \\ &= \int_{\mathbb{R}^{m_i} \times \widetilde{\mathbb{R}}^{m_i}} \|\mathbf{x} - \mathbf{y}\| \gamma_i^\dagger(d\mathbf{x}, d\mathbf{y}) \\ &= W_1(\hat{\mu}_i^\dagger, \mu_i^\dagger). \end{aligned}$$

Moreover, for any $\theta_i \in \Gamma(\hat{\mu}_i, \mu_i) \subset \mathcal{P}(\mathcal{X}_i \times \bar{\mathcal{X}}_i)$, let us define $\theta_i^\dagger \in \mathcal{P}(\mathbb{R}^{m_i} \times \widetilde{\mathbb{R}}^{m_i})$ by $\theta_i^\dagger(E) := \theta_i(E \cap (\mathcal{X}_i \times \bar{\mathcal{X}}_i))$ for all $E \in \mathcal{B}(\mathbb{R}^{m_i} \times \widetilde{\mathbb{R}}^{m_i})$. Then,

$$\begin{aligned} \int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} d\mathcal{X}_i(\mathbf{x}, \mathbf{y}) \theta_i(d\mathbf{x}, d\mathbf{y}) &= \int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} \|\mathbf{x} - \mathbf{y}\| \theta_i^\dagger(d\mathbf{x}, d\mathbf{y}) \\ &= \int_{\mathbb{R}^{m_i} \times \widetilde{\mathbb{R}}^{m_i}} \|\mathbf{x} - \mathbf{y}\| \theta_i^\dagger(d\mathbf{x}, d\mathbf{y}) \\ &\geq W_1(\hat{\mu}_i^\dagger, \mu_i^\dagger) \\ &= \int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} d\mathcal{X}_i(\mathbf{x}, \mathbf{y}) \gamma_i(d\mathbf{x}, d\mathbf{y}). \end{aligned}$$

This shows that γ_i is an optimal coupling between $\hat{\mu}_i$ and μ_i under the cost function $d_{\mathcal{X}_i}$. Consequently, by Definition 2.2.2, it holds that $\tilde{\mu} \in R(\hat{\mu}; \mu_1, \dots, \mu_N)$. The proof is now complete. \square

Proof of Proposition 3.1.2. Let us fix an arbitrary $i \in \{1, \dots, N\}$ and prove statement (i). Since $d_{\mathcal{X}_i}$ is continuous and non-negative, we have by the Kantorovich duality in the optimal transport theory (see, e.g., [60, Theorem 5.10]) that

$$\begin{aligned} W_1(\mu_i, \hat{\mu}_i) &= \inf_{\gamma \in \Gamma(\mu_i, \hat{\mu}_i)} \int_{\mathbb{R}^{m_i} \times \mathbb{R}^{m_i}} d_{\mathcal{X}_i}(\mathbf{z}, \mathbf{x}) \gamma(d\mathbf{z}, d\mathbf{x}) \\ &= \sup_{\phi \in \mathcal{L}^1(\mathbb{R}^{m_i}, \hat{\mu}_i)} \left\{ \int_{\mathbb{R}^{m_i}} \phi(\mathbf{x}) \hat{\mu}_i(d\mathbf{x}) - \int_{\mathbb{R}^{m_i}} \phi^{d_{\mathcal{X}_i}}(\mathbf{z}) \mu_i(d\mathbf{z}) \right\}, \end{aligned} \quad (5.11)$$

where $\phi^{d_{\mathcal{X}_i}}(\mathbf{z}) := \sup_{\mathbf{x} \in \mathbb{R}^{m_i}} \{\phi(\mathbf{x}) - d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{z})\}$ is known as the c -transform of ϕ (see, e.g., [60, Definition 5.7]; c refers to the cost function, i.e., $d_{\mathcal{X}_i}$ in our case). For a fixed $\mathbf{v} \in \mathbb{R}^{m_i}$, we have $d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{z}) \leq d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{v}) + d_{\mathcal{X}_i}(\mathbf{z}, \mathbf{v})$ for all $\mathbf{x}, \mathbf{z} \in \mathbb{R}^{m_i}$. Moreover, $d_{\mathcal{X}_i}(\cdot, \mathbf{v}) \in \mathcal{L}^1(\mathbb{R}^{m_i}, \hat{\mu}_i)$, and $d_{\mathcal{X}_i}(\cdot, \mathbf{v}) \in \mathcal{L}^1(\mathbb{R}^{m_i}, \mu_i)$. Therefore, by part (iii) of [60, Theorem 5.10], the supremum in (5.11) can be attained at some $\phi^* \in \mathcal{L}^1(\mathbb{R}^{m_i}, \hat{\mu}_i)$. We will show that

$$\int_{\mathbb{R}^{m_i}} \sup_{\mathbf{x} \in \mathbb{R}^{m_i}} \{\phi^*(\mathbf{x}) - d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{z})\} \mu_i(d\mathbf{z}) = \int_{\mathbb{R}^{m_i}} \max_{1 \leq j \leq J_i} \{\phi^*(\mathbf{x}_{i,j}) - d_{\mathcal{X}_i}(\mathbf{x}_{i,j}, \mathbf{z})\} \mu_i(d\mathbf{z}). \quad (5.12)$$

Suppose, for the sake of contradiction, that (5.12) does not hold. Then, since $\sup_{\mathbf{x} \in \mathbb{R}^{m_i}} \{\phi^*(\mathbf{x}) - d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{z})\} \geq \max_{1 \leq j \leq J_i} \{\phi^*(\mathbf{x}_{i,j}) - d_{\mathcal{X}_i}(\mathbf{x}_{i,j}, \mathbf{z})\}$ for all $\mathbf{z} \in \mathbb{R}^{m_i}$, there exist $\beta > 0$ and a set $E_\beta \subset \mathbb{R}^{m_i}$ given by

$$E_\beta := \left\{ \mathbf{z} \in \mathbb{R}^{m_i} : \sup_{\mathbf{x} \in \mathbb{R}^{m_i}} \{\phi^*(\mathbf{x}) - d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{z})\} - \max_{1 \leq j \leq J_i} \{\phi^*(\mathbf{x}_{i,j}) - d_{\mathcal{X}_i}(\mathbf{x}_{i,j}, \mathbf{z})\} > \beta \right\}$$

such that $\mu_i(E_\beta) > 0$. Subsequently, let us define $\phi' \in \mathcal{L}^1(\mathbb{R}^{m_i}, \hat{\mu}_i)$ as follows:

$$\phi'(\mathbf{x}) := \begin{cases} \phi^*(\mathbf{x}) & \text{if } \mathbf{x} = \mathbf{x}_{i,j} \text{ for some } j \in \{1, \dots, J_i\}, \\ \phi^*(\mathbf{x}) - \beta & \text{if } \mathbf{x} \neq \mathbf{x}_{i,j} \text{ for all } j \in \{1, \dots, J_i\}. \end{cases}$$

Then, by the definition of E_β , we have

$$\begin{aligned} \sup_{\mathbf{x} \in \mathbb{R}^{m_i}} \{\phi^*(\mathbf{x}) - d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{z})\} &\geq \sup_{\mathbf{x} \in \mathbb{R}^{m_i}} \{\phi'(\mathbf{x}) - d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{z})\} + \beta \quad \forall \mathbf{z} \in E_\beta, \\ \sup_{\mathbf{x} \in \mathbb{R}^{m_i}} \{\phi^*(\mathbf{x}) - d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{z})\} &\geq \sup_{\mathbf{x} \in \mathbb{R}^{m_i}} \{\phi'(\mathbf{x}) - d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{z})\} \quad \forall \mathbf{z} \in \mathbb{R}^{m_i} \setminus E_\beta. \end{aligned}$$

Hence,

$$\int_{\mathbb{R}^{m_i}} \sup_{\mathbf{x} \in \mathbb{R}^{m_i}} \{\phi^*(\mathbf{x}) - d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{z})\} \mu_i(d\mathbf{z}) - \int_{\mathbb{R}^{m_i}} \sup_{\mathbf{x} \in \mathbb{R}^{m_i}} \{\phi'(\mathbf{x}) - d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{z})\} \mu_i(d\mathbf{z}) \geq \beta \mu_i(E_\beta) > 0.$$

By the assumption that $\text{supp}(\hat{\mu}_i) = \{\mathbf{x}_{i,j} : 1 \leq j \leq J_i\}$, and since $\phi'(\mathbf{x}_{i,j}) = \phi^*(\mathbf{x}_{i,j})$ for all $j = 1, \dots, J_i$, we have

$$\begin{aligned} &\int_{\mathbb{R}^{m_i}} \phi'(\mathbf{x}) \hat{\mu}_i(d\mathbf{x}) - \int_{\mathbb{R}^{m_i}} \sup_{\mathbf{x} \in \mathbb{R}^{m_i}} \{\phi'(\mathbf{x}) - d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{z})\} \mu_i(d\mathbf{z}) \\ &> \int_{\mathbb{R}^{m_i}} \phi^*(\mathbf{x}) \hat{\mu}_i(d\mathbf{x}) - \int_{\mathbb{R}^{m_i}} \sup_{\mathbf{x} \in \mathbb{R}^{m_i}} \{\phi^*(\mathbf{x}) - d_{\mathcal{X}_i}(\mathbf{x}, \mathbf{z})\} \mu_i(d\mathbf{z}), \end{aligned}$$

which contradicts the optimality of ϕ^* . Thus, (5.12) holds, and we have

$$\begin{aligned} &\sup_{\phi \in \mathcal{L}^1(\mathbb{R}^{m_i}, \hat{\mu}_i)} \left\{ \int_{\mathbb{R}^{m_i}} \phi(\mathbf{x}) \hat{\mu}_i(d\mathbf{x}) - \int_{\mathbb{R}^{m_i}} \phi^{d_{\mathcal{X}_i}}(\mathbf{z}) \mu_i(d\mathbf{z}) \right\} \\ &= \int_{\mathbb{R}^{m_i}} \phi^*(\mathbf{x}) \hat{\mu}_i(d\mathbf{x}) - \int_{\mathbb{R}^{m_i}} \max_{1 \leq j \leq J_i} \{\phi^*(\mathbf{x}_{i,j}) - d_{\mathcal{X}_i}(\mathbf{x}_{i,j}, \mathbf{z})\} \mu_i(d\mathbf{z}) \\ &= \sum_{j=1}^{J_i} \alpha_{i,j} \phi^*(\mathbf{x}_{i,j}) - \int_{\mathbb{R}^{m_i}} \max_{1 \leq j \leq J_i} \{\phi^*(\mathbf{x}_{i,j}) - d_{\mathcal{X}_i}(\mathbf{x}_{i,j}, \mathbf{z})\} \mu_i(d\mathbf{z}), \end{aligned} \quad (5.13)$$

where the last expression depends only on $(\phi^*(\mathbf{x}_{i,j}))_{j=1:J_i}$. Let $\phi_{i,j}^* := \phi^*(\mathbf{x}_{i,j})$ for $j = 1, \dots, J_i$. Hence, (5.13) shows that the supremum in (3.1) is attained at $(\phi_{i,j}^*)_{j=1:J_i}$. This completes the proof of statement (i).

Statement (ii) can be established via the first-order optimality condition with respect to $(\phi_{i,j}^*)_{j=1:J_i}$. First, let us define the sets $(\tilde{V}_{i,j})_{j=1:J_i, i=1:N}$ as follows: for $i = 1, \dots, N, j = 1, \dots, J_i$, let

$$\tilde{V}_{i,j} := \left\{ \mathbf{z} \in \mathbb{R}^{m_i} : \phi_{i,j}^* - d_{\mathcal{X}_i}(\mathbf{x}_{i,j}, \mathbf{z}) > \phi_{i,j'}^* - d_{\mathcal{X}_i}(\mathbf{x}_{i,j'}, \mathbf{z}) \quad \forall j' \in \{1, \dots, J_i\} \setminus \{j\} \right\}. \quad (5.14)$$

Let us fix an arbitrary $i \in \{1, \dots, N\}$. The rest of the proof of statement (ii) is divided into two steps.

Step 1: showing that $\mu_i(\tilde{V}_{i,j}) = \mu_i(V_{i,j})$ for $j = 1, \dots, J_i$. Let us fix an arbitrary $j \in \{1, \dots, J_i\}$. Comparing (3.2) and (5.14), we have $\tilde{V}_{i,j} \subseteq V_{i,j}$ and

$$V_{i,j} \setminus \tilde{V}_{i,j} \subseteq \bigcup_{j' \in \{1, \dots, J_i\} \setminus \{j\}} \left\{ \mathbf{z} \in \mathbb{R}^{m_i} : d_{\mathcal{X}_i}(\mathbf{x}_{i,j}, \mathbf{z}) - d_{\mathcal{X}_i}(\mathbf{x}_{i,j'}, \mathbf{z}) = \phi_{i,j}^* - \phi_{i,j'}^* \right\}. \quad (5.15)$$

We will show that for any $\mathbf{y}_1, \mathbf{y}_2 \in \mathbb{R}^{m_i}$ with $\mathbf{y}_1 \neq \mathbf{y}_2$ and any $\beta \in \mathbb{R}$, the set

$$H(\mathbf{y}_1, \mathbf{y}_2, \beta) := \left\{ \mathbf{z} \in \mathbb{R}^{m_i} : \|\mathbf{y}_1 - \mathbf{z}\| - \|\mathbf{y}_2 - \mathbf{z}\| = \beta \right\} \quad (5.16)$$

has Lebesgue measure 0, which depends crucially on the assumption that the closed unit ball under the norm $\|\cdot\|$ is a strictly convex set. To that end, let $\mathbf{y}_1, \mathbf{y}_2 \in \mathbb{R}^{m_i}$, $\mathbf{y}_1 \neq \mathbf{y}_2$, and $\beta \in \mathbb{R}$ be arbitrary and fixed. We need to consider three separate cases.

Case 1: $\beta = \|\mathbf{y}_1 - \mathbf{y}_2\|$. In this case, we want to show that if $\mathbf{z} \in H(\mathbf{y}_1, \mathbf{y}_2, \beta)$, then \mathbf{z} , \mathbf{y}_1 , and \mathbf{y}_2 must lie on the same straight line. Suppose that $\mathbf{z} \in H(\mathbf{y}_1, \mathbf{y}_2, \beta)$. Then, either $\mathbf{z} = \mathbf{y}_2$ or the following equation holds:

$$\left\| \frac{\|\mathbf{y}_1 - \mathbf{y}_2\|}{\|\mathbf{y}_1 - \mathbf{y}_2\| + \|\mathbf{y}_2 - \mathbf{z}\|} \frac{\mathbf{y}_1 - \mathbf{y}_2}{\|\mathbf{y}_1 - \mathbf{y}_2\|} + \left(1 - \frac{\|\mathbf{y}_1 - \mathbf{y}_2\|}{\|\mathbf{y}_1 - \mathbf{y}_2\| + \|\mathbf{y}_2 - \mathbf{z}\|} \right) \frac{\mathbf{y}_2 - \mathbf{z}}{\|\mathbf{y}_2 - \mathbf{z}\|} \right\| = 1, \quad (5.17)$$

where $\left\| \frac{\mathbf{y}_1 - \mathbf{y}_2}{\|\mathbf{y}_1 - \mathbf{y}_2\|} \right\| = \left\| \frac{\mathbf{y}_2 - \mathbf{z}}{\|\mathbf{y}_2 - \mathbf{z}\|} \right\| = 1$ and $\frac{\|\mathbf{y}_1 - \mathbf{y}_2\|}{\|\mathbf{y}_1 - \mathbf{y}_2\| + \|\mathbf{y}_2 - \mathbf{z}\|} \in (0, 1)$. By the assumption that the closed unit ball is strictly convex, (5.17) implies that $\frac{\mathbf{y}_1 - \mathbf{y}_2}{\|\mathbf{y}_1 - \mathbf{y}_2\|} = \frac{\mathbf{y}_2 - \mathbf{z}}{\|\mathbf{y}_2 - \mathbf{z}\|}$. In both situations, \mathbf{z} is contained in the one-dimensional set $\{\xi \mathbf{y}_1 + (1 - \xi) \mathbf{y}_2 : \xi \in (-\infty, 0]\}$ and hence $H(\mathbf{y}_1, \mathbf{y}_2, \beta)$ has Lebesgue measure 0.

Case 2: $\beta = -\|\mathbf{y}_1 - \mathbf{y}_2\|$. In this case, we can repeat the same argument in Case 1 with the roles of \mathbf{y}_1 and \mathbf{y}_2 exchanged, and show that $H(\mathbf{y}_1, \mathbf{y}_2, \beta)$ is contained in the one-dimensional set $\{\xi \mathbf{y}_1 + (1 - \xi) \mathbf{y}_2 : \xi \in [1, \infty)\}$ and hence has Lebesgue measure 0.

