

Distributed Online Optimization for Multi-Agent Optimal Transport

Vishaal Krishnan^a, Sonia Martínez^b

^a*School of Engineering and Applied Sciences, Harvard University, Cambridge MA 02138 USA.*

^b*Department of Mechanical and Aerospace Engineering, University of California, San Diego, La Jolla CA 92093 USA.*

Abstract

We propose a scalable, distributed algorithm for the optimal transport of large-scale multi-agent systems. We formulate the problem as one of steering the collective towards a target probability measure while minimizing the total cost of transport, with the additional constraint of distributed implementation. Using optimal transport theory, we realize the solution as an iterative transport based on a stochastic proximal descent scheme. At each stage of the transport, the agents implement an online, distributed primal-dual algorithm to obtain local estimates of the Kantorovich potential for optimal transport from the current distribution of the collective to the target distribution. Using these estimates as their local objective functions, the agents then implement the transport by stochastic proximal descent. This two-step process is carried out recursively by the agents to converge asymptotically to the target distribution. We rigorously establish the underlying theoretical framework and convergence of the algorithm and test its behavior in numerical experiments.

Key words: Optimal transport, Stochastic optimization, Distributed online optimization, Multi-agent systems

1 Introduction

We consider the problem of designing distributed feedback control laws for optimally transporting a group of agents from an initial configuration, given by a probability measure μ_0 , to a target configuration specified by a probability measure μ^* over a domain Ω . Such a problem of transport of multi-agent collectives arises naturally in various settings, from the modeling of cell populations in biology, to engineering applications of coverage control and deployment in robotics and mobile sensing networks [9, 12, 27]. As these scenarios involve physical transport of resources, there is an associated cost of transport owing to energy considerations. Optimal transport theory [11, 35], which deals with the problem of rearranging probability measures while minimizing a cost of transport, presents an appropriate theoretical framework for the problem. Another consideration in the multi-agent setting is the scalability of implementation when the size of the collective increases, which underlines the need for distributed algorithms [9]. This need is fur-

ther exacerbated by limitations on sensing and communication typically present in these systems, whereby individual agents may only be able to sense/communicate with their spatial neighbors. However, existing formulations of the optimal transport problem result in solutions wherein the optimal transport routes for the individual agents depend on the distribution of the entire multi-agent system, which is a bottleneck for distributed implementation. The primary challenge in algorithm design, therefore, is in obtaining scalable distributed algorithms for large-scale implementation of optimal transport, which constitutes the aim of this paper.

Related work. Transport problems in robotics and mobile sensing network applications arise in the form of coverage control and deployment objectives, where the underlying goal is to steer a group of robots towards a target coverage profile over a spatial region. Among the approaches to the coverage control and deployment problem for large-scale multi-agent systems are transport by synthesis of Markov transition matrices [2, 4, 14], the use of continuum models [17, 21, 38] for transport, and coverage control by parameter tuning and/or boundary control of the reaction-advection-diffusion PDE [16, 37]. We note, however, that despite the potential for the application of optimal transport ideas to the multi-agent setting, as seen from the works [3, 20, 34, 39], a truly dis-

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Email addresses: vkrishnan@seas.harvard.edu (Vishaal Krishnan), soniamd@ucsd.edu (Sonia Martínez).

tributed formulation of optimal transport has remained open. While our preliminary work [22] was an attempt in this direction, we develop a rigorous theoretical framework for the design of distributed optimal transport algorithms in this paper. These works, however, present significant limitations either because they require centralized offline planning [20], or because of a need for costly computation and information exchange between agents [3]. This serves as a strong motivation for the development of a distributed iterative algorithm for optimal transport in this paper.

The applications of optimal transport in image processing and various engineering domains has motivated a search for efficient computational methods for the optimal transport problem [13, 25, 30]. Optimal transport from continuous to discrete probability distributions has been studied under the name of semi-discrete optimal transport, with connections to the problem of optimal quantization of probability measures, in [8]. While computational approaches to optimal transport often work with the static, Monge or Kantorovich formulations of the problem, investigations involving dynamical formulations was initiated by [5], where the authors recast the L^2 Monge-Kantorovich mass transfer problem in a fluid mechanics framework. This largely owes to notion of displacement interpolation originally introduced in [26]. [29] and [6] are other works in this vein. The problem of optimal transport was also explored from a stochastic control perspective in [1, 10, 28]. However, there has remained a gap in this literature with regard to distributed computation of optimal transport, which arises as a rather stringent constraint in multi-agent transport scenarios.

Contributions. In this work, we propose and investigate large-scale optimal transport of multi-agent collectives based on a scalable, distributed online optimization. Working with a reduction of the Kantorovich duality for metric costs conformal to the Euclidean metric, we note that the Kantorovich potential is almost everywhere differentiable and obtain a bound on the norm of its gradient. We then obtain a stochastic process for optimal iterative transport of probability measures based on Kantorovich duality, showing it to be equivalent to optimal transport along geodesics, and establish convergence of the sequence of probability measures generated by the process to the target probability measure with respect to the topology of weak convergence. We propose a distributed primal-dual algorithm to be implemented online by the agents to obtain local estimates of the Kantorovich potential, which are then used as local objectives in a proximal algorithm for transport. The paper contributes not only to the literature on computational methods for the optimal transport problem, but also presents a novel scalable, distributed approach to multi-agent optimal transport addressing a longstanding concern in the research on multi-agent systems.

Paper outline. In Section 2, we introduce the notation and mathematical preliminaries underlying the results presented in the rest of the paper. Our goal in this paper is to design an iterative transport process relying entirely on distributed computation for the optimal transport of a multi-agent system towards a target probability measure. To this end, we first design in Section 3 an iterative process for optimally transporting a probability measure onto a target measure with respect to an underlying transport cost on the spatial domain. We then obtain in Section 4 a distributed multi-agent optimal transport algorithm via a discretization of the transport process introduced in Section 3, which is then followed by an investigation of the behavior of the algorithm in numerical simulations. We then conclude with a brief summary of our results in Section 5.

2 Mathematical preliminaries

2.1 Notation

We first briefly introduce the notation adopted in the rest of the paper. We use $|\cdot|$ to denote the Euclidean norm in \mathbb{R}^d , for any $d \in \mathbb{N}$ (when $d = 1$, this denotes the absolute value). We use $\|\cdot\|$ for function space norms. The gradient operator in \mathbb{R}^d is represented as ∇ . For any $\Omega \subseteq \mathbb{R}^d$, $\partial\Omega \subseteq \mathbb{R}^d$ denotes its boundary, $\bar{\Omega} = \Omega \cup \partial\Omega$ its closure, and $\mathring{\Omega} = \Omega \setminus \partial\Omega$ its interior with respect to the standard Euclidean topology. We denote by (Ω, μ) the set Ω with an underlying measure μ . Given any $x \in \Omega \subset \mathbb{R}^d$, the set $B_r(x)$ is the closed d -ball of radius $r > 0$, centered at x . Furthermore, we denote by $B_r^c(x)$ the closed d -ball of radius r , centered at x , with respect to the metric c . We denote by $\mathcal{P}(\Omega)$ the space of probability measures over Ω . For a measurable mapping $\mathcal{T} : \Omega \rightarrow \Theta$, where Ω and Θ are measurable, we denote by $\mathcal{T}_\# \mu \in \mathcal{P}(\Theta)$ the pushforward measure of $\mu \in \mathcal{P}(\Omega)$ and we have $\mathcal{T}_\# \mu(B) = \mu(\mathcal{T}^{-1}(B))$, for all measurable $B \subseteq \Theta$. We use $\langle f, g \rangle$ to represent the inner product of functions $f, g : \Omega \rightarrow \mathbb{R}$ w.r.t. the Lebesgue measure vol , given by $\langle f, g \rangle = \int_\Omega fg \, \text{dvol}$. The set $\text{Lip}(\Omega)$ is the space of Lipschitz continuous functions on Ω . We denote by $L^p(\Omega, \mu)$ the space of p -integrable (measurable) functions on Ω , where the integration is carried out with the underlying measure μ (the Lebesgue measure is implied when μ is not specified), and by $W^{1,p}(\Omega, \mu)$ the space of p -integrable (measurable) functions with p -integrable (measurable) derivatives.

2.2 Monge and Kantorovich formulations of optimal transport

Let $\Omega \subseteq \mathbb{R}^d$ be a compact, convex domain, and let $\mu, \nu \in \mathcal{P}(\Omega)$ be absolutely continuous probability measures on Ω . Let $c : \Omega \times \Omega \rightarrow \mathbb{R}_{\geq 0}$ be a continuous function such that for $x, y \in \Omega$, $c(x, y)$ is the unit cost of transport from x to y . In the Monge (deterministic)

formulation, the optimal cost of transporting the probability measure μ onto ν is defined as the infimum of the transport cost over the set of maps for which ν is obtained as the pushforward measure of μ , as given below:

$$C_M(\mu, \nu) = \inf_{\substack{T: \Omega \rightarrow \Omega \\ T\# \mu = \nu}} \int_{\Omega} c(x, T(x)) d\mu(x). \quad (1)$$

The Kantorovich (probabilistic) formulation relaxes the Monge formulation (1) by defining the optimal cost of transporting the probability measure μ onto ν as the infimum of the transport cost over the set of joint probability measures $\Pi(\mu, \nu) \subset \mathcal{P}(\Omega \times \Omega)$, for which μ and ν are the respective marginals over Ω , as given below:

$$C_K(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int_{\Omega \times \Omega} c(x, y) d\pi(x, y). \quad (2)$$

Since Ω is a compact subset of \mathbb{R}^d and c is continuous over $\Omega \times \Omega$, it follows that the Kantorovich problem admits a solution [33]. Furthermore, the Kantorovich formulation can be shown [33] to be a relaxation of the Monge formulation, i.e. $C_M(\mu, \nu) = C_K(\mu, \nu)$, and we hereafter denote by $C(\mu, \nu) = C_M(\mu, \nu) = C_K(\mu, \nu)$. Furthermore, the Kantorovich formulation (2) admits the following dual formulation¹:

$$C(\mu, \nu) = \sup_{\phi, \psi \in L^1(\Omega)} \int_{\Omega} \phi(x) d\mu(x) + \int_{\Omega} \psi(y) d\nu(y) \quad \text{s.t.} \quad \phi(x) + \psi(y) \leq c(x, y). \quad (3)$$

The maximizers of the above dual formulation are pairs of functions (ϕ, ψ) called Kantorovich potentials. They occur at the boundary of the inequality constraint, thereby satisfying:

$$\begin{aligned} \phi(x) &= \inf_{y \in \Omega} (c(x, y) - \psi(y)), \\ \psi(y) &= \inf_{z \in \Omega} (c(z, y) - \phi(z)). \end{aligned} \quad (4)$$

We refer to (ϕ, ψ) defined above as a c -conjugate pair, and write $\psi = \phi^c$ to denote that ψ is the conjugate of ϕ .