Case 3: $\beta \neq \|\mathbf{y}_1 - \mathbf{y}_2\|$ and $\beta \neq -\|\mathbf{y}_1 - \mathbf{y}_2\|$. In this case, one can check that $H(\mathbf{y}_1, \mathbf{y}_2, \beta)$ has no intersection with the set $\{\xi \mathbf{y}_1 + (1 - \xi) \mathbf{y}_2 : \xi \in (-\infty, 0] \cup [1, \infty)\}$. Now, let us define $\mathbf{y}'_1(\lambda), \mathbf{y}'_2(\lambda)$ for $\lambda \in (0, 1)$ as follows:

$$\begin{aligned} \mathbf{y}'_1(\lambda) &:= \mathbf{y}_1 + \lambda(\mathbf{y}_2 - \mathbf{y}_1) = (1 - \lambda)\mathbf{y}_1 + \lambda\mathbf{y}_2, \\ \mathbf{y}'_2(\lambda) &:= \mathbf{y}_2 + \lambda(\mathbf{y}_2 - \mathbf{y}_1) = (1 + \lambda)\mathbf{y}_2 - \lambda\mathbf{y}_1. \end{aligned} \quad (5.18)$$

Then, by the definition of $H(\mathbf{y}_1, \mathbf{y}_2, \beta)$ in (5.16), we have for all $\lambda \in (0, 1)$ that

$$H(\mathbf{y}'_1(\lambda), \mathbf{y}'_2(\lambda), \beta) = H(\mathbf{y}_1, \mathbf{y}_2, \beta) + \lambda(\mathbf{y}_2 - \mathbf{y}_1). \quad (5.19)$$

Thus, $H(\mathbf{y}'_1(\lambda), \mathbf{y}'_2(\lambda), \beta)$ has the same Lebesgue measure as $H(\mathbf{y}_1, \mathbf{y}_2, \beta)$ for all $\lambda \in (0, 1)$ by the translation invariance of the Lebesgue measure. Now, let $\mathbf{z} \in H(\mathbf{y}_1, \mathbf{y}_2, \beta)$ be arbitrary. By (5.18), we have $\mathbf{y}_2 = \frac{1}{1+\lambda} \mathbf{y}'_2(\lambda) + \frac{\lambda}{1+\lambda} \mathbf{y}_1$ for all $\lambda \in (0, 1)$. Consequently, by (5.18) and the triangle inequality, we have for all $\lambda \in (0, 1)$ that

$$\|\mathbf{y}'_1(\lambda) - \mathbf{z}\| \leq \|(1 - \lambda)(\mathbf{y}_1 - \mathbf{z})\| + \|\lambda(\mathbf{y}_2 - \mathbf{z})\|, \quad (5.20)$$

$$\|\mathbf{y}_2 - \mathbf{z}\| \leq \left\| \frac{1}{1 + \lambda} (\mathbf{y}'_2(\lambda) - \mathbf{z}) \right\| + \left\| \frac{\lambda}{1 + \lambda} (\mathbf{y}_1 - \mathbf{z}) \right\|. \quad (5.21)$$

Again, by the assumption that the closed unit ball is strictly convex and the same argument used in Case 1, (5.20) is an equality only when $\frac{\mathbf{y}_1 - \mathbf{z}}{\|\mathbf{y}_1 - \mathbf{z}\|} = \frac{\mathbf{y}_2 - \mathbf{z}}{\|\mathbf{y}_2 - \mathbf{z}\|}$, which implies that $\mathbf{z} \in \{\xi \mathbf{y}_1 + (1 - \xi) \mathbf{y}_2 : \xi \in (-\infty, 0] \cup [1, \infty)\}$. However, this is impossible due to the assumption of Case 3. Similarly,

(5.21) is an equality only when $\frac{\mathbf{y}_1 - \mathbf{z}}{\|\mathbf{y}_1 - \mathbf{z}\|} = \frac{\mathbf{y}'_2(\lambda) - \mathbf{z}}{\|\mathbf{y}'_2(\lambda) - \mathbf{z}\|}$, which also leads to the impossible statement $\mathbf{z} \in \{\xi \mathbf{y}_1 + (1 - \xi) \mathbf{y}_2 : \xi \in (-\infty, 0] \cup [1, \infty)\}$. Thus, we have for all $\lambda \in (0, 1)$ that

$$\|\mathbf{y}'_1(\lambda) - \mathbf{z}\| < \|(1 - \lambda)(\mathbf{y}_1 - \mathbf{z})\| + \|\lambda(\mathbf{y}_2 - \mathbf{z})\| = (1 - \lambda)\|\mathbf{y}_1 - \mathbf{z}\| + \lambda\|\mathbf{y}_2 - \mathbf{z}\|, \quad (5.22)$$

$$\|\mathbf{y}_2 - \mathbf{z}\| < \left\| \frac{1}{1 + \lambda}(\mathbf{y}'_2(\lambda) - \mathbf{z}) \right\| + \left\| \frac{\lambda}{1 + \lambda}(\mathbf{y}_1 - \mathbf{z}) \right\| = \frac{1}{1 + \lambda}\|\mathbf{y}'_2(\lambda) - \mathbf{z}\| + \frac{\lambda}{1 + \lambda}\|\mathbf{y}_1 - \mathbf{z}\|. \quad (5.23)$$

By (5.22) and (5.23), it holds that

$$\|\mathbf{y}'_1(\lambda) - \mathbf{z}\| - \|\mathbf{y}'_2(\lambda) - \mathbf{z}\| < \|\mathbf{y}_1 - \mathbf{z}\| - \|\mathbf{y}_2 - \mathbf{z}\| = \beta, \quad (5.24)$$

which shows that $H(\mathbf{y}'_1(\lambda), \mathbf{y}'_2(\lambda), \beta) \cap H(\mathbf{y}_1, \mathbf{y}_2, \beta) = \emptyset$ for all $\lambda \in (0, 1)$. For $\lambda_1, \lambda_2 \in (0, 1)$ with $\lambda_1 < \lambda_2$, one can repeat the above argument with $\mathbf{y}_1, \mathbf{y}_2$ replaced by $\mathbf{y}'_1(\lambda_1), \mathbf{y}'_2(\lambda_1)$ (recall that $\|\mathbf{y}'_1(\lambda_1) - \mathbf{y}'_2(\lambda_1)\| = \|\mathbf{y}_1 - \mathbf{y}_2\|$ and the assumption of Case 3 still applies) to show that $H(\mathbf{y}'_1(\lambda_1), \mathbf{y}'_2(\lambda_1), \beta) \cap H(\mathbf{y}'_1(\lambda_2), \mathbf{y}'_2(\lambda_2), \beta) = \emptyset$. In summary, we have shown that the collection of sets $\{H(\mathbf{y}_1, \mathbf{y}_2, \beta) + \lambda(\mathbf{y}_2 - \mathbf{y}_1) : \lambda \in (0, 1)\}$ are pairwise disjoint. Now, let us denote by ν here the Lebesgue measure on \mathbb{R}^{m_i} , let $B(q) := \{\mathbf{z} \in \mathbb{R}^{m_i} : \|\mathbf{z}\| \leq q\}$ for $q > 0$, and let $H^{(n)}(\mathbf{y}_1, \mathbf{y}_2, \beta) := H(\mathbf{y}_1, \mathbf{y}_2, \beta) \cap B(n)$ for $n \in \mathbb{N}$. We hence have for all $n \in \mathbb{N}$ that

$$\bigcup_{\lambda \in (0, 1) \cap \mathbb{Q}} H^{(n)}(\mathbf{y}_1, \mathbf{y}_2, \beta) + \lambda(\mathbf{y}_2 - \mathbf{y}_1) \subset B(n + \|\mathbf{y}_1 - \mathbf{y}_2\|).$$

Therefore, by the translation invariance of ν , it holds that

$$\begin{aligned} \sum_{\lambda \in (0, 1) \cap \mathbb{Q}} \nu(H^{(n)}(\mathbf{y}_1, \mathbf{y}_2, \beta)) &= \sum_{\lambda \in (0, 1) \cap \mathbb{Q}} \nu(H^{(n)}(\mathbf{y}_1, \mathbf{y}_2, \beta) + \lambda(\mathbf{y}_2 - \mathbf{y}_1)) \\ &= \nu \left(\bigcup_{\lambda \in (0, 1) \cap \mathbb{Q}} (H^{(n)}(\mathbf{y}_1, \mathbf{y}_2, \beta) + \lambda(\mathbf{y}_2 - \mathbf{y}_1)) \right) \\ &\leq \nu(B(n + \|\mathbf{y}_1 - \mathbf{y}_2\|)) < \infty. \end{aligned}$$

Combining the three cases above, we have shown that for all $\mathbf{y}_1, \mathbf{y}_2 \in \mathbb{R}^{m_i}$ with $\mathbf{y}_1 \neq \mathbf{y}_2$, and for all $\beta \in \mathbb{R}$, the set $H(\mathbf{y}_1, \mathbf{y}_2, \beta)$ has Lebesgue measure 0. Consequently, the set on the right-hand side of (5.15) also has Lebesgue measure 0, and hence is also μ_i -negligible due to the assumption that μ_i is absolutely continuous with respect to the Lebesgue measure. Therefore, we conclude that $\mu_i(\tilde{V}_{i,j}) = \mu_i(V_{i,j})$ for $j = 1, \dots, J_i$.

Step 2: showing that $\mu_i(\tilde{V}_{i,j}) = \alpha_{i,j}$ for $j = 1, \dots, J_i$ via the first-order optimality condition with respect to $(\phi_{i,j}^)_{j=1:J_i}$.* In the following, we let ϕ^* denote the vector $(\phi_{i,1}^*, \dots, \phi_{i,J_i}^*)^\top$ and denote $\phi = (\phi_{i,1}, \dots, \phi_{i,J_i})^\top$ for any $\phi \in \mathbb{R}^{J_i}$. Let $h(\phi, \mathbf{z}) := \max_{1 \leq j \leq J_i} \{\phi_{i,j} - d_{\mathcal{X}_i}(\mathbf{x}_{i,j}, \mathbf{z})\}$ and let $\nabla h(\phi^*, \mathbf{z}) := (\mathbb{1}_{\tilde{V}_{i,1}}(\mathbf{z}), \dots, \mathbb{1}_{\tilde{V}_{i,J_i}}(\mathbf{z}))^\top \in \mathbb{R}^{J_i}$ for all $\phi \in \mathbb{R}^{J_i}$, $\mathbf{z} \in \mathbb{R}^{m_i}$. By the definition of $(\tilde{V}_{i,j})_{j=1:J_i}$ in (5.14), it holds for any $\mathbf{z} \in \tilde{V}_{i,j}$ and $\boldsymbol{\lambda} = (\lambda_1, \dots, \lambda_{J_i})^\top \in \mathbb{R}^{J_i}$ with $\|\boldsymbol{\lambda}\|_\infty$ small enough that

$$\phi_{i,j}^* + \lambda_j - d_{\mathcal{X}_i}(\mathbf{x}_{i,j}, \mathbf{z}) > \phi_{i,j'}^* + \lambda_{j'} - d_{\mathcal{X}_i}(\mathbf{x}_{i,j'}, \mathbf{z}) \quad \forall j' \in \{1, \dots, J_i\} \setminus \{j\}.$$

Thus, for every $\mathbf{z} \in \tilde{V}_{i,j}$, $h(\phi^* + \boldsymbol{\lambda}, \mathbf{z}) - h(\phi^*, \mathbf{z}) = \lambda_j$ for all $\boldsymbol{\lambda} = (\lambda_1, \dots, \lambda_{J_i})^\top$ with $\|\boldsymbol{\lambda}\|_\infty$ small enough. Consequently, it holds for all $\mathbf{z} \in \bigcup_{j=1}^{J_i} \tilde{V}_{i,j}$ that

$$\lim_{\boldsymbol{\lambda} \in \mathbb{R}^{J_i}, \boldsymbol{\lambda} \rightarrow \mathbf{0}} \frac{|h(\phi^* + \boldsymbol{\lambda}, \mathbf{z}) - h(\phi^*, \mathbf{z}) - \langle \nabla h(\phi^*, \mathbf{z}), \boldsymbol{\lambda} \rangle|}{\|\boldsymbol{\lambda}\|_2} = 0. \quad (5.25)$$

By Step 1, we have $\mu_i \left(\bigcup_{j=1}^{J_i} \tilde{V}_{i,j} \right) = \sum_{j=1}^{J_i} \mu_i(V_{i,j}) = 1$, and thus (5.25) holds for μ_i -almost every $\mathbf{z} \in \mathbb{R}^{m_i}$. Moreover, for all $\mathbf{z} \in \mathbb{R}^{m_i}$ and all $\boldsymbol{\lambda} \neq \mathbf{0}$, it holds that $|h(\phi^* + \boldsymbol{\lambda}, \mathbf{z}) - h(\phi^*, \mathbf{z})| \leq \|\boldsymbol{\lambda}\|_\infty$

and hence

$$\frac{|h(\phi^* + \lambda, z) - h(\phi^*, z) - \langle \nabla h(\phi^*, z), \lambda \rangle|}{\|\lambda\|_2} \leq \frac{\|\lambda\|_\infty + \|\lambda\|_\infty}{\|\lambda\|_2} \leq 2. \quad (5.26)$$

Let $u : \mathbb{R}^{J_i} \rightarrow \mathbb{R}$ denote the function being maximized in (3.1), i.e.,

$$u(\phi) := \sum_{j=1}^{J_i} \phi_{i,j} \alpha_{i,j} - \int_{\mathbb{R}^{m_i}} h(\phi, z) \mu_i(dz),$$

and let $\nabla u(\phi^*) := (\alpha_{i,1} - \mu_i(\tilde{V}_{i,1}), \dots, \alpha_{i,J_i} - \mu_i(\tilde{V}_{i,J_i}))^\top \in \mathbb{R}^{J_i}$. Then, by (5.25), (5.26), and the dominated convergence theorem, we have

$$\begin{aligned} & \lim_{\lambda \in \mathbb{R}^{J_i}, \lambda \rightarrow 0} \frac{|u(\phi^* + \lambda) - u(\phi^*) - \langle \nabla u(\phi^*), \lambda \rangle|}{\|\lambda\|_2} \\ &= \lim_{\lambda \in \mathbb{R}^{J_i}, \lambda \rightarrow 0} \left| \int_{\mathbb{R}^{m_i}} \frac{h(\phi^* + \lambda, z) - h(\phi^*, z) - \langle \nabla h(\phi^*, z), \lambda \rangle}{\|\lambda\|_2} \mu_i(dz) \right| \\ &\leq \lim_{\lambda \in \mathbb{R}^{J_i}, \lambda \rightarrow 0} \int_{\mathbb{R}^{m_i}} \frac{|h(\phi^* + \lambda, z) - h(\phi^*, z) - \langle \nabla h(\phi^*, z), \lambda \rangle|}{\|\lambda\|_2} \mu_i(dz) \\ &= \int_{\mathbb{R}^{m_i}} \lim_{\lambda \in \mathbb{R}^{J_i}, \lambda \rightarrow 0} \frac{|h(\phi^* + \lambda, z) - h(\phi^*, z) - \langle \nabla h(\phi^*, z), \lambda \rangle|}{\|\lambda\|_2} \mu_i(dz) \\ &= 0. \end{aligned}$$

Hence, u is differentiable at ϕ^* with gradient $\nabla u(\phi^*)$. Since u is a concave function that attains maximum at ϕ^* , we have by the first-order optimality condition that $\nabla u(\phi^*) = \mathbf{0}$ and hence, by Step 1, $\alpha_{i,j} = \mu_i(\tilde{V}_{i,j}) = \mu_i(V_{i,j})$ for $j = 1, \dots, J_i$. We have completed the proof of statement (ii).

Finally, let us prove statement (iii). For $i = 1, \dots, N$, let γ_i denote the law of (Y_i, X_i) . By the definition of (X_1, \dots, X_N) , the distribution of Y_i conditional on X_i given in (3.3), and statement (ii), we have for $i = 1, \dots, N$ and $E \in \mathcal{B}(\mathcal{X}_i)$ that

$$\begin{aligned} \gamma_i(E \times \mathcal{X}_i) &= \sum_{j=1}^{J_i} \gamma_i(E \times \{\mathbf{x}_{i,j}\}) \\ &= \sum_{j=1}^{J_i} \frac{\mu_i(E \cap V_{i,j})}{\mu_i(V_{i,j})} \alpha_{i,j} \\ &= \sum_{j=1}^{J_i} \mu_i(E \cap V_{i,j}) \\ &= \mu_i(E). \end{aligned}$$

Thus, we have $\gamma_i \in \Gamma(\mu_i, \hat{\mu}_i)$ for $i = 1, \dots, N$.

Let us now fix an arbitrary $i \in \{1, \dots, N\}$. Same as in the proof of statement (i), let $\phi^* \in \mathcal{L}^1(\mathbb{R}^{m_i}, \hat{\mu}_i)$ be a function at which the supremum in (5.11) is attained, let $\phi_{i,j}^* := \phi^*(\mathbf{x}_{i,j})$, $\phi^{*d_{X_i}}(z) := \sup_{\mathbf{x} \in \mathbb{R}^{m_i}} \{\phi^*(\mathbf{x}) - d_{X_i}(\mathbf{x}, z)\}$, and let S be the set given by

$$S := \left\{ z \in \mathbb{R}^{m_i} : \phi^{*d_{X_i}}(z) = \max_{1 \leq j \leq J_i} \{\phi^*(\mathbf{x}_{i,j}) - d_{X_i}(\mathbf{x}_{i,j}, z)\} \right\}.$$

We have by (5.12) that $\mu_i(S) = 1$. Moreover, by definition, we have $\phi^*(\mathbf{x}) - \phi^{*d_{X_i}}(z) \leq d_{X_i}(\mathbf{x}, z)$ for all $\mathbf{x}, z \in \mathbb{R}^{m_i}$. Recall that we have shown in the proof of statement (i) that the supremum in (3.1) is attained at $(\phi_{i,j}^*)_{j=1:J_i}$. Therefore, for $j = 1, \dots, J_i$ and for any $z \in V_{i,j} \cap S$, we have by the definition

of $V_{i,j}$ in (3.2) that

$$\begin{aligned}\phi^*(\mathbf{x}_{i,j}) - \phi^{*d\mathcal{X}_i}(\mathbf{z}) &= \phi^*(\mathbf{x}_{i,j}) - \max_{1 \leq j' \leq J_i} \{\phi^*(\mathbf{x}_{i,j'}) - d\mathcal{X}_i(\mathbf{x}_{i,j'}, \mathbf{z})\} \\ &= \phi^*(\mathbf{x}_{i,j}) - \phi^*(\mathbf{x}_{i,j}) + d\mathcal{X}_i(\mathbf{x}_{i,j}, \mathbf{z}) \\ &= d\mathcal{X}_i(\mathbf{x}_{i,j}, \mathbf{z}).\end{aligned}$$

Thus, $\phi^*(\mathbf{x}) - \phi^{*d\mathcal{X}_i}(\mathbf{z}) = d\mathcal{X}_i(\mathbf{x}, \mathbf{z})$ holds for all $(\mathbf{z}, \mathbf{x}) \in \bigcup_{j=1}^{J_i} [(V_{i,j} \cap S) \times \{\mathbf{x}_{i,j}\}]$. Moreover, by the definition of (X_1, \dots, X_N) and (3.3), we have

$$\gamma_i \left(\bigcup_{j=1}^{J_i} ((V_{i,j} \cap S) \times \{\mathbf{x}_{i,j}\}) \right) = \gamma_i \left(\bigcup_{j=1}^{J_i} (V_{i,j} \times \{\mathbf{x}_{i,j}\}) \right) = 1.$$

Therefore, by the equivalence of statements (a) and (d) in part (ii) of [60, Theorem 5.10], the infimum in (5.11) is attained at γ_i , and thus $\int_{\mathbb{R}^{m_i} \times \mathbb{R}^{m_i}} d\mathcal{X}_i(\mathbf{z}, \mathbf{x}) \gamma_i(d\mathbf{z}, d\mathbf{x}) = W_1(\mu_i, \hat{\mu}_i)$.

Lastly, let γ denote the law of $(X_1, \dots, X_N, Y_1, \dots, Y_N)$. Since γ satisfies all the required properties stated in Definition 2.2.2 and $\tilde{\mu}$ is the law of (Y_1, \dots, Y_N) , we have proved that $\tilde{\mu} \in R(\hat{\mu}, \mu_1, \dots, \mu_N)$. The proof is now complete. \square

5.4. Proof of results in Section 3.2. Before proving Proposition 3.2.5, let us first state and prove the following lemma which is a more general version of Proposition 3.2.5(i). This lemma is also crucial in the proof of Theorem 3.2.7.

Lemma 5.4.1. *Let $m \in \mathbb{N}$ and let $\mathcal{Y} \subseteq \mathbb{R}^m$. Let \mathfrak{C} be a polyhedral cover of \mathcal{Y} . Then, the sets in $\{\text{relint}(F) : F \in \mathfrak{F}(\mathfrak{C})\}$ are pairwise disjoint and $\bigcup_{F \in \mathfrak{F}(\mathfrak{C})} \text{relint}(F) = \bigcup_{C \in \mathfrak{C}} C$.*

Proof of Lemma 5.4.1. $\bigcup_{F \in \mathfrak{F}(\mathfrak{C})} \text{relint}(F) = \bigcup_{C \in \mathfrak{C}} C$ follows directly from [52, Theorem 18.2]. We will show that if $F, F' \in \mathfrak{F}(\mathfrak{C})$ and $F \neq F'$ then $\text{relint}(F) \cap \text{relint}(F') = \emptyset$. Suppose that $F \in \mathfrak{F}(\mathfrak{C})$ is a face of $C \in \mathfrak{C}$, $F' \in \mathfrak{F}(\mathfrak{C})$ is a face of $C' \in \mathfrak{C}$, and $\text{relint}(F) \cap \text{relint}(F') \neq \emptyset$. Then, by the definition of polyhedral covers in Definition 3.2.4, $C \cap C'$ is a face of both C and C' . Hence, $C \cap C'$ is a face of C and $\text{relint}(F) \cap \text{relint}(F') \subset F \cap F' \subseteq C \cap C'$. Since F is a convex set, $\text{relint}(F) \cap (C \cap C') \neq \emptyset$, and $C \cap C'$ is a face of C , we have by [52, Theorem 18.1] that $F \subseteq C \cap C'$. Then, by the definition of faces, F is a face of $C \cap C'$. It follows from the same argument that F' is also a face of $C \cap C'$, and thus $F = F'$ by [52, Corollary 18.1.2]. The proof is now complete. \square

Proof of Proposition 3.2.5. Statement (i) is a direct consequence of Lemma 5.4.1. To prove statement (ii), notice that for a fixed $F \in \mathfrak{F}(\mathfrak{C})$ and a fixed $\mathbf{x} \in F$, the representation of \mathbf{x} as a convex combination $\mathbf{x} = \sum_{\mathbf{w} \in V(F)} \lambda_{F,\mathbf{w}}(\mathbf{x}) \mathbf{w}$ where $\sum_{\mathbf{w} \in V(F)} \lambda_{F,\mathbf{w}}(\mathbf{x}) = 1$, $\lambda_{F,\mathbf{w}}(\mathbf{x}) \geq 0$ for all $\mathbf{w} \in V(F)$ is unique since F is an n -simplex with $0 \leq n \leq m$ and $V(F)$ is a set of $n+1$ affinely independent points. Moreover, under the additional assumption that $\mathbf{x} \in \text{relint}(F)$, we have $\lambda_{F,\mathbf{w}}(\mathbf{x}) > 0$ for all $\mathbf{w} \in V(F)$ by [52, Theorem 6.9] (with $\{C_1, \dots, C_m\} \leftarrow \{\{\mathbf{w}\} : \mathbf{w} \in V(F)\}$ in the notation of [52]).

Let us now prove statement (iii). To begin, let us prove that the functions $\{g_{\mathbf{v}} : \mathbf{v} \in V(\mathfrak{C})\}$ are continuous. To that end, let us fix an arbitrary $\mathbf{v} \in V(\mathfrak{C})$ and an arbitrary $F \in \mathfrak{F}(\mathfrak{C})$. Let $n := |V(F)| - 1$ and let $\{\mathbf{w}_0, \dots, \mathbf{w}_n\}$ be an arbitrary enumeration of $V(F)$. Let

$$\Delta_n := \left\{ (\alpha_0, \alpha_1, \dots, \alpha_n)^\top : \sum_{i=0}^n \alpha_i = 1, \alpha_i \geq 0 \forall 0 \leq i \leq n \right\},$$

and let $h_n : \Delta_n \rightarrow F$ be given by

$$h_n(\alpha_0, \dots, \alpha_n) := \sum_{i=0}^n \alpha_i \mathbf{w}_i \quad \forall (\alpha_0, \dots, \alpha_n)^\top \in \Delta_n.$$

By the same argument as in the proof of statement (ii), h_n is a continuous bijection whose inverse is also continuous. Moreover, let $u_{\mathbf{v}} : \Delta_n \rightarrow \mathbb{R}$ be given by

$$u_{\mathbf{v}}(\alpha_0, \dots, \alpha_n) := \begin{cases} \alpha_0 & \text{if } \mathbf{v} = \mathbf{w}_0, \\ \dots & \\ \alpha_n & \text{if } \mathbf{v} = \mathbf{w}_n, \\ 0 & \text{if } \mathbf{v} \neq \mathbf{w}_i \forall 0 \leq i \leq n \end{cases} \quad \forall (\alpha_0, \dots, \alpha_n)^\top \in \Delta_n.$$

Now, for any $\mathbf{x} \in \text{relint}(F')$ where F' is a non-empty face of F , we repeat the argument in the proof of statement (ii) to represent $\mathbf{x} = \sum_{\mathbf{w} \in V(F')} \lambda_{F,\mathbf{w}}(\mathbf{x})\mathbf{w}$ where $\sum_{\mathbf{w} \in V(F')} \lambda_{F,\mathbf{w}}(\mathbf{x}) = 1$, $\lambda_{F,\mathbf{w}}(\mathbf{x}) > 0$ for all $\mathbf{w} \in V(F')$, and $\lambda_{F,\mathbf{w}}(\mathbf{x}) = 0$ for all $\mathbf{w} \in V(F) \setminus V(F')$. Thus, we have by (3.5) that

$$g_v(\mathbf{x}) = \sum_{\mathbf{w} \in V(F')} \lambda_{F,\mathbf{w}}(\mathbf{x}) \mathbb{1}_{\{\mathbf{w}=v\}} = \sum_{\mathbf{w} \in V(F)} \lambda_{F,\mathbf{w}}(\mathbf{x}) \mathbb{1}_{\{\mathbf{w}=v\}}.$$

Since $\bigcup_{F'} \text{relint}(F') = F$ by [52, Theorem 18.2], this shows that

$$g_v(\mathbf{x}) = u_v(h_n^{-1}(\mathbf{x})) \quad \forall \mathbf{x} \in F, \quad (5.27)$$

which shows that g_v is continuous on F . Subsequently, since g_v is continuous on each of the finitely many closed sets in $\mathfrak{F}(\mathfrak{C})$, g_v is also continuous on $\bigcup_{C \in \mathfrak{C}} C$ by statement (i).

From the definition in (3.5), one can check that $\{g_v : v \in V(\mathfrak{C})\}$ satisfy the property (IFB1). For $v, v' \in V(\mathfrak{C})$, it holds that $v' \in \text{relint}(\{v'\})$. Thus, (3.5) shows that $g_v(v') = \mathbb{1}_{\{v=v'\}}$ and hence the property (IFB2) holds. To show that the properties (IFB3) and (IFB4) hold, let us fix an arbitrary $F \in \mathfrak{F}(\mathfrak{C})$ and an arbitrary $\mathbf{x} \in F$. By the unique representation $\mathbf{x} = \sum_{\mathbf{w} \in V(F)} \lambda_{F,\mathbf{w}}(\mathbf{x})\mathbf{w}$ in the proof of statement (i) as well as (5.27), we have $\sum_{v \in V(F)} g_v(\mathbf{x}) = \sum_{v \in V(F)} \lambda_{F,v}(\mathbf{x}) = 1$. This proves that $\{g_v : v \in V(\mathfrak{C})\}$ satisfy the property (IFB3). Moreover, for any $v' \in V(\mathfrak{C}) \setminus V(F)$, we have by (5.27) that $g_{v'}(\mathbf{x}) = 0$, thus proving the property (IFB4). Finally, since $\bigcup_{C \in \mathfrak{C}} C$ is bounded, we have $D(\mathfrak{C}) = \emptyset$ and thus the properties (IFB5) and (IFB6) hold vacuously. The proof is now complete. \square

Proof of Proposition 3.2.6. Let us first introduce some notations used in this proof. For $i = 1, \dots, m$, we denote the i -th standard basis vector of \mathbb{R}^m by e_i . Moreover, we denote the m -dimensional vector with all entries equal to one by $\mathbf{1}$, i.e., $\mathbf{1} := \underbrace{(1, \dots, 1)}_{m \text{ times}}^\top$, and denote the m -dimensional vector with all

entries equal to ∞ by ∞ . For $\mathbf{x} = (x_1, \dots, x_m)^\top, \mathbf{x}' = (x'_1, \dots, x'_m)^\top \in (\mathbb{R} \cup \{-\infty, \infty\})^m$, we let $(\mathbf{x}, \mathbf{x}') := \{(z_1, \dots, z_m)^\top \in \mathbb{R}^m : x_i < z_i < x'_i \forall 1 \leq i \leq m\}$, $(\mathbf{x}, \mathbf{x}') := \{(z_1, \dots, z_m)^\top \in \mathbb{R}^m : x_i < z_i \leq x'_i \forall 1 \leq i \leq m\}$, and $[\mathbf{x}, \mathbf{x}'] := \{(z_1, \dots, z_m)^\top \in \mathbb{R}^m : x_i \leq z_i \leq x'_i \forall 1 \leq i \leq m\}$. Let us remark that the definition of \mathcal{G} in (3.6) can be equivalently written as:

$$\begin{aligned} \mathcal{G} = & \left\{ \mathbb{R}^m \ni (x_1, \dots, x_m)^\top \mapsto \max \left\{ \beta_1^{-1}(x_1 - \kappa_1), \dots, \beta_m^{-1}(x_m - \kappa_m), 0 \right\} \in \mathbb{R} : \right. \\ & \left. \kappa_i \in \{\kappa_{i,0}, \dots, \kappa_{i,n_i}, \infty\} \forall 1 \leq i \leq m \right\} \quad (5.28) \\ & \cup \left\{ \mathbb{R}^m \ni (x_1, \dots, x_m)^\top \mapsto x_i \in \mathbb{R} : 1 \leq i \leq m \right\}. \end{aligned}$$

Throughout this proof, we adopt the definition of \mathcal{G} in (5.28) for notational simplicity.

To begin, one can observe from the definition of \mathfrak{C} that

$$\begin{aligned} \mathfrak{F}(\mathfrak{C}) = & \left\{ I_1 \times \dots \times I_m : \right. \\ & \left. I_i \in \left\{ (-\infty, \kappa_{i,0}], \{\kappa_{i,0}\}, [\kappa_{i,0}, \kappa_{i,1}], \dots, [\kappa_{i,n_i-1}, \kappa_{i,n_i}], \{\kappa_{i,n_i}\}, [\kappa_{i,n_i}, \infty) \right\} \forall 1 \leq i \leq m \right\}, \quad (5.29) \end{aligned}$$

and that

$$\begin{aligned} V(\mathfrak{C}) = & \times_{i=1}^m \{\kappa_{i,0}, \dots, \kappa_{i,n_i}\}, \quad (5.30) \\ D(\mathfrak{C}) = & \{-e_1, e_1, \dots, -e_m, e_m\}. \end{aligned}$$

Let us define $\mathbf{T} : \mathbb{R}^m \rightarrow \mathbb{R}^m$ as follows:

$$\mathbf{T}(x_1, \dots, x_m) := (\beta_1^{-1}(x_1 - \underline{\kappa}_1), \dots, \beta_m^{-1}(x_m - \underline{\kappa}_m))^\top.$$

Notice that \mathbf{T} is affine and bijective, and that $\mathbf{T}(V(\mathfrak{C})) = \times_{i=1}^m \{0, \dots, n_i\}$. The rest of the proof is divided into four steps.

Step 1: defining the function $M(\cdot; \mathbf{j}', \mathbf{j})$ and showing its relation to a probability measure. For $i = 1, \dots, m$, let $L_i := \{0, \dots, n_i\}$, $J_i := \{0, \dots, n_i - 1, \infty\}$, $\bar{J}_i := \{-\infty, 0, \dots, n_i - 1, \infty\}$, $K_{i,L} :=$

$\{-\infty, 0, \dots, n_i - 1, n_i\}$, and $K_{i,R} := \{0, \dots, n_i - 1, n_i, \infty\}$. For $i = 1, \dots, m$ and $j \in \bar{J}_i$, let $p_i(j)$ denote the predecessor of j in \bar{J}_i , i.e.,

$$p_i(j) := \begin{cases} -\infty & \text{if } j = -\infty \text{ or } j = 0, \\ j - 1 & \text{if } j \in \{1, \dots, n_i - 1\}, \\ n_i - 1 & \text{if } j = \infty. \end{cases}$$

For $i = 1, \dots, m$, let $l_i(j) := \min\{j, n_i\} \in L_i$ for all $j \in J_i$, and let $q_{i,L} : K_{i,L} \rightarrow J_i$, $q_{i,R} : K_{i,R} \rightarrow J_i$, $q_{i,L}^\dagger : J_i \rightarrow K_{i,L}$, and $q_{i,R}^\dagger : J_i \rightarrow K_{i,R}$ be defined as

$$q_{i,L}(k_L) := \begin{cases} 0 & \text{if } k_L = -\infty, \\ k_L & \text{if } k_L \in \{0, \dots, n_i - 1\}, \\ \infty & \text{if } k_L = n_i, \end{cases} \quad q_{i,R}(k_R) := \begin{cases} k_R & \text{if } k_R \in \{0, \dots, n_i - 1\}, \\ \infty & \text{if } k_R = n_i \text{ or } k_R = \infty, \end{cases}$$

$$q_{i,L}^\dagger(j) := \begin{cases} -\infty & \text{if } j = 0, \\ j & \text{if } j \in \{1, \dots, n_i - 1\}, \\ n_i & \text{if } j = \infty, \end{cases} \quad q_{i,R}^\dagger(j) := j,$$

for all $k_L \in K_{i,L}$, $k_R \in K_{i,R}$, $j \in J_i$. Moreover, let $\mathbf{L} := \times_{i=1}^m L_i$, $\mathbf{J} := \times_{i=1}^m J_i$, $\bar{\mathbf{J}} = \times_{i=1}^m \bar{J}_i$, $\mathbf{K}_L := \times_{i=1}^m K_{i,L}$, $\mathbf{K}_R := \times_{i=1}^m K_{i,R}$, and let $\mathbf{p} : \bar{\mathbf{J}} \rightarrow \bar{\mathbf{J}}$, $\mathbf{l} : \mathbf{J} \rightarrow \mathbf{L}$, $\mathbf{q}_L : \mathbf{K}_L \rightarrow \mathbf{J}$, $\mathbf{q}_R : \mathbf{K}_R \rightarrow \mathbf{J}$, $\mathbf{q}_L^\dagger : \mathbf{J} \rightarrow \mathbf{K}_L$, and $\mathbf{q}_R^\dagger : \mathbf{J} \rightarrow \mathbf{K}_R$ be defined as follows:

$$\begin{aligned} \mathbf{p}(j_1, \dots, j_m) &:= (p_1(j_1), \dots, p_m(j_m))^\top & \forall (j_1, \dots, j_m)^\top \in \bar{\mathbf{J}}, \\ \mathbf{l}(j_1, \dots, j_m) &:= (l_1(j_1), \dots, l_m(j_m))^\top & \forall (j_1, \dots, j_m)^\top \in \mathbf{J}, \\ \mathbf{q}_L(k_1, \dots, k_m) &:= (q_{1,L}(k_1), \dots, q_{m,L}(k_m))^\top & \forall (k_1, \dots, k_m)^\top \in \mathbf{K}_L, \\ \mathbf{q}_R(k_1, \dots, k_m) &:= (q_{1,R}(k_1), \dots, q_{m,R}(k_m))^\top & \forall (k_1, \dots, k_m)^\top \in \mathbf{K}_R, \\ \mathbf{q}_L^\dagger(j_1, \dots, j_m) &:= (q_{1,L}^\dagger(j_1), \dots, q_{m,L}^\dagger(j_m))^\top & \forall (j_1, \dots, j_m)^\top \in \mathbf{J}, \\ \mathbf{q}_R^\dagger(j_1, \dots, j_m) &:= (q_{1,R}^\dagger(j_1), \dots, q_{m,R}^\dagger(j_m))^\top & \forall (j_1, \dots, j_m)^\top \in \mathbf{J}. \end{aligned}$$