3 Optimal iterative transport of measures

We first briefly describe the setting for the multi-agent optimal transport problem addressed in this paper. We consider a compact and convex domain $\Omega \subset \mathbb{R}^d$ across which N agents are initially independently and identically distributed according to an absolutely continuous probability measure $\mu_0 \in \mathcal{P}(\Omega)$, i.e., the initial agent positions $\{x_1(0), \dots, x_N(0)\}$ are independently generated

¹ Strong duality holds for the Kantorovich formulation (c.f. Theorem 5.10 in [35]).

as $x_i(0) \sim \mu_0$ for any $i \in \{1, \dots, N\}$. Our goal in this paper is to design an iterative transport process to steer the agents towards an absolutely continuous target probability measure $\mu^* \in \mathcal{P}(\Omega)$, while minimizing the net cost of transport measured with respect to an underlying metric c on Ω . In particular, we restrict the transport cost c to the class of distance functions induced by a Riemannian metric conformal to the Euclidean one, as stated in the following assumption:

Assumption 1 (Conformal distance) *Let $c : \Omega \times \Omega \rightarrow \mathbb{R}_{\geq 0}$ be a distance function on Ω conformal to the Euclidean distance (with a strictly positive conformal factor $\xi \in C^1(\Omega)$), i.e., for any $x, y \in \Omega$, $c(x, y)$ is given by:*

$$c(x, y) = \inf_{\substack{\gamma \in C^1([0, 1]; \Omega); \\ \gamma(0) = x, \gamma(1) = y}} \int_0^1 \xi(\gamma(t)) |\dot{\gamma}(t)| dt. \quad (5)$$

The restriction to a conformal metric affords us the flexibility to penalize transport through certain regions of the domain relative to other regions via the conformal factor, therefore allowing for the possibility of modeling physical obstacles and uneven terrain in real environments with relative ease. The following lemma² establishes a reduction of the Kantorovich duality (3) for conformal metric costs:

Lemma 1 (Local Lipschitz bound) *Let $c : \Omega \times \Omega \rightarrow \mathbb{R}_{\geq 0}$ be a metric on Ω conformal to the Euclidean distance, with a strictly positive conformal factor $\xi \in C^1(\Omega)$. (a) The conjugate of the Kantorovich potential in (4) satisfies $\phi^c = -\phi$ and $|\phi(x) - \phi(y)| \leq c(x, y)$ for all $x, y \in \Omega$. (b) Furthermore, the Kantorovich potential is differentiable almost everywhere in Ω , with $|\nabla \phi| \leq \xi$ a.e.*

Proof sketch. We provide a sketch of the proof here. (a) employs similar arguments as in the proof of the Kantorovich duality [35]. The fact that the c -conjugate ϕ^c of ϕ satisfies $\phi^c = -\phi$ and the Lipschitz property of ϕ follows from a combination of (4) and the triangle inequality property of c . (b) The almost everywhere differentiability of ϕ is a consequence of Rademacher's theorem owing to the Lipschitz property of ϕ . The bound on the gradient of ϕ follows from taking the limit on the Lipschitz bound on ϕ along geodesics of Ω equipped with the metric c ; see [23] for further details. •

It follows from Lemma 1 that for absolutely continuous probability measures $\mu, \mu^* \in \mathcal{P}(\Omega)$, the optimal transport cost for the transport of μ onto μ^* can be written

² We refer the reader to the extended version [23] for the detailed proofs of the results in the paper.

as:

$$C(\mu, \mu^*) = \sup_{\phi \in W^{1,\infty}(\Omega, \mu)} \int_{\Omega} \phi \left(1 - \frac{d\mu^*}{d\mu}\right) d\mu, \quad \text{s.t. } |\nabla \phi| \leq \xi, \quad \mu - \text{a.e. in } \Omega, \quad (6)$$

where $d\mu^*/d\mu$ is the Radon-Nikodym derivative. With $G_{\phi}(x) = [|\nabla \phi(x)|^2 - \xi(x)^2]/2$, we can rewrite the constraint in Problem (6) as $G_{\phi} \leq 0$, μ -a.e. in Ω . Furthermore, we have $G_{\phi} \geq -\xi^2/2$ for any $\phi \in W^{1,\infty}(\Omega, \mu)$. Therefore, it follows that $G_{\phi} \in L^{\infty}(\Omega, \mu)$, and the Lagrange multiplier corresponding to the constraint $G_{\phi} \leq 0$ then belongs to $L^{\infty}(\Omega, \mu)^*$, the dual space of $L^{\infty}(\Omega, \mu)$. Since $L^{\infty}(\Omega, \mu)^*$ is isomorphic [15] to $\text{ba}(\Omega, \mu)$ ³, we get that $\lambda(G_{\phi}) = \frac{1}{2} \int_{\Omega} (|\nabla \phi|^2 - |\xi|^2) \rho d\lambda$. The Lagrangian functional $L : W^{1,\infty}(\Omega, \mu) \times L^{\infty}(\Omega, \mu)_{\geq 0}^* \rightarrow \mathbb{R}$ can now be defined as follows:

$$L(\phi, \lambda) = - \int_{\Omega} \phi \left(1 - \frac{d\mu^*}{d\mu}\right) d\mu + \lambda(G_{\phi}).$$

The following theorem establishes the existence of a (global) maximizer for Problem (6), also called a Kantorovich potential, and characterizes the saddle points of the Lagrangian L :

Theorem 1 (First-order optimality conditions) *Let $\mu, \mu^* \in \mathcal{P}(\Omega)$ be absolutely continuous probability measures with densities $\rho, \rho^* \in L^1(\Omega)$. Problem (6) has a global maximizer $\phi_{\mu \rightarrow \mu^*} \in W^{1,\infty}(\Omega, \mu)$. The Lagrangian L has a saddle point $(\phi_{\mu \rightarrow \mu^*}, \lambda_{\mu \rightarrow \mu^*}) \in W^{1,\infty}(\Omega, \mu) \times L^1(\Omega, \mu)_{\geq 0}$. Moreover, $(\phi_{\mu \rightarrow \mu^*}, \lambda_{\mu \rightarrow \mu^*})$ satisfies the first-order optimality conditions:*