Observe that $\mathbf{l}(\cdot)$ is a bijection between \mathbf{J} and $\mathbf{T}(V(\mathfrak{C}))$, and that

$$\mathbf{q}_L^\dagger(\mathbf{q}_L(\mathbf{k}_L)) \leq \mathbf{k}_L, \quad \mathbf{q}_R^\dagger(\mathbf{q}_R(\mathbf{k}_R)) \geq \mathbf{k}_R \quad \forall \mathbf{k}_L \in \mathbf{K}_L, \mathbf{k}_R \in \mathbf{K}_R. \quad (5.31)$$

Furthermore, one can observe from (5.29) that every $F \in \mathfrak{F}(\mathfrak{C})$ satisfies

$$\begin{aligned} \mathbf{T}(F) &\in \left\{ I_1 \times \dots \times I_m : I_i \in \{(-\infty, 0], \{0\}, [0, 1], \dots, [n_i - 1, n_i], \{n_i\}, [n_i, \infty)\} \forall 1 \leq i \leq m \right\} \\ &\subset \left\{ \left(\times_{i=1}^m [k_{i,L}, k_{i,R}] \right) \cap \mathbb{R}^m : k_{i,L} \in K_{i,L}, k_{i,R} \in K_{i,R}, k_{i,L} \leq k_{i,R} \forall 1 \leq i \leq m \right\}. \end{aligned} \quad (5.32)$$

Next, for every $\mathbf{k} = (k_1, \dots, k_m)^\top \in \mathbf{K}_R$, let us denote the function $\mathbb{R}^m \ni (x_1, \dots, x_m)^\top \mapsto \max\{(x_1 - k_1), \dots, (x_m - k_m), 0\} \in \mathbb{R}$ by $b(\cdot; \mathbf{k})$, i.e.,

$$b(x_1, \dots, x_m; \mathbf{k}) := \max\{(x_1 - k_1), \dots, (x_m - k_m), 0\} \quad \forall (x_1, \dots, x_m)^\top \in \mathbb{R}^m.$$

For every $\mathbf{k} = (k_1, \dots, k_m)^\top \in \mathbf{K}_R$, we have

$$(x_1, \dots, x_m)^\top \mapsto b(\mathbf{T}(x_1, \dots, x_m); \mathbf{k}) = \max\{\beta_1^{-1}(x_1 - \underline{\kappa}_1) - k_1, \dots, \beta_m^{-1}(x_m - \underline{\kappa}_m) - k_m, 0\}.$$

For $i = 1, \dots, m$, we have

$$\begin{aligned} \underline{\kappa}_i + \beta_i k_i &= \begin{cases} \kappa_{i,k_i} & \text{if } k_i \in \{0, \dots, n_i\}, \\ \infty & \text{if } k_i = \infty \end{cases} \\ &\in \{\kappa_{i,0}, \dots, \kappa_{i,n_i}, \infty\}, \end{aligned}$$

and thus we have by (5.28) that $b(\mathbf{T}(\cdot); \mathbf{k}) \in \text{span}_1(\mathcal{G})$ for all $\mathbf{k} \in \mathbf{K}_R$. Subsequently, for all $\mathbf{j}, \mathbf{j}' \in \bar{\mathcal{J}}$ with $\mathbf{j}' \leq \mathbf{j}$, let us define $Q(\cdot; \mathbf{j}) : \mathbb{R}^m \rightarrow \mathbb{R}$ and $M(\cdot; \mathbf{j}', \mathbf{j}) : \mathbb{R}^m \rightarrow \mathbb{R}$ by

$$Q(\mathbf{x}; \mathbf{j}) := \begin{cases} 1 - b(\mathbf{x}; \mathbf{j}) + b(\mathbf{x}; \mathbf{j} + \mathbf{1}) & \text{if } \mathbf{j} \in \mathcal{J}, \\ 0 & \text{if } \mathbf{j} \in \bar{\mathcal{J}} \setminus \mathcal{J}. \end{cases} \quad (5.33)$$

$$M(\mathbf{x}; \mathbf{j}', \mathbf{j}) := \sum_{\boldsymbol{\iota}=(\iota_1, \dots, \iota_m) \in \{0,1\}^m} (-1)^{\sum_{i=1}^m \iota_i} Q(\mathbf{x}; \boldsymbol{\sigma}(\mathbf{p}(\mathbf{j}'), \mathbf{j}, \boldsymbol{\iota})), \quad (5.34)$$

where $\boldsymbol{\sigma} : (\mathbb{R} \cup \{-\infty, \infty\})^m \times (\mathbb{R} \cup \{-\infty, \infty\})^m \times \{0, 1\}^m \rightarrow (\mathbb{R} \cup \{-\infty, \infty\})^m$ is defined by

$$\boldsymbol{\sigma}((y'_1, \dots, y'_m)^\top, (y_1, \dots, y_m)^\top, (\iota_1, \dots, \iota_m)) := (\sigma(y'_1, y_1, \iota_1), \dots, \sigma(y'_m, y_m, \iota_m))^\top, \\ \text{where } \sigma(y', y, \iota) := \begin{cases} y & \text{if } \iota = 0, \\ y' & \text{if } \iota = 1. \end{cases}$$

Since $b(\mathbf{T}(\cdot); \mathbf{k}) \in \text{span}_1(\mathcal{G})$ for all $\mathbf{k} \in \mathbf{K}_R$, it follows from (5.33) and (5.34) that

$$Q(\mathbf{T}(\cdot); \mathbf{j}) \in \text{span}_1(\mathcal{G}) \text{ and } M(\mathbf{T}(\cdot); \mathbf{j}', \mathbf{j}) \in \text{span}_1(\mathcal{G}) \quad \text{for all } \mathbf{j}, \mathbf{j}' \in \bar{\mathcal{J}} \text{ such that } \mathbf{j}' \leq \mathbf{j}. \quad (5.35)$$

By (5.33), for every $\mathbf{j} = (j_1, \dots, j_m)^\top \in \bar{\mathcal{J}}$ and $\mathbf{x} = (x_1, \dots, x_m)^\top \in \mathbb{R}^m$, $Q(\mathbf{x}; \mathbf{j})$ can be explicitly expressed as

$$Q(\mathbf{x}; \mathbf{j}) = 1 \wedge \left(1 - \max_{1 \leq i \leq m} \{x_i - j_i\} \right)^+ = \min_{1 \leq i \leq m} \left\{ (j_i - (x_i - 1))^+ \wedge 1 \right\}. \quad (5.36)$$

For every $\mathbf{x} = (x_1, \dots, x_m)^\top \in \mathbb{R}^m$, let us define $\tilde{Q}(\cdot; \mathbf{x}) : (\mathbb{R} \cup \{-\infty, \infty\})^m \rightarrow \mathbb{R}$ by

$$\tilde{Q}(\mathbf{y}; \mathbf{x}) := \min_{1 \leq i \leq m} \left\{ (y_i - (x_i - 1))^+ \wedge 1 \right\} \quad \forall \mathbf{y} = (y_1, \dots, y_m)^\top \in (\mathbb{R} \cup \{-\infty, \infty\})^m. \quad (5.37)$$

By (5.36), we have $\tilde{Q}(\mathbf{j}; \mathbf{x}) = Q(\mathbf{x}; \mathbf{j})$ for all $\mathbf{x} \in \mathbb{R}^m$ and $\mathbf{j} \in \bar{\mathcal{J}}$. Notice that for any $x_i \in \mathbb{R}$,

$$y_i \mapsto (y_i - (x_i - 1))^+ \wedge 1 = \begin{cases} 0 & \text{if } -\infty \leq y_i < x_i - 1, \\ y_i - (x_i - 1) & \text{if } x_i - 1 \leq y_i \leq x_i, \\ 1 & \text{if } x_i < y_i \leq \infty \end{cases}$$

corresponds to the distribution function of a random variable which is uniformly distributed on the interval $[x_i - 1, x_i]$. Consequently, for every $\mathbf{x} \in \mathbb{R}^m$, we have by the definition of the comonotonicity copula and Sklar's theorem (see, e.g., [45, Equation (5.7) & Equation (5.3) & Theorem 5.3]) that $\tilde{Q}(\cdot; \mathbf{x})$ is the distribution function of a random vector which is uniformly distributed on the line segment $\{\mathbf{x} - \lambda \mathbf{1} : 0 \leq \lambda \leq 1\}$. Let $\mu_{\mathbf{x}}$ be the law of this random vector, i.e., $\mu_{\mathbf{x}}$ satisfies

$$\mu_{\mathbf{x}}((-\infty, \mathbf{y}]) = \tilde{Q}(\mathbf{y}; \mathbf{x}) \quad \forall \mathbf{y} \in (\mathbb{R} \cup \{-\infty, \infty\})^m. \quad (5.38)$$

In particular, it holds that

$$\mu_{\mathbf{x}}((\mathbf{x} - \mathbf{1}, \mathbf{x})) = 1. \quad (5.39)$$

By (5.34), (5.38), and the identity

$$\mathbb{1}_{(\mathbf{y}', \mathbf{y}]}(\mathbf{x}) = \sum_{\boldsymbol{\iota}=(\iota_1, \dots, \iota_m) \in \{0,1\}^m} (-1)^{\sum_{i=1}^m \iota_i} \mathbb{1}_{(-\infty, \boldsymbol{\sigma}(\mathbf{y}', \mathbf{y}, \boldsymbol{\iota})]}(\mathbf{x}) \\ \forall \mathbf{x} \in \mathbb{R}^m, \forall \mathbf{y}, \mathbf{y}' \in (\mathbb{R} \cup \{-\infty, \infty\})^m \text{ such that } \mathbf{y}' \leq \mathbf{y},$$

we have

$$M(\mathbf{x}; \mathbf{j}', \mathbf{j}) = \mu_{\mathbf{x}}((\mathbf{p}(\mathbf{j}'), \mathbf{j}]) \quad \forall \mathbf{j}, \mathbf{j}' \in \bar{\mathcal{J}} \text{ with } \mathbf{j}' \leq \mathbf{j}. \quad (5.40)$$

Step 2: deriving three additional properties of $M(\cdot; \mathbf{j}', \mathbf{j})$. For the first two properties, let us first fix an arbitrary $i \in \{1, \dots, m\}$ and consider $j, j', \hat{j} \in \mathcal{J}_i$ with $j' \leq j$. In the case where $\hat{j} > j$, we have

$j \leq \hat{j} - 1, j \leq n_i - 1, \hat{j} \geq 1$, and hence we get

$$\begin{aligned} (l_i(\hat{j}) - 1, l_i(\hat{j})) \cap (p_i(j'), j] &= \begin{cases} (\hat{j} - 1, \hat{j}) \cap (p_i(j'), j] & \text{if } \hat{j} \in \{1, \dots, n_i - 1\}, \\ (n_i - 1, n_i) \cap (p_i(j'), j] & \text{if } \hat{j} = \infty \end{cases} \\ &= \emptyset \end{aligned}$$

as well as

$$\begin{aligned} (q_{i,L}^\dagger(j') - 1, q_{i,R}^\dagger(j)) \cap (p_i(\hat{j}), \hat{j}] &= \begin{cases} (q_{i,L}^\dagger(j') - 1, j) \cap (\hat{j} - 1, \hat{j}] & \text{if } \hat{j} \in \{1, \dots, n_i - 1\}, \\ (q_{i,L}^\dagger(j') - 1, j) \cap (n_i - 1, \infty] & \text{if } \hat{j} = \infty \end{cases} \\ &= \emptyset. \end{aligned}$$

On the other hand, in the case where $\hat{j} < j'$, we have $j' \geq 1, \hat{j} \leq j' - 1, \hat{j} \leq n_i - 1$, and hence we get

$$\begin{aligned} (l_i(\hat{j}) - 1, l_i(\hat{j})) \cap (p_i(j'), j] &= \begin{cases} (\hat{j} - 1, \hat{j}) \cap (j' - 1, j] & \text{if } j' \in \{1, \dots, n_i - 1\}, \\ (\hat{j} - 1, \hat{j}) \cap (n_i - 1, \infty] & \text{if } j' = \infty \end{cases} \\ &= \emptyset \end{aligned}$$

as well as

$$\begin{aligned} (q_{i,L}^\dagger(j') - 1, q_{i,R}^\dagger(j)) \cap (p_i(\hat{j}), \hat{j}] &= \begin{cases} (j' - 1, j) \cap (p_i(\hat{j}), \hat{j}] & \text{if } \hat{j} \in \{1, \dots, n_i - 1\}, \\ (n_i - 1, j) \cap (p_i(\hat{j}), \hat{j}] & \text{if } \hat{j} = \infty \end{cases} \\ &= \emptyset. \end{aligned}$$

Therefore, we can conclude that for all $j, j', \hat{j} \in J_i$ with $j' \leq j$, if $j' \leq \hat{j} \leq j$ does not hold, then $(l_i(\hat{j}) - 1, l_i(\hat{j})) \cap (p_i(j'), j] = \emptyset$ and $(q_{i,L}^\dagger(j') - 1, q_{i,R}^\dagger(j)) \cap (p_i(\hat{j}), \hat{j}] = \emptyset$. These observations extend to the vector case. Specifically, for all $\mathbf{j}, \mathbf{j}', \hat{\mathbf{j}} \in \mathbf{J}$ with $\mathbf{j}' \leq \mathbf{j}$, we have:

$$\mathbf{j}' \leq \hat{\mathbf{j}} \leq \mathbf{j} \text{ does not hold} \quad \Rightarrow \quad \begin{cases} (\mathbf{l}(\hat{\mathbf{j}}) - \mathbf{1}, \mathbf{l}(\hat{\mathbf{j}})) \cap (\mathbf{p}(\mathbf{j}'), \mathbf{j}] = \emptyset, \\ (\mathbf{q}_L^\dagger(\mathbf{j}') - \mathbf{1}, \mathbf{q}_R^\dagger(\mathbf{j})) \cap (\mathbf{p}(\hat{\mathbf{j}}), \hat{\mathbf{j}}] = \emptyset. \end{cases} \quad (5.41)$$

Consequently, for all $\mathbf{j}, \mathbf{j}', \hat{\mathbf{j}} \in \mathbf{J}$ such that $\mathbf{j}' \leq \mathbf{j}$ holds and $\mathbf{j}' \leq \hat{\mathbf{j}} \leq \mathbf{j}$ does not hold, we have by (5.40), (5.41), and (5.39) that

$$M(\mathbf{l}(\hat{\mathbf{j}}); \mathbf{j}', \mathbf{j}) = \mu_{\mathbf{l}(\hat{\mathbf{j}})}((\mathbf{p}(\mathbf{j}'), \mathbf{j}]) = \mu_{\mathbf{l}(\hat{\mathbf{j}})}((\mathbf{l}(\hat{\mathbf{j}}) - \mathbf{1}, \mathbf{l}(\hat{\mathbf{j}})) \cap (\mathbf{p}(\mathbf{j}'), \mathbf{j}]) = 0, \quad (5.42)$$

and that for all $\mathbf{x} \in \mathbb{R}^m$ such that $\mathbf{q}_L^\dagger(\mathbf{j}') \leq \mathbf{x} \leq \mathbf{q}_R^\dagger(\mathbf{j})$,

$$\begin{aligned} M(\mathbf{x}; \hat{\mathbf{j}}, \hat{\mathbf{j}}) &= \mu_{\mathbf{x}}((\mathbf{p}(\hat{\mathbf{j}}), \hat{\mathbf{j}}]) \\ &= \mu_{\mathbf{x}}((\mathbf{x} - \mathbf{1}, \mathbf{x}) \cap (\mathbf{p}(\hat{\mathbf{j}}), \hat{\mathbf{j}}]) \\ &\leq \mu_{\mathbf{x}}((\mathbf{q}_L^\dagger(\mathbf{j}') - \mathbf{1}, \mathbf{q}_R^\dagger(\mathbf{j})) \cap (\mathbf{p}(\hat{\mathbf{j}}), \hat{\mathbf{j}}]) \\ &= 0. \end{aligned} \quad (5.43)$$

We have thus finished deriving the first two properties (5.42) and (5.43) of $M(\cdot; \mathbf{j}', \mathbf{j})$. To derive the third property of $M(\cdot; \mathbf{j}', \mathbf{j})$, let us again fix an arbitrary $i \in \{1, \dots, m\}$ and observe that for any $j, j' \in J_i$ and $x \in \mathbb{R}$ such that $j' \leq j$ and $q_{i,L}^\dagger(j') \leq x \leq q_{i,R}^\dagger(j)$, we have $p_i(j') \leq q_{i,L}^\dagger(j') - 1 \leq x - 1$ and $x \leq j$. Extending this observation to the vector case, for all $\mathbf{j}, \mathbf{j}' \in \mathbf{J}$ and $\mathbf{x} \in \mathbb{R}^m$ such that $\mathbf{j}' \leq \mathbf{j}$ and $\mathbf{q}_L^\dagger(\mathbf{j}') \leq \mathbf{x} \leq \mathbf{q}_R^\dagger(\mathbf{j})$, we have $(\mathbf{x} - \mathbf{1}, \mathbf{x}) \subset (\mathbf{p}(\mathbf{j}'), \mathbf{j}]$. Hence, by (5.40) and (5.39), we have

$$1 \geq M(\mathbf{x}; \mathbf{j}', \mathbf{j}) = \mu_{\mathbf{x}}((\mathbf{p}(\mathbf{j}'), \mathbf{j}]) \geq \mu_{\mathbf{x}}((\mathbf{x} - \mathbf{1}, \mathbf{x})) = 1, \quad (5.44)$$

showing that $M(\mathbf{x}; \mathbf{j}', \mathbf{j}) = 1$. In particular, since $\mathbf{q}_L^\dagger(\mathbf{j}) \leq \mathbf{l}(\mathbf{j}) \leq \mathbf{q}_R^\dagger(\mathbf{j})$ for all $\mathbf{j} \in \mathbf{J}$, we have

$$M(\mathbf{l}(\mathbf{j}); \mathbf{j}, \mathbf{j}) = 1 \quad \forall \mathbf{j} \in \mathbf{J}. \quad (5.45)$$

Step 3: defining $\{g_{\mathbf{v}} : \mathbf{v} \in V(\mathcal{C})\}$ and proving the properties (IFB1)–(IFB4). Recall that $\mathbf{T}(V(\mathcal{C})) = \mathbf{l}(\mathbf{J})$ and hence $V(\mathcal{C}) = \mathbf{T}^{-1}(\mathbf{l}(\mathbf{J}))$. Thus, from now on, we index the members of $V(\mathcal{C})$ by $\mathbf{v}(\mathbf{j}) := \mathbf{T}^{-1}(\mathbf{l}(\mathbf{j}))$ for $\mathbf{j} \in \mathbf{J}$. For every $\mathbf{j} \in \mathbf{J}$, let us define $g_{\mathbf{v}(\mathbf{j})}(\mathbf{x}) := M(\mathbf{T}(\mathbf{x}); \mathbf{j}, \mathbf{j})$ for all $\mathbf{x} \in \mathbb{R}^m$. We

have by (5.35) that $g_{v(j)} \in \text{span}_1(\mathcal{G})$ and that $g_{v(j)}$ is continuous. In the following, we prove that the functions $\{g_{v(j)} : j \in \mathbf{J}\}$ satisfy the properties (IFB1)–(IFB4).

It follows directly from (5.40) that the property (IFB1) is satisfied. For all $j \in \mathbf{J}$, it follows from (5.45) that

$$g_{v(j)}(v(j)) = M(\mathbf{T}(v(j)); j, j) = M(\mathbf{l}(j); j, j) = 1.$$

Moreover, for all $j, \hat{j} \in \mathbf{J}$ such that $j \neq \hat{j}$, letting $j' = j$ in (5.42) leads to

$$g_{v(j)}(v(\hat{j})) = M(\mathbf{T}(v(\hat{j})); j, j) = M(\mathbf{l}(\hat{j}); j, j) = 0.$$

Hence, the property (IFB2) is satisfied.

Since by definition $Q(\mathbf{x}; j) = 0$ for all $\mathbf{x} \in \mathbb{R}^m$ if $j \in \bar{\mathbf{J}} \setminus \mathbf{J}$, we have $g_{v(j)}(\cdot) \in \text{span}_1(\{Q(\mathbf{T}(\cdot); j') : j' \in \mathbf{J}\})$ for all $j \in \mathbf{J}$. Moreover, we have $g_{v(j)}(v(j')) = \mathbb{1}_{\{j=j'\}}$ for all $j, j' \in \mathbf{J}$ by the property (IFB2), and hence $\{g_{v(j)} : j \in \mathbf{J}\}$ are linearly independent. Subsequently, since $\{g_{v(j)} : j \in \mathbf{J}\}$ and $\{Q(\mathbf{T}(\cdot); j) : j \in \mathbf{J}\}$ have the same finite cardinality, it follows that every $h \in \text{span}_1(\{Q(\mathbf{T}(\cdot); j) : j \in \mathbf{J}\})$ satisfies

$$h(\mathbf{x}) = \sum_{j \in \mathbf{J}} h(v(j))g_{v(j)}(\mathbf{x}) \quad \forall \mathbf{x} \in \mathbb{R}^m, \quad (5.46)$$

that is, every $h \in \text{span}_1(\{Q(\mathbf{T}(\cdot); j) : j \in \mathbf{J}\})$ is uniquely characterized by the values of $(h(v(j)))_{j \in \mathbf{J}}$. To prove the properties (IFB3) and (IFB4), let us fix an arbitrary $F \in \mathfrak{F}(\mathcal{C})$, which, by (5.32), satisfies $\mathbf{T}(F) = [\mathbf{k}_L, \mathbf{k}_R]$ for some $\mathbf{k}_L = (k_{1,L}, \dots, k_{m,L})^\top \in \mathbf{K}_L$ and $\mathbf{k}_R = (k_{1,R}, \dots, k_{m,R})^\top \in \mathbf{K}_R$ such that $\mathbf{k}_L \leq \mathbf{k}_R$. In addition, let us fix an arbitrary $\hat{j} = (\hat{j}_1, \dots, \hat{j}_m)^\top \in \mathbf{J}$ such that $\mathbf{l}(\hat{j}) \notin \mathbf{T}(F)$. Since $\mathbf{T}(\cdot)$ is a bijection, we have $v(\hat{j}) = \mathbf{T}^{-1}(\mathbf{l}(\hat{j})) \notin F$ and thus $v(\hat{j}) \in V(\mathcal{C}) \setminus V(F)$. Now, let us consider the function $M(\mathbf{T}(\cdot); \mathbf{q}_L(\mathbf{k}_L), \mathbf{q}_R(\mathbf{k}_R))$. Since every $\mathbf{y} \in \mathbf{T}(F)$ satisfies $\mathbf{k}_L \leq \mathbf{y} \leq \mathbf{k}_R$, it follows from (5.31) that

$$\mathbf{q}_L^\dagger(\mathbf{q}_L(\mathbf{k}_L)) \leq \mathbf{T}(\mathbf{x}) \leq \mathbf{q}_R^\dagger(\mathbf{q}_R(\mathbf{k}_R)) \quad \forall \mathbf{x} \in F. \quad (5.47)$$

Since $\mathbf{q}_L(\mathbf{k}_L) \leq \mathbf{q}_R(\mathbf{k}_R)$, we have by (5.47) and (5.44) that

$$M(\mathbf{T}(\mathbf{x}); \mathbf{q}_L(\mathbf{k}_L), \mathbf{q}_R(\mathbf{k}_R)) = 1 \quad \forall \mathbf{x} \in F. \quad (5.48)$$

In particular, we have $M(\mathbf{T}(\mathbf{x}); \mathbf{q}_L(\mathbf{k}_L), \mathbf{q}_R(\mathbf{k}_R)) = 1$ for all $\mathbf{x} \in V(F)$. On the other hand, $\mathbf{l}(\hat{j}) \notin \mathbf{T}(F)$ implies that there exists $i \in \{1, \dots, m\}$ such that either $l_i(\hat{j}_i) < k_{i,L}$ or $l_i(\hat{j}_i) > k_{i,R}$ holds. If $l_i(\hat{j}_i) < k_{i,L}$, then we have $k_{i,L} \geq 1$, $\hat{j}_i \neq \infty$, and hence $\hat{j}_i = l_i(\hat{j}_i) < k_{i,L} \leq q_{i,L}(k_{i,L})$. Alternatively, if $l_i(\hat{j}_i) > k_{i,R}$, then we have $k_{i,R} \leq n_i - 1$, and hence $\hat{j}_i > k_{i,R} = q_{i,R}(k_{i,R})$. In both cases, $\mathbf{q}_L(\mathbf{k}_L) \leq \hat{j} \leq \mathbf{q}_R(\mathbf{k}_R)$ does not hold, and we have by (5.42) that

$$M(\mathbf{T}(v(\hat{j})); \mathbf{q}_L(\mathbf{k}_L), \mathbf{q}_R(\mathbf{k}_R)) = M(\mathbf{l}(\hat{j}); \mathbf{q}_L(\mathbf{k}_L), \mathbf{q}_R(\mathbf{k}_R)) = 0.$$

To summarize the properties of $M(\mathbf{T}(\cdot); \mathbf{q}_L(\mathbf{k}_L), \mathbf{q}_R(\mathbf{k}_R))$, we have $M(\mathbf{T}(\mathbf{x}); \mathbf{q}_L(\mathbf{k}_L), \mathbf{q}_R(\mathbf{k}_R)) = 1$ for all $\mathbf{x} \in V(F)$, and $M(\mathbf{T}(\mathbf{x}); \mathbf{q}_L(\mathbf{k}_L), \mathbf{q}_R(\mathbf{k}_R)) = 0$ for all $\mathbf{x} \in V(\mathcal{C}) \setminus V(F)$. Consequently, by (5.46) and the fact that $M(\mathbf{T}(\cdot); \mathbf{q}_L(\mathbf{k}_L), \mathbf{q}_R(\mathbf{k}_R)) \in \text{span}_1(\{Q(\mathbf{T}(\cdot); j) : j \in \mathbf{J}\})$, it holds that

$$M(\mathbf{T}(\mathbf{x}); \mathbf{q}_L(\mathbf{k}_L), \mathbf{q}_R(\mathbf{k}_R)) = \sum_{j \in \mathbf{J}, v(j) \in V(F)} g_{v(j)}(\mathbf{x}) \quad \forall \mathbf{x} \in \mathbb{R}^m. \quad (5.49)$$

It follows from (5.49) and (5.48) that the property (IFB3) is satisfied. Moreover, since $\mathbf{q}_L(\mathbf{k}_L) \leq \hat{j} \leq \mathbf{q}_R(\mathbf{k}_R)$ does not hold, by (5.47) and (5.43), it holds for all $\mathbf{x} \in F$ that $g_{v(\hat{j})}(\mathbf{x}) = M(\mathbf{T}(\mathbf{x}); \hat{j}, \hat{j}) = 0$, which proves that the property (IFB4) is satisfied.

Step 4: defining $\{\bar{g}_{\mathbf{u}} : \mathbf{u} \in D(\mathcal{C})\}$ and proving the properties (IFB5) and (IFB6). Recall from (5.30) that $D(\mathcal{C}) = \{-\mathbf{e}_1, \mathbf{e}_1, \dots, -\mathbf{e}_m, \mathbf{e}_m\}$. For $i = 1, \dots, m$, let us define the continuous functions $\bar{g}_{\mathbf{e}_i} : \mathbb{R}^m \rightarrow \mathbb{R}$ and $\bar{g}_{-\mathbf{e}_i} : \mathbb{R}^m \rightarrow \mathbb{R}$ by

$$\begin{aligned} \bar{g}_{\mathbf{e}_i}(x_1, \dots, x_m) &:= \theta \max\{x_i - \kappa_{i,n_i}, 0\} \in \text{span}_1(\mathcal{G}), \\ \bar{g}_{-\mathbf{e}_i}(x_1, \dots, x_m) &:= \theta \max\{\kappa_{i,0} - x_i, 0\} = \theta \kappa_{i,0} - \theta x_i + \theta \max\{x_i - \kappa_{i,0}, 0\} \in \text{span}_1(\mathcal{G}), \end{aligned} \quad (5.50)$$

where $\theta \geq 1$ is a constant that satisfies $\|\mathbf{x}\| \leq \theta \|\mathbf{x}\|_1$ for all $\mathbf{x} \in \mathbb{R}^m$, which exists due to the equivalence of norms on a Euclidean space. The property **(IFB5)** follows immediately from the definitions in **(5.50)**. To prove the property **(IFB6)**, let us fix $F \in \mathfrak{F}(\mathcal{C})$ with $D(F) \neq \emptyset$ and $\mathbf{x} = (x_1, \dots, x_m)^\top \in F$. By **(5.29)**, F can be expressed as $F = I_1 \times \dots \times I_m$, where $I_i \in \{(-\infty, \kappa_{i,0}], \{\kappa_{i,0}\}, [\kappa_{i,0}, \kappa_{i,1}], \dots, [\kappa_{i,n_i-1}, \kappa_{i,n_i}], \{\kappa_{i,n_i}\}, [\kappa_{i,n_i}, \infty)\}$ for $i = 1, \dots, m$. Observe that for $i = 1, \dots, m$, $\mathbf{e}_i \in D(F)$ if and only if $I_i = [\kappa_{i,n_i}, \infty)$, and that $-\mathbf{e}_i \in D(F)$ if and only if $I_i = (-\infty, \kappa_{i,0}]$. For $i = 1, \dots, m$, let us define \tilde{I}_i as follows:

$$\tilde{I}_i := \begin{cases} \{\kappa_{i,n_i}\} & \text{if } \mathbf{e}_i \in D(F), \\ \{\kappa_{i,0}\} & \text{if } -\mathbf{e}_i \in D(F), \\ I_i & \text{if } \mathbf{e}_i \notin D(F) \text{ and } -\mathbf{e}_i \notin D(F). \end{cases}$$

Since \tilde{I}_i is bounded for $i = 1, \dots, m$, we have $\tilde{I}_1 \times \dots \times \tilde{I}_m = \text{conv}(V(F))$. Now, let us construct $\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(m)}$ by the following procedure.

- (a) Let $\mathbf{x}^{(0)} = \mathbf{x}$.
- (b) For $i = 1, \dots, m$, define $\mathbf{x}^{(i)}$ as follows:
 - if $\mathbf{e}_i \in D(F)$, let $\mathbf{x}^{(i)} = \mathbf{x}^{(i-1)} - \max\{x_i - \kappa_{i,n_i}, 0\}\mathbf{e}_i$;
 - if $-\mathbf{e}_i \in D(F)$, let $\mathbf{x}^{(i)} = \mathbf{x}^{(i-1)} + \max\{\kappa_{i,0} - x_i, 0\}\mathbf{e}_i$;
 - if $\mathbf{e}_i \notin D(F)$ and $-\mathbf{e}_i \notin D(F)$, let $\mathbf{x}^{(i)} = \mathbf{x}^{(i-1)}$.

Let $x_j^{(i)}$ denote the j -th component of $\mathbf{x}^{(i)}$. For $i = 1, \dots, m$, it follows from the above procedure that $x_i^{(i)} = \kappa_{i,n_i} \in \tilde{I}_i$ if $\mathbf{e}_i \in D(F)$, $x_i^{(i)} = \kappa_{i,0} \in \tilde{I}_i$ if $-\mathbf{e}_i \in D(F)$, and that $x_i^{(i)} = x_i \in \tilde{I}_i$ if $\mathbf{e}_i \notin D(F)$ and $-\mathbf{e}_i \notin D(F)$. Thus, we have $\mathbf{x}^{(m)} \in \tilde{I}_1 \times \dots \times \tilde{I}_m = \text{conv}(V(F))$. Moreover, we have

$$\|\mathbf{x}^{(i)} - \mathbf{x}^{(i-1)}\|_1 = \begin{cases} \max\{x_i - \kappa_{i,n_i}, 0\} = \theta^{-1} \bar{g}_{\mathbf{e}_i}(\mathbf{x}) & \text{if } \mathbf{e}_i \in D(F), \\ \max\{\kappa_{i,0} - x_i, 0\} = \theta^{-1} \bar{g}_{-\mathbf{e}_i}(\mathbf{x}) & \text{if } -\mathbf{e}_i \in D(F), \\ 0 & \text{if } \mathbf{e}_i \notin D(F) \text{ and } -\mathbf{e}_i \notin D(F). \end{cases}$$

Consequently, it holds that

$$\begin{aligned} \min_{\mathbf{y} \in \text{conv}(V(F))} \{\|\mathbf{x} - \mathbf{y}\|\} &\leq \|\mathbf{x} - \mathbf{x}^{(m)}\| \\ &\leq \sum_{i=1}^m \|\mathbf{x}^{(i)} - \mathbf{x}^{(i-1)}\| \\ &\leq \sum_{i=1}^m \theta \|\mathbf{x}^{(i)} - \mathbf{x}^{(i-1)}\|_1 \\ &= \sum_{\mathbf{u} \in D(F)} \bar{g}_{\mathbf{u}}(\mathbf{x}). \end{aligned}$$

Thus, the property **(IFB6)** is satisfied. The proof is now complete. \square

Proof of Theorem 3.2.7. Let $\mathcal{Y}^\dagger := \bigcup_{C \in \mathcal{C}} C$. It follows from Lemma 5.4.1 that $\{\text{relint}(F) : F \in \mathfrak{F}(\mathcal{C})\}$ is a disjoint partition of \mathcal{Y}^\dagger . The rest of the proof is divided into five steps.

Step 1: decomposing a fixed probability measure $\mu \in \mathcal{P}_1(\mathcal{Y})$ into a mixture of probability measures each concentrated on $\text{relint}(F)$ for a face $F \in \mathfrak{F}(\mathcal{C})$. Let us fix an arbitrary $\mu \in \mathcal{P}_1(\mathcal{Y})$. Let us define $\mu^\dagger \in \mathcal{P}_1(\mathcal{Y}^\dagger)$ by $\mu^\dagger(E) := \mu(E \cap \mathcal{Y})$ for all $E \in \mathcal{B}(\mathcal{Y}^\dagger)$, and define $\mathfrak{F}_{\mu^\dagger}(\mathcal{C}) := \{F \in \mathfrak{F}(\mathcal{C}) : \mu^\dagger(\text{relint}(F)) > 0\}$. Then, $\mu^\dagger\left(\bigcup_{F \in \mathfrak{F}_{\mu^\dagger}(\mathcal{C})} \text{relint}(F)\right) = 1$. For each $F \in \mathfrak{F}_{\mu^\dagger}(\mathcal{C})$, let us define $\mu_F^\dagger \in \mathcal{P}_1(\mathcal{Y}^\dagger)$ as follows:

$$d\mu_F^\dagger := \frac{\mathbb{1}_{\text{relint}(F)}}{\mu^\dagger(\text{relint}(F))} d\mu^\dagger.$$

Thus, for any $E \in \mathcal{B}(\mathcal{Y}^\dagger)$, $\sum_{F \in \mathfrak{F}_{\mu^\dagger}(\mathcal{C})} [\mu^\dagger(\text{relint}(F)) \mu_F^\dagger(E)] = \mu^\dagger\left(\left[\bigcup_{F \in \mathfrak{F}_{\mu^\dagger}(\mathcal{C})} \text{relint}(F)\right] \cap E\right) = \mu^\dagger(E)$ and hence $\sum_{F \in \mathfrak{F}_{\mu^\dagger}(\mathcal{C})} \mu^\dagger(\text{relint}(F)) \mu_F^\dagger(d\mathbf{x}) = \mu^\dagger(d\mathbf{x})$.