(1) *Stationarity: The saddle point $(\phi_{\mu \rightarrow \mu^*}, \lambda_{\mu \rightarrow \mu^*})$ weakly satisfies the Poisson equation,*

$$-\frac{1}{\rho} \nabla \cdot (\rho \lambda_{\mu \rightarrow \mu^*} \nabla \phi_{\mu \rightarrow \mu^*}) = 1 - \frac{\rho^*}{\rho}, \quad \mu - \text{a.e. in } \Omega, \\ \rho \lambda_{\mu \rightarrow \mu^*} \nabla \phi_{\mu \rightarrow \mu^*} \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega,$$

where \mathbf{n} is the outward normal to the boundary $\partial\Omega$.

(2) *Feasibility: $\lambda_{\mu \rightarrow \mu^*} \geq 0$ and $|\nabla \phi_{\mu \rightarrow \mu^*}| \leq \xi$, μ -a.e. in Ω .*

(3) *Complementary slackness: $\lambda_{\mu \rightarrow \mu^*} (|\nabla \phi_{\mu \rightarrow \mu^*}| - \xi) = 0$, μ -a.e. in Ω .*

Proof sketch. The proof follows along the following steps.

(i) *Existence of Kantorovich potential ϕ :* First, the Kan-

³ The space of bounded finitely additive measures on Ω that are absolutely continuous w.r.t. μ .

torovich duality (6) can be rewritten the as

$$C(\mu, \mu^*) = - \inf_{\phi \in W^{1,\infty}(\Omega, \mu)} \underbrace{\mathbb{E}_{\mu^*}[\phi]}_{\triangleq L_{\mu^*}(\phi)}, \quad \text{s.t. } \begin{cases} \mathbb{E}_{\mu}[\phi] = 0, \\ |\nabla \phi| \leq \xi, \quad \mu - \text{a.e.} \end{cases}$$

by exploiting the fact that the optimization is invariant under vertical shifts. Second, the set $\mathcal{L}(\Omega, \mu) = \{\phi \in W^{1,\infty}(\Omega, \mu) \mid \mathbb{E}_{\mu}[\phi] = 0, \quad |\nabla \phi| \leq \xi, \quad \mu - \text{a.e.}\}$ is closed, convex and bounded. Since the objective functional L_{μ^*} is convex and lower semicontinuous, a minimizing sequence $\{\phi_n\}_{n \in \mathbb{N}}$ in $\mathcal{L}(\Omega, \mu)$ for L_{μ^*} , such that $\phi_n \in \mathcal{L}(\Omega, \mu)$ and $\lim_{n \rightarrow \infty} L_{\mu^*}(\phi_n) = \inf_{\phi \in \mathcal{L}(\Omega, \mu)} L_{\mu^*}(\phi)$ can be shown to be uniformly bounded and uniformly equicontinuous. Therefore, by the Arzelà-Ascoli Theorem [32], there exists a uniformly convergent subsequence $\{\phi_{n_j}\}_{j \in \mathbb{N}}$, with the limit $\phi^* \in \mathcal{L}(\Omega, \mu)$. By the continuity and convexity of L_{μ^*} , we get that ϕ^* is a global minimizer of L_{μ^*} .

(ii) *Saddle points of Lagrangian functional L :* It is possible to apply Theorem 3.6 in [7] to infer that the set of Lagrange multipliers corresponding to the minimizer $\bar{\phi}$ is a non-empty, convex, bounded and weakly- $*$ compact subset of $L^{\infty}(\Omega)_{\geq 0}^*$, and the set of Lagrange multipliers is the same for any minimizer $\bar{\phi}$. Moreover, we note that $(-\infty, 0]$ is a closed convex cone, and it follows from Theorem 3.4-(iii) in [7] that for any Lagrange multiplier $\bar{\lambda}$, the pair $(\bar{\phi}, \bar{\lambda})$ is a saddle point of the Lagrangian functional L .

For $\phi \in W^{1,\infty}(\Omega)$ and a variation $\eta \in W^{1,\infty}(\Omega)$, the directional derivative of L_{λ} at ϕ along η is given by:

$$L'_{\lambda}(\phi, \eta) = \lim_{\epsilon \rightarrow 0^+} \frac{1}{\epsilon} \int_{\Omega} \epsilon \eta (-\rho + \rho^*) d\text{vol} \\ + \frac{1}{2\epsilon} \int_{\Omega} (\epsilon^2 |\nabla \eta|^2 + 2\epsilon \nabla \phi \cdot \nabla \eta) d\lambda \\ = - \int_{\Omega} \eta (\rho - \rho^*) d\text{vol} + \int_{\Omega} \nabla \phi \cdot \nabla \eta d\lambda.$$

By the Minimax theorem and since $(\bar{\phi}, \bar{\lambda})$ is a saddle point for the Lagrangian L , for any feasible $\tilde{\phi}$ and $\lambda \geq 0$, we must have $\int_{\Omega} (|\nabla \tilde{\phi}|^2 - |\xi|^2) d\bar{\lambda} \leq 0$, from which it follows that $|\nabla \tilde{\phi}|^2 \leq |\xi|^2$ a.e. in Ω as $\bar{\lambda} \in \text{ba}(\Omega)_{\geq 0}$. We also have:

$$L(\bar{\phi}, 0) = - \int_{\Omega} \bar{\phi} (\rho - \rho^*) d\text{vol} \leq L(\bar{\phi}, \bar{\lambda}) = \min_{\phi} L(\phi, \bar{\lambda}) \\ \leq L(\bar{\phi}, \bar{\lambda}) = - \int_{\Omega} \bar{\phi} (\rho - \rho^*) d\text{vol} + \int_{\Omega} (|\nabla \bar{\phi}|^2 - |\xi|^2) d\bar{\lambda} \\ \leq - \int_{\Omega} \bar{\phi} (\rho - \rho^*) d\text{vol},$$

where the first inequality is due to the saddle point definition, the second equality follows from the Minimax theorem, the last inequality from the fact that $\bar{\phi}$ is a feasible solution. All inequalities are indeed equalities, and we therefore see that *complementary slackness* holds in the form $\int_{\Omega} (|\nabla \bar{\phi}|^2 - |\xi|^2) d\bar{\lambda} = 0$.

Since the pair $(\bar{\phi}, \bar{\lambda})$ is a saddle point of L , it is also a stationary point of L and we have $L'_{\bar{\lambda}}(\bar{\phi}, \eta) = 0$ for any $\eta \in W^{1,\infty}(\Omega)$, and we get the *stationarity* condition $\int_{\Omega} \eta(\rho - \rho^*) d\text{vol} = \int_{\Omega} \nabla \bar{\phi} \cdot \nabla \eta d\bar{\lambda}$.

(iii) *Improved regularity of Lagrange multipliers*: Finally a stronger regularity for the Lagrange multipliers $\bar{\lambda}$ can be established and thus of the saddle point $(\bar{\phi}, \bar{\lambda})$.

Under stronger regularity of the saddle point $(\bar{\phi}, \bar{\lambda})$, the stationarity condition can be expressed as:

$$\begin{aligned} \int_{\Omega} (\rho - \rho^*) \eta d\text{vol} &= \int_{\Omega} \bar{\lambda} \nabla \bar{\phi} \cdot \nabla \eta d\text{vol} \\ &= - \int_{\Omega} \nabla \cdot (\bar{\lambda} \nabla \bar{\phi}) \eta d\text{vol} + \int_{\partial\Omega} \bar{\lambda} \nabla \bar{\phi} \cdot \mathbf{n} \eta dS \end{aligned}$$

where we have used the divergence theorem to obtain the final equality, with S as the surface measure on $\partial\Omega$. As the above holds for any variation $\eta \in W^{1,\infty}(\Omega)$, it must follow that $-\nabla \cdot (\bar{\lambda} \nabla \bar{\phi}) = \rho - \rho^*$ in Ω and $\bar{\lambda} \nabla \bar{\phi} \cdot \mathbf{n} = 0$ on $\partial\Omega$, and if we do not suppose stronger regularity of the saddle point $(\bar{\phi}, \bar{\lambda})$, the equations must be hold weakly. Therefore, the saddle point $(\bar{\phi}, \bar{\lambda})$ weakly satisfies $-\nabla \cdot (\bar{\lambda} \nabla \bar{\phi}) = \rho - \rho^*$ in Ω and $\bar{\lambda} \nabla \bar{\phi} \cdot \mathbf{n} = 0$ on $\partial\Omega$.

The above correspond to the necessary KKT conditions. Conversely, any solution pair $(\bar{\phi}, \bar{\lambda})$ which satisfies the above KKT conditions results in a saddle point for the Lagrangian and it is a solution to the original optimization problem.

Having characterized the Kantorovich potential via the saddle points of the Lagrangian L , in what follows we devise a stochastic process to achieve iterative optimal transport to the target measure μ^* . We obtain a formulation of optimal transport of probability measures in which the net transport of a given initial probability measure μ_0 onto a target probability measure μ^* is carried out by a stochastic process. However, we first require the following lemma which establishes that the optimal transport can be decomposed into multiple stages:

Lemma 2 (Decomposition of optimal transport cost) *Given atomless probability measures $\mu, \mu^* \in \mathcal{P}(\Omega)$, the cost of optimal transport from μ to μ^* satisfies:*

$$C(\mu, \mu^*) = \min_{\nu \in \mathcal{P}(\Omega)} C(\mu, \nu) + C(\nu, \mu^*).$$

Proof sketch. Lemma 2 is a consequence of the metric property of C , which can be established using the triangle inequality for c along minimum-length geodesics within the Monge formulation (1). •

We note that Lemma 2 allows for the decomposition of optimal transport into an iterative process. By exploiting this decomposition, we will be able to integrate “small transport steps” with distributed multi-agent computations that approximate the Kantorovich potential of optimal transport, as explained in the following section. Thus, as a first step, we evaluate decompositions for which the individual stage costs are upper bounded by an $\epsilon > 0$, as established by the following theorem:

Theorem 2 (Stochastic process for optimal iterative transport) *Let $\epsilon > 0$ and let $\{X(k)\}_{k \in \mathbb{N}}$ be a stochastic process with absolutely continuous marginals $\mu_k \in \mathcal{P}(\Omega)$ (i.e., $X(k) \sim \mu_k$ for every $k \in \mathbb{N}$) such that for (measurable) $B \subseteq \Omega$ the following holds*

$$\mathbb{P}[X(k+1) \in B \mid X(k) = x] = \frac{\ell(B \cap \mathcal{M}_{\mu_k}^{\epsilon}(x))}{\ell(\mathcal{M}_{\mu_k}^{\epsilon}(x))} \quad (7)$$

with the set $\mathcal{M}_{\mu}^{\epsilon}(x) = \arg \min_{z \in B_{\epsilon}^c(x)} c(x, z) + \phi_{\mu \rightarrow \mu^*}(z)$, where ℓ denotes the arclength (or induced Lebesgue) measure. Then, the sequence $\{\mu_k\}_{k \in \mathbb{N}}$ satisfies

$$\begin{aligned} \mu_{k+1} \in \arg \min_{\nu \in \mathcal{P}(\Omega)} \{C(\mu_k, \nu) + C(\nu, \mu^*), \\ \text{s.t. } C(\mu_k, \nu) \leq \epsilon\}, \end{aligned} \quad (8)$$

and $C(\mu_k, \mu^*) \rightarrow 0$, as $k \rightarrow \infty$.