Step 2: approximating the mixture component concentrated on $\text{relint}(F)$ by a discrete probability measure concentrated on $V(F)$. For each $F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C})$, let us define $\hat{\mu}_F^\dagger$ as follows:

$$\hat{\mu}_F^\dagger(d\mathbf{x}) := \sum_{\mathbf{v} \in V(F)} \left(\int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\mu_F^\dagger \right) \delta_{\mathbf{v}}(d\mathbf{x}),$$

where $\delta_{\mathbf{v}}$ denotes the Dirac measure at \mathbf{v} . Then,

$$\begin{aligned} \hat{\mu}_F^\dagger(\mathcal{Y}^\dagger) &= \sum_{\mathbf{v} \in V(F)} \int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\mu_F^\dagger \\ &= \int_{\mathcal{Y}^\dagger} \left(\sum_{\mathbf{v} \in V(F)} g_{\mathbf{v}} \right) d\mu_F^\dagger \\ &= \frac{1}{\mu^\dagger(\text{relint}(F))} \int_{\mathcal{Y}^\dagger} \left(\sum_{\mathbf{v} \in V(F)} g_{\mathbf{v}} \right) \mathbb{1}_{\text{relint}(F)} d\mu^\dagger \\ &= \frac{\mu^\dagger(\text{relint}(F))}{\mu^\dagger(\text{relint}(F))} \\ &= 1, \end{aligned}$$

where the fourth equality is due to the property (IFB3) of $\{g_{\mathbf{v}} : \mathbf{v} \in V(\mathfrak{C})\}$. Since $\int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\mu_F^\dagger \geq 0$ by the property (IFB1), we thus have $\hat{\mu}_F^\dagger \in \mathcal{P}_1(\mathcal{Y}^\dagger)$. Moreover, for every $\mathbf{v} \in V(F)$, we have by the property (IFB2) that

$$\int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\hat{\mu}_F^\dagger = \sum_{\mathbf{v}' \in V(F)} \left[\left(\int_{\mathcal{Y}^\dagger} g_{\mathbf{v}'} d\mu_F^\dagger \right) g_{\mathbf{v}}(\mathbf{v}') \right] = \int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\mu_F^\dagger.$$

Furthermore, for every $\mathbf{v} \in V(\mathfrak{C}) \setminus V(F)$, we have by the property (IFB4) that

$$\int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\hat{\mu}_F^\dagger = 0 = \int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\mu_F^\dagger.$$

We have thus shown that

$$\int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\hat{\mu}_F^\dagger = \int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\mu_F^\dagger \quad \forall \mathbf{v} \in V(\mathfrak{C}), \forall F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C}). \quad (5.51)$$

Step 3: controlling the W_1 -distance between the mixture component concentrated on $\text{relint}(F)$ and its discrete approximation. For each $F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C})$, let $T_F : F \rightarrow F$ be a Borel measurable mapping such that

$$F \ni \mathbf{x} \mapsto T_F(\mathbf{x}) \in \arg \min_{\mathbf{y} \in \text{conv}(V(F))} \{\|\mathbf{x} - \mathbf{y}\|\}.$$

Such a mapping exists by [10, Proposition 7.33]. Let γ_F denote an optimal coupling of μ_F^\dagger and $\hat{\mu}_F^\dagger$ under the cost $(\mathbf{x}, \mathbf{y}) \mapsto \|\mathbf{x} - \mathbf{y}\|$ and let us fix an arbitrary $\tilde{\gamma}_F \in \Gamma(\mu_F^\dagger \circ T_F^{-1}, \hat{\mu}_F^\dagger)$. By the definition of T_F ,

$$\begin{aligned} \int_{\mathcal{Y}^\dagger \times \mathcal{Y}^\dagger} \|\mathbf{x} - \mathbf{y}\| \gamma_F(d\mathbf{x}, d\mathbf{y}) &= W_1(\mu_F^\dagger, \hat{\mu}_F^\dagger) \\ &\leq W_1(\mu_F^\dagger, \mu_F^\dagger \circ T_F^{-1}) + W_1(\mu_F^\dagger \circ T_F^{-1}, \hat{\mu}_F^\dagger) \\ &\leq \int_{\mathcal{Y}^\dagger} \|\mathbf{x} - T_F(\mathbf{x})\| \mu_F^\dagger(d\mathbf{x}) + \int_{\mathcal{Y}^\dagger \times \mathcal{Y}^\dagger} \|\mathbf{x} - \mathbf{y}\| \tilde{\gamma}_F(d\mathbf{x}, d\mathbf{y}) \\ &= \int_{\mathcal{Y}^\dagger} \min_{\mathbf{y} \in \text{conv}(V(F))} \{\|\mathbf{x} - \mathbf{y}\|\} \mu_F^\dagger(d\mathbf{x}) + \int_{\mathcal{Y}^\dagger \times \mathcal{Y}^\dagger} \|\mathbf{x} - \mathbf{y}\| \tilde{\gamma}_F(d\mathbf{x}, d\mathbf{y}). \end{aligned} \quad (5.52)$$

If $D(F) = \emptyset$, then $\text{conv}(V(F)) = F$ and thus $\min_{\mathbf{y} \in \text{conv}(V(F))} \{\|\mathbf{x} - \mathbf{y}\|\} = 0$ for all $\mathbf{x} \in F$. If $D(F) \neq \emptyset$, then by the properties **(IFB5)** and **(IFB6)** of $\{\bar{g}_{\mathbf{u}} : \mathbf{u} \in D(\mathfrak{C})\}$, we have

$$\begin{aligned} \int_{\mathcal{Y}^\dagger} \min_{\mathbf{y} \in \text{conv}(V(F))} \{\|\mathbf{x} - \mathbf{y}\|\} \mu_F^\dagger(d\mathbf{x}) &\leq \int_{\mathcal{Y}^\dagger} \sum_{\mathbf{u} \in D(F)} \bar{g}_{\mathbf{u}}(\mathbf{x}) \mu_F^\dagger(d\mathbf{x}) \\ &\leq \sum_{\mathbf{u} \in D(\mathfrak{C})} \int_{\mathcal{Y}^\dagger} \bar{g}_{\mathbf{u}} d\mu_F^\dagger. \end{aligned} \quad (5.53)$$

Moreover, since $\text{supp}(\tilde{\gamma}_F) \subset \text{conv}(V(F)) \times \text{conv}(V(F))$ and by a convex maximization argument $\max_{\mathbf{x}, \mathbf{y} \in \text{conv}(V(F))} \{\|\mathbf{x} - \mathbf{y}\|\} = \max_{\mathbf{v}, \mathbf{v}' \in V(F)} \{\|\mathbf{v} - \mathbf{v}'\|\}$, we have

$$\begin{aligned} \int_{\mathcal{Y}^\dagger \times \mathcal{Y}^\dagger} \|\mathbf{x} - \mathbf{y}\| \tilde{\gamma}_F(d\mathbf{x}, d\mathbf{y}) &\leq \max_{\mathbf{x}, \mathbf{y} \in \text{conv}(V(F))} \{\|\mathbf{x} - \mathbf{y}\|\} \\ &= \max_{\mathbf{v}, \mathbf{v}' \in V(F)} \{\|\mathbf{v} - \mathbf{v}'\|\} \\ &\leq \max_{\mathfrak{C} \in \mathfrak{C}} \max_{\mathbf{v}, \mathbf{v}' \in V(\mathfrak{C})} \{\|\mathbf{v} - \mathbf{v}'\|\} \\ &= \eta(\mathfrak{C}). \end{aligned} \quad (5.54)$$

Combining **(5.52)**, **(5.53)**, and **(5.54)**, we get

$$\int_{\mathcal{Y}^\dagger \times \mathcal{Y}^\dagger} \|\mathbf{x} - \mathbf{y}\| \gamma_F(d\mathbf{x}, d\mathbf{y}) \leq \eta(\mathfrak{C}) + \sum_{\mathbf{u} \in D(\mathfrak{C})} \int_{\mathcal{Y}^\dagger} \bar{g}_{\mathbf{u}} d\mu_F^\dagger. \quad (5.55)$$

Step 4: taking the mixture of the discrete probability measures to make a discrete approximation of the original probability measure and controlling their W_1 -distance. Now that we have defined $\mu_F^\dagger \in \mathcal{P}_1(\mathcal{Y}^\dagger)$, $\hat{\mu}_F^\dagger \in \mathcal{P}_1(\mathcal{Y}^\dagger)$, and $\gamma_F \in \Gamma(\mu_F^\dagger, \hat{\mu}_F^\dagger)$ for each $F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C})$, let us define $\hat{\mu}^\dagger$ and γ by

$$\begin{aligned} \hat{\mu}^\dagger(d\mathbf{x}) &:= \sum_{F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C})} \mu^\dagger(\text{relint}(F)) \hat{\mu}_F^\dagger(d\mathbf{x}), \\ \gamma(d\mathbf{x}, d\mathbf{y}) &:= \sum_{F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C})} \mu^\dagger(\text{relint}(F)) \gamma_F(d\mathbf{x}, d\mathbf{y}). \end{aligned}$$

Since $\mu^\dagger\left(\bigcup_{F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C})} \text{relint}(F)\right) = 1$, we have $\hat{\mu}^\dagger \in \mathcal{P}_1(\mathcal{Y}^\dagger)$ and $\gamma \in \Gamma(\mu^\dagger, \hat{\mu}^\dagger)$. By the property **(IFB2)** and **(5.51)**, it holds for all $\mathbf{v} \in V(\mathfrak{C})$ that

$$\begin{aligned} \hat{\mu}^\dagger(\{\mathbf{v}\}) &= \int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\hat{\mu}^\dagger \\ &= \sum_{F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C})} \mu^\dagger(\text{relint}(F)) \int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\hat{\mu}_F^\dagger \\ &= \sum_{F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C})} \mu^\dagger(\text{relint}(F)) \int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\mu_F^\dagger \\ &= \sum_{F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C})} \int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} \mathbb{1}_{\text{relint}(F)} d\mu^\dagger \\ &= \int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\mu^\dagger. \end{aligned} \quad (5.56)$$

Moreover, by (5.55),

$$\begin{aligned}
\int_{\mathcal{Y}^\dagger \times \mathcal{Y}^\dagger} \|\mathbf{x} - \mathbf{y}\| \gamma(d\mathbf{x}, d\mathbf{y}) &= \sum_{F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C})} \mu^\dagger(\text{relint}(F)) \int_{\mathcal{Y}^\dagger \times \mathcal{Y}^\dagger} \|\mathbf{x} - \mathbf{y}\| \gamma_F(d\mathbf{x}, d\mathbf{y}) \\
&\leq \sum_{F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C})} \mu^\dagger(\text{relint}(F)) \left(\eta(\mathfrak{C}) + \sum_{\mathbf{u} \in D(\mathfrak{C})} \int_{\mathcal{Y}^\dagger} \bar{g}_{\mathbf{u}} d\mu_F^\dagger \right) \\
&= \eta(\mathfrak{C}) + \sum_{\mathbf{u} \in D(\mathfrak{C})} \sum_{F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C})} \mu^\dagger(\text{relint}(F)) \int_{\mathcal{Y}^\dagger} \bar{g}_{\mathbf{u}} d\mu_F^\dagger \\
&= \eta(\mathfrak{C}) + \sum_{\mathbf{u} \in D(\mathfrak{C})} \sum_{F \in \mathfrak{F}_{\mu^\dagger}(\mathfrak{C})} \int_{\mathcal{Y}^\dagger} \bar{g}_{\mathbf{u}} \mathbb{1}_{\text{relint}(F)} d\mu^\dagger \\
&= \eta(\mathfrak{C}) + \sum_{\mathbf{u} \in D(\mathfrak{C})} \int_{\mathcal{Y}^\dagger} \bar{g}_{\mathbf{u}} d\mu^\dagger \\
&= \eta(\mathfrak{C}) + \sum_{\mathbf{u} \in D(\mathfrak{C})} \int_{\mathcal{Y}} \bar{g}_{\mathbf{u}} d\mu.
\end{aligned}$$

Thus, $W_1(\mu^\dagger, \hat{\mu}^\dagger) \leq \int_{\mathcal{Y}^\dagger \times \mathcal{Y}^\dagger} \|\mathbf{x} - \mathbf{y}\| \gamma(d\mathbf{x}, d\mathbf{y}) \leq \eta(\mathfrak{C}) + \sum_{\mathbf{u} \in D(\mathfrak{C})} \int_{\mathcal{Y}} \bar{g}_{\mathbf{u}} d\mu$.

Step 5: showing that if $\mu \stackrel{\mathcal{G}}{\sim} \nu$, then μ and ν lead to the same discrete approximation. Finally, let us take an arbitrary $\nu \in \mathcal{P}_1(\mathcal{Y})$ such that $\mu \stackrel{\mathcal{G}}{\sim} \nu$. Let us repeat Step 1 to Step 4 above to construct $\nu^\dagger, \hat{\nu}^\dagger \in \mathcal{P}_1(\mathcal{Y}^\dagger)$. By the same arguments above, we have

$$W_1(\nu^\dagger, \hat{\nu}^\dagger) \leq \eta(\mathfrak{C}) + \sum_{\mathbf{u} \in D(\mathfrak{C})} \int_{\mathcal{Y}} \bar{g}_{\mathbf{u}} d\nu = \eta(\mathfrak{C}) + \sum_{\mathbf{u} \in D(\mathfrak{C})} \int_{\mathcal{Y}} \bar{g}_{\mathbf{u}} d\mu,$$

where the equality is due to the assumption that $\{\bar{g}_{\mathbf{u}} : \mathbf{u} \in D(\mathfrak{C})\} \subset \text{span}_1(\mathcal{G})$. Moreover, by (5.56) and the assumption that $\{g_{\mathbf{v}} : \mathbf{v} \in V(\mathfrak{C})\} \subset \text{span}_1(\mathcal{G})$, we have

$$\hat{\nu}^\dagger(\{\mathbf{v}\}) = \int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\nu^\dagger = \int_{\mathcal{Y}} g_{\mathbf{v}} d\nu = \int_{\mathcal{Y}} g_{\mathbf{v}} d\mu = \int_{\mathcal{Y}^\dagger} g_{\mathbf{v}} d\mu^\dagger = \hat{\mu}^\dagger(\{\mathbf{v}\}) \quad \forall \mathbf{v} \in V(\mathfrak{C}). \quad (5.57)$$

But since $\text{supp}(\mu^\dagger) \subseteq V(\mathfrak{C})$ and $\text{supp}(\nu^\dagger) \subseteq V(\mathfrak{C})$, (5.57) implies that $\mu^\dagger = \nu^\dagger$. Thus, it holds that $W_1(\mu^\dagger, \nu^\dagger) \leq W_1(\mu^\dagger, \hat{\mu}^\dagger) + W_1(\nu^\dagger, \hat{\nu}^\dagger) \leq 2 \left(\eta(\mathfrak{C}) + \sum_{\mathbf{u} \in D(\mathfrak{C})} \int_{\mathcal{Y}} \bar{g}_{\mathbf{u}} d\mu \right)$. Let $\theta^\dagger \in \Gamma(\mu^\dagger, \nu^\dagger) \subset \mathcal{P}(\mathcal{Y}^\dagger \times \mathcal{Y}^\dagger)$ be an optimal coupling of μ^\dagger and ν^\dagger under the cost function $(\mathbf{x}, \mathbf{y}) \mapsto \|\mathbf{x} - \mathbf{y}\|$. Since $\theta^\dagger(\mathcal{Y} \times \mathcal{Y}) = 1$, let us define $\theta \in \mathcal{P}(\mathcal{Y} \times \mathcal{Y})$ by $\theta(E) := \theta^\dagger(E)$ for all $E \in \mathcal{B}(\mathcal{Y} \times \mathcal{Y})$. Then, we have $\theta \in \Gamma(\mu, \nu)$ and

$$\begin{aligned}
W_1(\mu, \nu) &\leq \int_{\mathcal{Y} \times \mathcal{Y}} d_{\mathcal{Y}}(\mathbf{x}, \mathbf{y}) \theta(d\mathbf{x}, d\mathbf{y}) \\
&= \int_{\mathcal{Y}^\dagger \times \mathcal{Y}^\dagger} \|\mathbf{x} - \mathbf{y}\| \theta^\dagger(d\mathbf{x}, d\mathbf{y}) \\
&= W_1(\mu^\dagger, \nu^\dagger) \\
&\leq 2 \left(\eta(\mathfrak{C}) + \sum_{\mathbf{u} \in D(\mathfrak{C})} \int_{\mathcal{Y}} \bar{g}_{\mathbf{u}} d\mu \right).
\end{aligned}$$