Proof sketch. (a) To see that process (7) achieves (8), we recall from (4) and Lemma 1 that for the transport $\mu_k \rightarrow \mu^*$, and for any $x \in \Omega$, we have:

$$\phi_{\mu_k \rightarrow \mu^*}(x) = \inf_{y \in \Omega} c(x, y) + \phi_{\mu_k \rightarrow \mu^*}(y). \quad (9)$$

Using the fact that $\phi_{\mu_k \rightarrow \mu^*}(x) \leq c(x, y) + \phi_{\mu_k \rightarrow \mu^*}(y)$ and $c(x, y) = c(x, z) + c(z, y)$ for any (and only) z on a minimum-length geodesic from x to y , substituting for any z on the minimum-length geodesic in (12), we can infer that every point on a length-minimizing geodesic is also a minimizer. The set of minimizers $\mathcal{M}_{\mu_k}^{\epsilon}(x)$ in (7) therefore correspond to the segments of the length-minimizing geodesics (from the current iterate to the minimizers of (12)) contained in the ϵ -ball B_{ϵ}^c centered at the current iterate. We then use Theorem 5.10 in [35] to infer that the optimal transport plans $\pi_k \in \mathcal{P}(\Omega \times \Omega)$ (with μ_k and μ^* as the marginals) are supported in the set:

$$\Gamma = \{(x, y) \in \Omega \times \Omega \mid \phi_{\mu_k \rightarrow \mu^*}(x) - \phi_{\mu_k \rightarrow \mu^*}(y) = c(x, y)\}.$$

With $\Gamma_x = \{y \in \Omega \mid (x, y) \in \Gamma\}$ and $\Gamma_x^{\epsilon} = \Gamma_x \cap B_{\epsilon}^c(x)$ for all $x \in \Omega$, we see that Γ_x^{ϵ} is the set of minimizers

$\mathcal{M}_{\mu_k}^\epsilon(x)$ in (7). Now, for any transport map \tilde{T}_k from μ_k to μ^* , we get $\phi_{\mu_k \rightarrow \mu^*}(x) \leq c(x, \tilde{T}_k(x)) + \phi_{\mu_k \rightarrow \mu^*}(\tilde{T}_k(x))$. It then follows that:

$$\begin{aligned} & \int_{\Omega} \left(\phi_{\mu_k \rightarrow \mu^*}(x) - \phi_{\mu_k \rightarrow \mu^*}(\tilde{T}_k(x)) \right) d\mu_k(x) \\ &= \int_{\Omega} \phi_{\mu_k \rightarrow \mu^*} d\mu_k - \int_{\Omega} \phi_{\mu_k \rightarrow \mu^*} d\mu^* \\ &\leq \int_{\Omega} c(x, \tilde{T}_k(x)) d\mu_k(x). \end{aligned}$$

We see that the LHS is the optimal transport cost obtained from the Kantorovich dual formulation, while an infimum over the RHS w.r.t. \tilde{T}_k would again yield the optimal transport cost from the Monge formulation and an equality would then be attained. Using the fact that the Monge problem attains a minimum, the above correspondence between the Monge problem and the process (7), and from the proof of Lemma 2, it follows that the optimal transport cost $C(\mu_k, \mu^*)$ can be decomposed as in (8) by the process (7).

(b) Furthermore, to see that process (7) achieves convergence $C(\mu_k, \mu^*) \rightarrow 0$, we first note that every x^+ , where x^+ be a sample drawn uniformly at random from the set of minimizers $\arg \min_{z \in B_\epsilon^c(x)} c(x, z) + \phi_{\mu \rightarrow \mu^*}(z)$, satisfies $c(x^+, T_{\mu \rightarrow \mu^*}(x)) \leq c(x, T_{\mu \rightarrow \mu^*}(x))$. Since this holds for any sample x of X , we get that the random variable X^+ obtained from the single update of X , with $X^+ \sim \mu^+$, is such that $C(\mu^+, \mu^*) \leq C(\mu, \mu^*)$. Therefore, the sequence of measures $\{\mu_k\}_{k \in \mathbb{N}}$ corresponding to the process $\{X_k\}_{k \in \mathbb{N}}$ satisfies $C(\mu_{k+1}, \mu^*) \leq C(\mu_k, \mu^*)$ for all $k \in \mathbb{N}$, and applying the monotone convergence theorem, we get that $C(\mu_k, \mu^*) \rightarrow C$. By Prokhorov's Theorem [35], from which we get that $\mathcal{P}(\Omega)$ is compact w.r.t. the topology of weak convergence, and the fact that μ_k lies on the (unique) geodesic between μ_0 and μ^* , it follows that there exists an accumulation point $\bar{\mu}$ on the geodesic between μ_0 and μ^* such that $\mu_k \rightarrow \bar{\mu}$. This implies that $C(\bar{\mu}, \bar{\mu}^+) = 0$, where $\bar{\mu}^+ \in \mathcal{P}(\Omega)$ is obtained from a one step update of $\bar{X} \sim \bar{\mu}$. Furthermore, from Section (a) of the proof, it follows that the process (7) results in optimal transport from $\bar{\mu}$ to $\bar{\mu}^+$. We can then establish that μ^* is the only accumulation point and the sequence $\{\mu_k\}_{k \in \mathbb{N}}$ converges to μ^* as $k \rightarrow \infty$ w.r.t. the topology of weak convergence in $\mathcal{P}(\Omega)$, i.e., $C(\mu_k, \mu^*) \rightarrow 0$. To see this, we consider

$$\begin{aligned} \eta &= C(\bar{\mu}, \mu^*) = \int_{\Omega} c(x, T_{\bar{\mu} \rightarrow \mu^*}(x)) d\bar{\mu}(x) \\ &= \int_{\Omega} \min_{z \in B_\epsilon^c(x)} [c(x, z) + c(z, T_{\mu \rightarrow \mu^*}(x))] d\bar{\mu}(x) \\ &= \int_{\Omega} \frac{1}{\ell(\mathcal{M}_{\bar{\mu}}^\epsilon(x))} \int_{z \in \mathcal{M}_{\bar{\mu}}^\epsilon(x)} [c(x, z) \\ &\quad + c(z, T_{\mu \rightarrow \mu^*}(x))] d\ell(z) d\bar{\mu}(x) \\ &= C(\bar{\mu}, \bar{\mu}^+) \end{aligned}$$

$$+ \int_{\Omega} \frac{1}{\ell(\mathcal{M}_{\bar{\mu}}^\epsilon(x))} \int_{z \in \mathcal{M}_{\bar{\mu}}^\epsilon(x)} c(z, T_{\mu \rightarrow \mu^*}(x)) d\ell(z) d\bar{\mu}(x)$$

From $C(\bar{\mu}, \bar{\mu}^+) = 0$ (since $\bar{\mu}$ is an accumulation point), we get

$$\int_{\Omega} \frac{1}{\ell(\mathcal{M}_{\bar{\mu}}^\epsilon(x))} \int_{z \in \mathcal{M}_{\bar{\mu}}^\epsilon(x)} c(z, T_{\mu \rightarrow \mu^*}(x)) d\ell(z) d\bar{\mu}(x) = \eta$$

which implies that $\bar{\mu}$ -a.e. in Ω

$$c(x, T_{\bar{\mu} \rightarrow \mu^*}(x)) = \frac{1}{\ell(\mathcal{M}_{\bar{\mu}}^\epsilon(x))} \int_{z \in \mathcal{M}_{\bar{\mu}}^\epsilon(x)} c(z, T_{\mu \rightarrow \mu^*}(x)) d\ell(z).$$

Since for $z \in \mathcal{M}_{\bar{\mu}}^\epsilon(x)$ we have $c(z, T_{\mu \rightarrow \mu^*}(x)) \leq c(x, T_{\mu \rightarrow \mu^*}(x))$, it follows that $\mathcal{M}_{\bar{\mu}}^\epsilon(x) = \{x\}$, $\bar{\mu}$ -a.e. in Ω , which is the case if and only if $T_{\bar{\mu} \rightarrow \mu^*}(x) = x$, i.e., $C(\bar{\mu}, \mu^*) = 0$, and we get a contradiction.

Some comments on Theorem 2 are in order. We note that for a given $\mu \in \mathcal{P}(\Omega)$, at any $x \in \Omega$, the set of minimizers $\mathcal{M}_\mu^\epsilon(x)$ is the segment of the geodesic from x to its image $T_{\mu \rightarrow \mu^*}(x)$ (the optimal transport map from μ to μ^*) that lies within the ϵ -ball centered at x . The update of the stochastic process involves uniformly sampling from this set. By limiting the update to distributions that are close in the sense of optimal transport, we achieve various objectives: first, we can account for the physical limitations of robots arising from the multi-agent setting wherein the agents cannot take arbitrarily large steps. Second, we can integrate such short displacement steps with distributed computations, as explained in the next section. Third, we also note that the resulting iterative process opens the door for feedback-based implementations, applicable to Model Predictive Control and tracking time-varying μ^* .

4 Multi-agent implementation

4.1 Multi-agent optimal transport algorithm

We now obtain an implementable algorithm for multi-agent transport by the stochastic process (7), via a discretization of the Kantorovich potential. At the culmination of the previous section, it becomes evident that while the process (7) achieves optimal iterative transport of absolutely continuous measures, multi-agent systems are intrinsically represented by discrete measures, whereby we are faced with the problem of obtaining an appropriate discretization and an implementable algorithm for the transport process. To this end, we first discretize Problem (6) onto a Voronoi partition generated by the positions of the agents and devising a primal-dual algorithm to solve the discretized problem. We then note that the primal-dual algorithm for the

multi-agent system is Laplacian-based, thereby being intrinsically distributed in nature, i.e., requiring communication only between immediate neighbors on the Delaunay graph corresponding to the Voronoi partition. This crucial fact enables scalable large-scale implementation of multi-agent optimal transport. In what follows, we first develop the underlying structure for a discretization of Problem (6), followed by the distributed primal-dual algorithm.