In the particular case where \mathfrak{C} contains only bounded sets, we have $D(\mathfrak{C}) = \emptyset$ and thus $W_1(\mu, \nu) \leq 2\eta(\mathfrak{C})$. The proof is now complete. \square

Proof of Corollary 3.2.8. For $i = 1, \dots, m$, let $\mathcal{I}_i := \{(-\infty, \kappa_{i,0}], [\kappa_{i,0}, \kappa_{i,1}], \dots, [\kappa_{i,n_i-1}, \kappa_{i,n_i}], [\kappa_{i,n_i}, \infty)\}$, and let $\mathfrak{C} := \{I_1 \times \dots \times I_m : I_i \in \mathcal{I}_i \forall 1 \leq i \leq m\}$. By letting $\beta_1 = \dots = \beta_m = \beta$ in (3.6) and Proposition 3.2.6 and then multiplying each function $\mathbb{R}^m \ni (x_1, \dots, x_m)^\top \mapsto (\max_{i \in L} \{\beta^{-1}(x_i -$

$\kappa_{i,j_i})^+\} \in \mathbb{R}$ in (3.6) by the positive constant β , it follows that \mathfrak{C} is a polyhedral cover of \mathcal{Y} and \mathcal{G} defined in (3.7) is an interpolation function basis associated with \mathfrak{C} . Since $V(\mathfrak{C}) = \times_{i=1}^m \{\kappa_{i,0}, \dots, \kappa_{i,n_i}\}$, we have

$$\eta(\mathfrak{C}) := \max_{C \in \mathfrak{C}} \max_{\mathbf{v}, \mathbf{v}' \in V(C)} \{\|\mathbf{v} - \mathbf{v}'\|\} = \|\beta \mathbf{1}\| \leq \theta \beta \|\mathbf{1}\|_1 = \theta m \beta, \quad (5.58)$$

where $\mathbf{1}$ denotes the vector in \mathbb{R}^m with all entries equal to 1. Moreover, it follows from (5.30) that $D(\mathfrak{C}) = \{-e_1, e_1, \dots, -e_m, e_m\}$. Therefore, let us define \bar{g}_{e_i} and \bar{g}_{-e_i} for $i = 1, \dots, m$ by (5.50). Subsequently,

$$\sum_{\mathbf{u} \in D(\mathfrak{C})} \int_{\mathcal{Y}} \bar{g}_{\mathbf{u}} d\mu = \sum_{i=1}^m \int_{\mathcal{Y}} \bar{g}_{-e_i} + \bar{g}_{e_i} d\mu = \sum_{i=1}^m \int_{\mathbb{R}} \theta(\kappa_{i,0} - x_i)^+ + \theta(x_i - \kappa_{i,n_i})^+ \mu_i(dx_i). \quad (5.59)$$

Combining (5.58) and (5.59), it follows from Theorem 3.2.7 that (3.8) holds.

To prove the last statement in Corollary 3.2.8, let us fix an arbitrary $\epsilon > 0$ and let $\beta = \frac{\epsilon}{4\theta m}$. For $i = 1, \dots, m$, it holds by the dominated convergence theorem that there exists $\underline{\kappa}_i \in \mathbb{R}$ such that

$$\int_{\mathbb{R}} (\underline{\kappa}_i - x_i)^+ \mu_i(dx_i) \leq \frac{\epsilon}{8\theta m}.$$

Subsequently, by applying the dominated convergence theorem again, there exists $n_i \in \mathbb{N}$ such that

$$\int_{\mathbb{R}} (x_i - \underline{\kappa}_i - n_i \beta)^+ \mu_i(dx_i) \leq \frac{\epsilon}{8\theta m}.$$

With this choice of β , $(\underline{\kappa}_i)_{i=1:m}$, and $(n_i)_{i=1:m}$, we have by (3.8) that

$$\begin{aligned} \bar{W}_{1,\mu}([\mu]_{\mathcal{G}}) &\leq 2\theta \left(m\beta + \sum_{i=1}^m \int_{\mathbb{R}} (\kappa_{i,0} - x_i)^+ + (x_i - \kappa_{i,n_i})^+ \mu_i(dx_i) \right) \\ &\leq 2\theta \left(m \frac{\epsilon}{4\theta m} + \sum_{i=1}^m \left(\frac{\epsilon}{8\theta m} + \frac{\epsilon}{8\theta m} \right) \right) \\ &= \frac{2\theta \epsilon}{2\theta} \\ &= \epsilon. \end{aligned}$$

The proof is now complete. \square

5.5. Proof of results in Section 4.1. Before proving Proposition 4.1.1, let us first establish the following lemma.

Lemma 5.5.1. *Let \mathcal{Y} be a compact subset of a Euclidean space, let \mathfrak{C} be a polyhedral cover of \mathcal{Y} such that $\bigcup_{C \in \mathfrak{C}} C = \mathcal{Y}$, and let continuous real-valued functions $\{g_{\mathbf{t}} : \mathbf{t} \in V(\mathfrak{C})\}$ on \mathcal{Y} satisfy the properties (IFB1)–(IFB4) with respect to \mathfrak{C} . Let $k := |V(\mathfrak{C})| - 1$ and enumerate $V(\mathfrak{C})$ arbitrarily by $V(\mathfrak{C}) = \{\mathbf{t}_0, \mathbf{t}_1, \dots, \mathbf{t}_k\}$. Let $\mathcal{G} := \{g_{\mathbf{t}_j} : 1 \leq j \leq k\}$, and let*

$$\mathcal{Y} \ni \mathbf{x} \mapsto \mathbf{g}(\mathbf{x}) := (g_{\mathbf{t}_1}(\mathbf{x}), \dots, g_{\mathbf{t}_k}(\mathbf{x}))^T \in \mathbb{R}^k.$$

Then, \mathcal{G} is an interpolation function basis associated with \mathfrak{C} and

$$\text{conv}(\{\mathbf{g}(\mathbf{x}) : \mathbf{x} \in \mathcal{Y}\}) = \left\{ (z_1, \dots, z_k)^T : z_1 \geq 0, \dots, z_k \geq 0, \sum_{j=1}^k z_j \leq 1 \right\}, \quad (5.60)$$

that is, $\text{conv}(\{\mathbf{g}(\mathbf{x}) : \mathbf{x} \in \mathcal{Y}\})$ is a k -simplex with vertices $\{\mathbf{0}, \mathbf{e}_1, \dots, \mathbf{e}_k\}$ where \mathbf{e}_j denotes the j -th standard basis vector of \mathbb{R}^k .

Proof of Lemma 5.5.1. Note that since \mathcal{Y} is bounded, $D(\mathfrak{C}) = \emptyset$ and thus \mathcal{G} vacuously satisfy (IFB5) and (IFB6). Hence, \mathcal{G} is an interpolation function basis associated with \mathfrak{C} . Moreover, since $\bigcup_{C \in \mathfrak{C}} C = \mathcal{Y}$, we have $V(\mathfrak{C}) \subset \mathcal{Y}$. In addition, we have by the property (IFB2) that $\mathbf{g}(\mathbf{t}_0) = \mathbf{0}$ and $\mathbf{g}(\mathbf{t}_j) = \mathbf{e}_j$ for $j = 1, \dots, k$. Consequently,

$$\begin{aligned} \text{conv}(\{\mathbf{g}(\mathbf{x}) : \mathbf{x} \in \mathcal{Y}\}) &\supseteq \text{conv}(\{\mathbf{0}, \mathbf{e}_1, \dots, \mathbf{e}_k\}) \\ &= \left\{ (z_1, \dots, z_k)^T : z_1 \geq 0, \dots, z_k \geq 0, \sum_{j=1}^k z_j \leq 1 \right\}. \end{aligned}$$

On the other hand, we have by the property **(IFB1)** that $g_{t_j}(\mathbf{x}) \geq 0$ for all $\mathbf{x} \in \mathcal{Y}$ and $j = 0, \dots, k$. Moreover, for any $F \in \mathfrak{F}(\mathcal{C})$ and any $\mathbf{x} \in F$, it holds by the properties **(IFB3)** and **(IFB4)** that $\sum_{0 \leq j \leq k, t_j \in V(F)} g_{t_j}(\mathbf{x}) = 1$ and that $\sum_{0 \leq j \leq k, t_j \notin V(F)} g_{t_j}(\mathbf{x}) = 0$. We thus have $\sum_{j=0}^k g_{t_j}(\mathbf{x}) = 1$ for all $\mathbf{x} \in \mathcal{Y}$. Consequently, we have for all $\mathbf{x} \in \mathcal{Y}$ that

$$\mathbf{g}(\mathbf{x}) = (g_{t_1}(\mathbf{x}), \dots, g_{t_k}(\mathbf{x}))^\top \in \left\{ (z_1, \dots, z_k)^\top : z_1 \geq 0, \dots, z_k \geq 0, \sum_{j=1}^k z_j \leq 1 \right\},$$

which, by the convexity of $\{(z_1, \dots, z_k)^\top : z_1 \geq 0, \dots, z_k \geq 0, \sum_{j=1}^k z_j \leq 1\}$, implies that

$$\text{conv}(\{\mathbf{g}(\mathbf{x}) : \mathbf{x} \in \mathcal{Y}\}) \subseteq \left\{ (z_1, \dots, z_k)^\top : z_1 \geq 0, \dots, z_k \geq 0, \sum_{j=1}^k z_j \leq 1 \right\}.$$

This completes the proof. \square

Proof of Proposition 4.1.1. For $i = 1, \dots, N$, let $\mathbf{g}_i : \mathcal{X}_i \rightarrow \mathbb{R}^{m_i}$ and $\mathbf{v}_i \in \mathbb{R}^{m_i}$ be defined as follows:

$$\begin{aligned} x_i &\mapsto \mathbf{g}_i(x_i) := (g_{i,1}(x_i), \dots, g_{i,m_i}(x_i))^\top, \\ \mathbf{v}_i &:= \left(\int_{\mathcal{X}_i} g_{i,1} d\mu_i, \dots, \int_{\mathcal{X}_i} g_{i,m_i} d\mu_i \right)^\top. \end{aligned}$$

Subsequently, let $K_i \subset \mathbb{R}^{m_i}$ be defined as follows:

$$K_i := \text{conv}(\{\mathbf{g}_i(\mathbf{x}_i) : \mathbf{x}_i \in \mathcal{X}_i\}).$$

It follows from (2.12) and (2.13) that

$$\text{conv}(\{\mathbf{g}(\mathbf{x}) : \mathbf{x} \in \mathcal{X}\}) = \bigtimes_{i=1}^N K_i, \quad (5.61)$$

$$\mathbf{v} = (\mathbf{v}_1^\top, \dots, \mathbf{v}_N^\top)^\top. \quad (5.62)$$

Let us fix an arbitrary $i \in \{1, \dots, N\}$. By Lemma 5.5.1,

$$K_i = \left\{ (z_1, \dots, z_{m_i})^\top : z_1 \geq 0, \dots, z_{m_i} \geq 0, \sum_{j=1}^{m_i} z_j \leq 1 \right\}.$$

Moreover, since \mathcal{G}_i satisfies properties **(IFB3)** and **(IFB4)**, it holds for any $F \in \mathfrak{F}(\mathcal{C}_i)$ and any $\mathbf{x} \in F$ that $\sum_{0 \leq j \leq m_i, t_j \in V(F)} g_{i,t_j}(\mathbf{x}) = 1$ and $\sum_{0 \leq j \leq m_i, t_j \notin V(F)} g_{i,t_j}(\mathbf{x}) = 0$. Thus, for all $\mathbf{x}_i \in \mathcal{X}_i$, we have $\sum_{j=0}^{m_i} g_{i,j}(\mathbf{x}_i) = 1$ and hence $\sum_{j=0}^{m_i} \int_{\mathcal{X}_i} g_{i,j} d\mu_i = 1$. Since it holds by assumption that $\int_{\mathcal{X}_i} g_{i,j} d\mu_i > 0$ for $j = 0, 1, \dots, m_i$, we have $\sum_{j=1}^{m_i} \int_{\mathcal{X}_i} g_{i,j} d\mu_i = 1 - \int_{\mathcal{X}_i} g_{i,0} d\mu_i < 1$, which implies that $\mathbf{v}_i \in \text{int}(K_i)$. Consequently, by (5.61) and (5.62), $\mathbf{v} \in \text{int}(\times_{i=1}^N K_i) = \text{int}(\text{conv}(\{\mathbf{g}(\mathbf{x}) : \mathbf{x} \in \mathcal{X}\}))$. The boundedness of the set of optimizers of **(MMOT*_{relax})** then follows from Theorem 2.3.1(iv). \square

Proof of Theorem 4.1.3. Statement (i) follows from Proposition 4.1.1 and the equivalence between (i) and (iii) in [35, Corollary 9.3.1]. Due to the compactness of $\mathcal{X}_1, \dots, \mathcal{X}_N$ and the continuity of functions in $\mathcal{G}_1, \dots, \mathcal{G}_N$, the set $\{\mathbf{g}(\mathbf{x}) : \mathbf{x} \in \mathcal{X}\}$ is bounded. Moreover, the global maximization problem in Line 4 is bounded from above. Therefore, statement (ii) follows from [35, Theorem 11.2] with $g(\cdot, \cdot) \leftarrow (\mathcal{X} \times \mathbb{R}^{1+m} \ni (\mathbf{x}, (y_0, \mathbf{y})) \mapsto -(y_0 + \langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle - f(\mathbf{x})) \in \mathbb{R})$.

In order to prove statements (iii), (iv), and (v), we will show that $(\hat{y}_0, \hat{\mathbf{y}})$ is a feasible solution of **(MMOT*_{relax})** with objective value equal to $\text{MMOT}_{\text{relax}}^{\text{LB}}$ and that $\hat{\mu}$ is a feasible solution of **(MMOT_{relax})** with objective value equal to $\text{MMOT}_{\text{relax}}^{\text{UB}}$. Subsequently, since Line 5, Line 6, and Line 10 guarantee that $\text{MMOT}_{\text{relax}}^{\text{UB}} - \text{MMOT}_{\text{relax}}^{\text{LB}} = s^{(r)} \leq \epsilon$, statements (iii), (iv), and (v) will follow from the weak duality in Theorem 2.3.1(i). On the one hand, by Line 4 and Line 11, it holds for any $\mathbf{x} \in \mathcal{X}$ that

$$\begin{aligned} \hat{y}_0 + \langle \hat{\mathbf{y}}, \mathbf{g}(\mathbf{x}) \rangle - f(\mathbf{x}) &= y_0^{(r)} - s^{(r)} + \langle \mathbf{y}^{(r)}, \mathbf{g}(\mathbf{x}) \rangle - f(\mathbf{x}) \\ &= \left(y_0^{(r)} + \langle \mathbf{y}^{(r)}, \mathbf{g}(\mathbf{x}) \rangle - f(\mathbf{x}) \right) - \max_{\mathbf{x}' \in \mathcal{X}} \left\{ y_0^{(r)} + \langle \mathbf{y}^{(r)}, \mathbf{g}(\mathbf{x}') \rangle - f(\mathbf{x}') \right\} \\ &\leq 0. \end{aligned}$$

Moreover, it follows from Line 3, Line 10, and Line 11 that $\hat{y}_0 + \langle \hat{\mathbf{y}}, \mathbf{v} \rangle = y_0^{(r)} - s^{(r)} + \langle \mathbf{y}^{(r)}, \mathbf{v} \rangle = \phi^{(r)} - s^{(r)} = \text{MMOT}_{\text{relax}}^{\text{LB}}$. This shows that $(\hat{y}_0, \hat{\mathbf{y}})$ is a feasible solution of **(MMOT*_{relax})** with objective

value $\text{MMOT}_{\text{relax}}^{\text{LB}}$. On the other hand, by Line 3, $(\mu_x^{(r)})_{x \in \mathcal{X}^{\dagger(r)}}$ is an optimizer of the following LP problem, which corresponds to the dual of the LP problem in Line 3:

$$\begin{aligned} & \underset{(\mu_x)_{x \in \mathcal{X}^{\dagger(r)}}}{\text{minimize}} && \sum_{x \in \mathcal{X}^{\dagger(r)}} f(x) \mu_x \\ & \text{subject to} && \sum_{x \in \mathcal{X}^{\dagger(r)}} \mu_x = 1, \\ & && \sum_{x \in \mathcal{X}^{\dagger(r)}} g(x) \mu_x = v, \\ & && \mu_x \geq 0 \quad \forall x \in \mathcal{X}^{\dagger(r)}. \end{aligned} \tag{5.63}$$

Consequently, by Line 12, (2.12), and (2.13), $\hat{\mu}$ is a positive Borel measure with $\hat{\mu}(\mathcal{X}) = \sum_{x \in \mathcal{X}^{\dagger(r)}} \mu_x^{(r)} = 1$ and $\int_{\mathcal{X}} g_{i,j} \circ \pi_i d\hat{\mu} = \sum_{x \in \mathcal{X}^{\dagger(r)}} g_{i,j} \circ \pi_i(x) \mu_x^{(r)} = \int_{\mathcal{X}_i} g_{i,j} d\mu_i$ for $j = 1, \dots, m_i, i = 1, \dots, N$, which shows that $\hat{\mu} \in \Gamma([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})$. Moreover, since $\mathcal{X}^{\dagger(r)} \supset \mathcal{X}^{\dagger(0)}$ by Line 8, it follows from the assumption about $\mathcal{X}^{\dagger(0)}$ in Remark 4.1.2 that the LP problem in Line 3 is feasible and bounded from above. Subsequently, we have by the strong duality of LP problems that $\int_{\mathcal{X}} f d\hat{\mu} = \sum_{x \in \mathcal{X}^{\dagger(r)}} f(x) \mu_x^{(r)} = \phi^{(r)}$. Since $\text{MMOT}_{\text{relax}}^{\text{UB}} = \phi^{(r)}$ by Line 10, $\hat{\mu}$ is a feasible solution of $(\text{MMOT}_{\text{relax}}^{\text{UB}})$ with objective value $\text{MMOT}_{\text{relax}}^{\text{UB}}$. The proof is now complete. \square

5.6. Proof of results in Section 4.2.

Proof of Lemma 4.2.1. For any $x, x' \in D$, it holds by the L_f -Lipschitz continuity of f that $f(x) \leq f(x') + L_f d_{\mathcal{Y}}(x, x')$. Subsequently, taking the infimum over $x' \in D$ yields $f(x) \leq \tilde{f}(x)$. Moreover, $\tilde{f}(x) \leq f(x) + L_f d_{\mathcal{Y}}(x, x) = f(x)$, which proves that $\tilde{f}(x) = f(x)$ for all $x \in D$. To prove the L_f -Lipschitz continuity of \tilde{f} , let $x_1, x_2 \in \tilde{D}$ be arbitrary. Then, it holds for any $x' \in D$ that $\tilde{f}(x_2) \leq f(x') + L_f d_{\mathcal{Y}}(x_2, x') \leq f(x') + L_f d_{\mathcal{Y}}(x_1, x_2) + L_f d_{\mathcal{Y}}(x_1, x')$ and hence

$$\tilde{f}(x_2) - L_f d_{\mathcal{Y}}(x_1, x_2) \leq \inf_{x' \in D} \{f(x') + L_f d_{\mathcal{Y}}(x_1, x')\} = \tilde{f}(x_1).$$

Subsequently, exchanging the roles of x_1 and x_2 yields $|\tilde{f}(x_1) - \tilde{f}(x_2)| \leq L_f d_{\mathcal{Y}}(x_1, x_2)$, which shows that \tilde{f} is L_f -Lipschitz continuous. The proof is now complete. \square

Proof of Theorem 4.2.3. Statement (i) follows from the compactness of $\mathcal{X}_1, \dots, \mathcal{X}_N$ and Proposition 3.2.5 as well as the procedure for constructing a simplicial cover introduced before Proposition 3.2.5. To prove statement (ii), notice that by Lines 3–6, the condition (CPD1) in Remark 4.1.2 holds with respect to $(\mathcal{X}_i)_{i=1:N} \leftarrow (\tilde{\mathcal{X}}_i)_{i=1:N}$. Moreover, the condition (A2) implies that $\int_{\tilde{\mathcal{X}}_i} g_{i,j} d\mu_i^{\dagger} = \int_{\mathcal{X}_i} g_{i,j} d\mu_i > 0$ for $j = 0, 1, \dots, m_i, i = 1, \dots, N$, showing that the condition (CPD2) holds with respect to $(\mathcal{X}_i)_{i=1:N} \leftarrow (\tilde{\mathcal{X}}_i)_{i=1:N}, (\mu_i)_{i=1:N} \leftarrow (\mu_i^{\dagger})_{i=1:N}$. Hence, statement (ii) follows from Theorem 4.1.3(i) (with $(\mathcal{X}_i)_{i=1:N} \leftarrow (\tilde{\mathcal{X}}_i)_{i=1:N}, \mathcal{X} \leftarrow \tilde{\mathcal{X}}, f \leftarrow \tilde{f}$).

Next, let us prove statements (iii) and (iv). Since we have by Line 11 that $\text{supp}(\mu_i^{\dagger}) \subseteq \mathcal{X}_i$ for $i = 1, \dots, N$, it holds that every $\mu^{\dagger} \in \Gamma(\mu_1^{\dagger}, \dots, \mu_N^{\dagger})$ satisfies $\text{supp}(\mu^{\dagger}) \subseteq \mathcal{X}$. In particular, since $\tilde{\mu}^{\dagger} \in \Gamma(\mu_1^{\dagger}, \dots, \mu_N^{\dagger})$ and $\tilde{\mu}(E) = \tilde{\mu}^{\dagger}(E)$ for all $E \in \mathcal{B}(\mathcal{X})$ by Line 12, we have $\text{supp}(\tilde{\mu}^{\dagger}) \subseteq \mathcal{X}$ and thus $\tilde{\mu} \in \Gamma(\mu_1, \dots, \mu_N)$. Moreover, since $\tilde{f}(x) = f(x)$ for all $x \in \mathcal{X}$, we also get

$$\int_{\mathcal{X}} f d\tilde{\mu} = \int_{\tilde{\mathcal{X}}} \tilde{f} d\tilde{\mu}^{\dagger}, \tag{5.64}$$

$$\inf_{\mu^{\dagger} \in \Gamma(\mu_1^{\dagger}, \dots, \mu_N^{\dagger})} \left\{ \int_{\tilde{\mathcal{X}}} \tilde{f} d\mu^{\dagger} \right\} = \inf_{\mu \in \Gamma(\mu_1, \dots, \mu_N)} \left\{ \int_{\mathcal{X}} f d\mu \right\}. \tag{5.65}$$

Furthermore, we obtain from Theorem 4.1.3(iii) and Theorem 4.1.3(v) (with $(\mathcal{X}_i)_{i=1:N} \leftarrow (\tilde{\mathcal{X}}_i)_{i=1:N}$, $\mathcal{X} \leftarrow \tilde{\mathcal{X}}$, $f \leftarrow \tilde{f}$, $(\mu_i)_{i=1:N} \leftarrow (\mu_i^\dagger)_{i=1:N}$) that

$$\text{MMOT}_{\text{relax}}^{\text{LB}} \leq \sup_{y_0 \in \mathbb{R}, \mathbf{y} \in \mathbb{R}^m} \left\{ y_0 + \langle \mathbf{y}, \mathbf{v} \rangle : y_0 + \langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle \leq \tilde{f}(\mathbf{x}) \ \forall \mathbf{x} \in \tilde{\mathcal{X}} \right\} \leq \text{MMOT}_{\text{relax}}^{\text{UB}}, \quad (5.66)$$

$$\text{MMOT}_{\text{relax}}^{\text{UB}} - \text{MMOT}_{\text{relax}}^{\text{LB}} \leq \epsilon, \quad (5.67)$$

$$\int_{\tilde{\mathcal{X}}} \tilde{f} \, d\tilde{\mu} = \text{MMOT}_{\text{relax}}^{\text{UB}}. \quad (5.68)$$

Combining Line 13, (5.66), (5.65), and Theorem 2.3.1(i) yields

$$\begin{aligned} \text{MMOT}^{\text{LB}} &= \text{MMOT}_{\text{relax}}^{\text{LB}} \\ &\leq \sup_{y_0 \in \mathbb{R}, \mathbf{y} \in \mathbb{R}^m} \left\{ y_0 + \langle \mathbf{y}, \mathbf{v} \rangle : y_0 + \langle \mathbf{y}, \mathbf{g}(\mathbf{x}) \rangle \leq \tilde{f}(\mathbf{x}) \ \forall \mathbf{x} \in \tilde{\mathcal{X}} \right\} \\ &\leq \inf_{\mu^\dagger \in \Gamma(\mu_1^\dagger, \dots, \mu_N^\dagger)} \left\{ \int_{\tilde{\mathcal{X}}} \tilde{f} \, d\mu^\dagger \right\} \\ &= \inf_{\mu \in \Gamma(\mu_1, \dots, \mu_N)} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} \\ &\leq \int_{\mathcal{X}} f \, d\tilde{\mu} \\ &= \text{MMOT}^{\text{UB}}. \end{aligned} \quad (5.69)$$

On the other hand, combining Line 13, (5.67), (5.68), and (5.64) leads to

$$\begin{aligned} \text{MMOT}^{\text{UB}} - \text{MMOT}^{\text{LB}} &= \int_{\mathcal{X}} f \, d\tilde{\mu} - \text{MMOT}_{\text{relax}}^{\text{LB}} \\ &= \left(\int_{\mathcal{X}} f \, d\tilde{\mu} - \text{MMOT}_{\text{relax}}^{\text{UB}} \right) + (\text{MMOT}_{\text{relax}}^{\text{UB}} - \text{MMOT}_{\text{relax}}^{\text{LB}}) \\ &\leq \left(\int_{\mathcal{X}} f \, d\tilde{\mu} - \int_{\tilde{\mathcal{X}}} \tilde{f} \, d\tilde{\mu} \right) + \epsilon \\ &= \left(\int_{\tilde{\mathcal{X}}} \tilde{f} \, d\tilde{\mu}^\dagger - \int_{\tilde{\mathcal{X}}} \tilde{f} \, d\tilde{\mu} \right) + \epsilon. \end{aligned} \quad (5.70)$$

Subsequently, since $\tilde{\mu}^\dagger \in R(\hat{\mu}; \mu_1^\dagger, \dots, \mu_N^\dagger)$, it follows from Corollary 2.2.9(i) (with $(\mathcal{X}_i)_{i=1:N} \leftarrow (\tilde{\mathcal{X}}_i)_{i=1:N}$, $\mathcal{X} \leftarrow \tilde{\mathcal{X}}$, $f \leftarrow \tilde{f}$, $(\mu_i)_{i=1:N} \leftarrow (\mu_i^\dagger)_{i=1:N}$, $\tilde{\mu} \leftarrow \tilde{\mu}^\dagger$) that

$$\int_{\tilde{\mathcal{X}}} \tilde{f} \, d\tilde{\mu}^\dagger - \int_{\tilde{\mathcal{X}}} \tilde{f} \, d\tilde{\mu} \leq \sum_{i=1}^N L_f \overline{W}_{1, \mu_i^\dagger}([\mu_i^\dagger]_{\mathcal{G}_i}). \quad (5.71)$$

By Theorem 3.2.7 and Line 3, we have

$$\overline{W}_{1, \mu_i^\dagger}([\mu_i^\dagger]_{\mathcal{G}_i}) \leq 2\eta(\mathfrak{C}_i) \leq \frac{\tilde{\epsilon} - \epsilon}{NL_f} \quad \forall 1 \leq i \leq N. \quad (5.72)$$

We combine (5.70), (5.71), and (5.72) to obtain $\text{MMOT}^{\text{UB}} - \text{MMOT}^{\text{LB}} \leq \tilde{\epsilon}$. This completes the proof of statement (iii). Finally, (5.69) implies that

$$\int_{\mathcal{X}} f \, d\tilde{\mu} - \inf_{\mu \in \Gamma(\mu_1, \dots, \mu_N)} \left\{ \int_{\mathcal{X}} f \, d\mu \right\} \leq \text{MMOT}^{\text{UB}} - \text{MMOT}^{\text{LB}} = \hat{\epsilon},$$

thus proving statement (iv). \square

APPENDIX A. MIXED-INTEGER LINEAR PROGRAMMING FORMULATION OF THE GLOBAL OPTIMIZATION PROBLEM IN THE NUMERICAL EXAMPLE

In this section, we discuss how the global optimization problem in Line 4 of Algorithm 1 can be numerically solved under the setting of Section 4.3. Let us assume that $(\mathcal{X}_i)_{i=1:N}$, $(\mathcal{C}_i)_{i=1:N}$, $(\mathcal{G}_i)_{i=1:N}$ are defined as in Section 4.3. Instead of (4.1), we assume that $f : \mathcal{X} \rightarrow \mathbb{R}$ takes a more general form:

$$f(\mathbf{x}) := \left(\sum_{k=1}^{K^+} \max \{ \langle \mathbf{a}_{k,i}^+, \mathbf{x} \rangle + b_{k,i}^+ : 1 \leq i \leq I_k^+ \} \right) - \left(\sum_{k=1}^{K^-} \max \{ \langle \mathbf{a}_{k,i}^-, \mathbf{x} \rangle + b_{k,i}^- : 1 \leq i \leq I_k^- \} \right), \quad (\text{A.1})$$

where $K^+, K^- \in \mathbb{N}_0$, $\mathbf{a}_{k,i}^+ \in \mathbb{R}^N$, $b_{k,i}^+ \in \mathbb{R}$, $I_k^+ \in \mathbb{N}$ for $i = 1, \dots, I_k^+$, $k = 1, \dots, K^+$, and $\mathbf{a}_{k,i}^- \in \mathbb{R}^N$, $b_{k,i}^- \in \mathbb{R}$, $I_k^- \in \mathbb{N}$ for $i = 1, \dots, I_k^-$, $k = 1, \dots, K^-$. Notice that (A.1) represents a general continuous piece-wise affine function on a Euclidean space, and it contains (4.1) as a special case; see [46, Definition 3.1 & Lemma EC.2.2] for some properties of this class of functions. Under the setting of Section 4.3 and given $y_0 \in \mathbb{R}$, $(y_{i,j})_{j=1:m_i, i=1:N} \subset \mathbb{R}$, the global maximization problem in Line 4 is equivalent (up to the addition of a minus sign) to the following global minimization problem:

$$\begin{aligned} & \underset{(x_i)}{\text{minimize}} && f(x_1, \dots, x_N) - \left(y_0 + \sum_{i=1}^N \sum_{j=1}^{m_i} y_{i,j} g_{i,j}(x_i) \right) \\ & \text{subject to} && \underline{\kappa}_i \leq x_i \leq \bar{\kappa}_i \quad \forall 1 \leq i \leq N. \end{aligned} \quad (\text{A.2})$$

Through the introduction of auxiliary variables, (A.2) can be equivalently formulated into a mixed-integer linear programming problem. Let \mathbf{x} denote $(x_1, \dots, x_N)^\top$ and set $y_{i,0} := 0$ for $i = 1, \dots, N$. The mixed-integer linear programming formulation of (A.2) is given by:

$$\begin{aligned} & \underset{\substack{(x_i), (\lambda_k), (\zeta_k), (s_{k,i}), (\delta_{k,i}), \\ (z_{i,j}), (l_{i,j})}}{\text{minimize}} && \left(\sum_{k=1}^{K^+} \lambda_k \right) - \left(\sum_{k=1}^{K^-} \zeta_k \right) - \left(y_0 + \sum_{i=1}^N \sum_{j=1}^{m_i} (y_{i,j} - y_{i,j-1}) z_{i,j} \right) \\ & \text{subject to} && \text{for } k = 1, \dots, K^+ : \\ & && \begin{cases} \lambda_k \in \mathbb{R}, \\ \langle \mathbf{a}_{k,i}^+, \mathbf{x} \rangle + b_{k,i}^+ \leq \lambda_k \quad \forall 1 \leq i \leq I_k^+, \end{cases} \\ & && \text{for } k = 1, \dots, K^- : \\ & && \begin{cases} \zeta_k \in \mathbb{R}, s_{k,i} \in \mathbb{R}, \delta_{k,i} \in \{0, 1\} & \forall 1 \leq i \leq I_k^-, \\ \langle \mathbf{a}_{k,i}^-, \mathbf{x} \rangle + b_{k,i}^- + s_{k,i} = \zeta_k & \forall 1 \leq i \leq I_k^-, \\ 0 \leq s_{k,i} \leq M_{k,i}(1 - \delta_{k,i}) & \forall 1 \leq i \leq I_k^-, \\ \sum_{i=1}^{I_k^-} \delta_{k,i} = 1, \end{cases} \\ & && \text{for } i = 1, \dots, N : \\ & && \begin{cases} z_{i,j} \in \mathbb{R} & \forall 1 \leq j \leq m_i, \\ l_{i,j} \in \{0, 1\} & \forall 1 \leq j \leq m_i - 1, \\ z_{i,1} \leq 1, z_{i,m_i} \geq 0, \\ z_{i,j+1} \leq l_{i,j} \leq z_{i,j} & \forall 1 \leq j \leq m_i - 1, \\ \kappa_{i,0} + \sum_{j=1}^{m_i} (\kappa_{i,j} - \kappa_{i,j-1}) z_{i,j} = x_i, \end{cases} \end{aligned} \quad (\text{A.3})$$

where for $k = 1, \dots, K^-$ and $i = 1, \dots, I_k^-$, $M_{k,i}$ is a constant given by

$$M_{k,i} := \max \left\{ \langle \mathbf{a}_{k,i'}^- - \mathbf{a}_{k,i}^-, \mathbf{x} \rangle + b_{k,i'}^- - b_{k,i}^- : \mathbf{x} \in \mathcal{X}, 1 \leq i' \leq I_k^- \right\}.$$

This formulation consists of two parts. The first part lifts the epigraph of f to a higher-dimensional space involving continuous auxiliary variables and binary-valued auxiliary variables, which follows [46, Lemma EC.2.8] (with $\mathbf{a}_{k,i} \leftarrow \mathbf{a}_{k,i}^+$, $b_{k,i} \leftarrow b_{k,i}^+$, $I_k \leftarrow I_k^+$ if $\xi_k = 1$, $\mathbf{a}_{k,i} \leftarrow \mathbf{a}_{k,i}^-$, $b_{k,i} \leftarrow b_{k,i}^-$,

$I_k \leftarrow I_k^-, \delta_{k,i} \leftarrow s_{k,i}, \iota_{k,i} \leftarrow \delta_{k,i}$ if $\xi_k = -1$ in the notation of [46]). The second part of the formulation lifts the epigraph of each one-dimensional continuous piece-wise affine function $[\underline{\kappa}_i, \bar{\kappa}_i] \ni x_i \mapsto -\left(\sum_{j=1}^{m_i} y_{i,j} g_{i,j}(x_i)\right) \in \mathbb{R}$ into a higher-dimensional space involving continuous auxiliary variables and binary-valued auxiliary variables, which follows [58, Equations (11a) & (11b)] (with $x \leftarrow x_i, K \leftarrow m_i, k \leftarrow j, d_0 \leftarrow \kappa_{i,0}, d_k \leftarrow \kappa_{i,j}, \delta_k \leftarrow z_{i,j}, f(d_0) \leftarrow 0, f(d_k) \leftarrow -y_{i,j}, y_k \leftarrow \iota_{i,j}$ in the notation of [58]).

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