Let $\{x_i(0)\}_{i=1}^N$ be the positions of the N agents, distributed independently and identically according to a probability measure μ_0 . The idea is to transport the agents by the iterative process (7) to obtain $\{x_i(k)\}_{i=1}^N$ at any time k . Let $\hat{\mu}_N(k) = \frac{1}{N} \sum_{i=1}^N \delta_{x_i(k)}$ be the empirical measure generated by the agents $\{x_i(k)\}_{i=1}^N$ at time k . To this end, we formulate a (finite) N -dimensional distributed optimization to be implemented by the agents to obtain local estimates of the Kantorovich potential. We approximate the true Kantorovich potential by a $\Phi^d : \mathbb{N} \times \Omega \rightarrow \mathbb{R}$ generated by an (finite) N -dimensional vector $\phi(k) = (\phi^1(k), \dots, \phi^N(k)) \in \mathbb{R}^N$, such that $\Phi^d(k, x_i(k)) = \phi^i(k)$ for $i \in \{1, \dots, N\}$ and $\Phi^d(k, x)$ for $x \in \Omega \setminus \{x_1(k), \dots, x_N(k)\}$ is defined by a suitable multivariate interpolation. In particular, let $\{\mathcal{V}_i(k)\}_{i=1}^N$ be the Voronoi partition of Ω generated by $\{x_1(k), \dots, x_N(k)\}$ w.r.t. the metric c , and $\Phi^d = \sum_{i=1}^N \phi^{\mathcal{V}_i(k)}$ (decomposed into a sum of N functions $\phi^{\mathcal{V}_i(k)}$ with supports $\mathcal{V}_i(k)$). We assume that at time k , the agents i, j corresponding to neighboring cells $\mathcal{V}_i(k)$ and $\mathcal{V}_j(k)$ are connected by an edge, which defines a connected graph $G(k) = (\{x_i(k)\}_{i=1}^N, E(k))$ (where $E(k)$ is the edge set of the graph $G(k)$ at time k).

Dropping the index k (as is clear from context), the finite dimensional approximation of the Kantorovich duality (6) for the transport between $\hat{\mu}_N$ and μ^* , restricted to the graph G , is given by:

$$\begin{aligned} \max_{(\phi^1, \dots, \phi^N)} \quad & \sum_{i=1}^N \left(\frac{1}{N} \cdot \phi^i - \mathbb{E}_{\mu^*}[\phi^{\mathcal{V}_i}] \right) \\ \text{s.t.} \quad & |\phi^i - \phi^j| \leq c(x_i, x_j), \quad \forall (i, j) \in E. \end{aligned} \quad (10)$$

We call (10) a restriction of (6) to the graph G because we only impose the constraint $|\phi^i - \phi^j| \leq c(x_i, x_j)$ on neighbors i, j on the graph.

We note that Theorem 2 guarantees convergence of the algorithm solving (10) exactly at each stage k in the limit $N \rightarrow \infty$, when the closure of these samples are equal to the support of μ_k . When N is finite, there always will be an approximation error, which is expected to lead to an approximate convergence. This is what it is verified in the simulations later.

We solve the optimization problem (10) by a primal-dual

algorithm, and its solution is used to update the agent positions by (7). We take Φ^d here to be a simple function, such that $\phi^{\mathcal{V}_i}(x) = \phi^i$ for $x \in \mathcal{V}_i$. The Lagrangian for the problem (10), with Φ^d a simple function and $c(x_i, x_j) = c_{ij}$, is given by:

$$\begin{aligned} L_d = & - \sum_{i=1}^N \phi^i \left[\frac{1}{N} - \mu^*(\mathcal{V}_i) \right] \\ & + \frac{1}{2} \sum_{i=1}^N \sum_{j \in \mathcal{N}_i} \lambda_{ij} \left[|\phi^i - \phi^j|^2 - c_{ij}^2 \right], \end{aligned}$$

and the primal-dual algorithm (with step size τ) is given by (for $i \in \{1, \dots, N\}$ and $j \in \mathcal{N}_i$):

$$\begin{aligned} \phi^i(l+1) &= \phi^i(l) - \tau \sum_{j \in \mathcal{N}_i} \lambda_{ij}(l) (\phi^i(l) - \phi^j(l)) \\ & \quad + \left(\frac{1}{N} - \mu^*(\mathcal{V}_i) \right), \\ \lambda_{ij}(l+1) &= \max \left\{ 0, \lambda_{ij}(l) + \tau \left[\frac{1}{2} |\phi^i(l) - \phi^j(l)|^2 - c_{ij}^2 \right] \right\}. \end{aligned} \quad (11)$$

The term $\sum_{j \in \mathcal{N}_i} \lambda_{ij}(l) (\phi^i(l) - \phi^j(l))$ in (11) is the action of the weighted Laplacian matrix (with weights $\lambda_{ij}(l)$) on $\phi(l)$. We note from the structure of the above algorithm that it renders itself to a distributed implementation by the agents, where agent i uses information from its neighbors $j \in \mathcal{N}_i$ to update ϕ^i and $\{\lambda_{ij}\}_{j \in \mathcal{N}_i}$.

At the end of every step $x_i(k) \mapsto x_i(k+1)$ from (7), the agent i assigns $\phi^i \leftarrow \Phi_k^d(x_i(k+1))$ as the initial condition for the primal algorithm (11) at the time step $k+1$ of the transport. Moreover, we are interested in an online implementation of the transport, in that the agents do not wait for convergence of the distributed primal-dual algorithm but carry out n iterations of it for every update step (7), as outlined formally in the algorithm below.

Remark 1 (Optimize-then-discretize vs discretize-then-optimize) It can be seen that the key ingredient of the multi-agent optimal transport Algorithm 1 is the distributed computation by the agents of the (discretized) Kantorovich potential which is the maximizer in (6). This can be achieved either via a discretization of the PDE characterizing the first-order optimality condition for the Kantorovich potential, namely the optimize-then-discretize approach, or by first discretizing the infinite-dimensional optimization problem (6) over a partition (e.g., Voronoi) of the domain and then solving the finite-dimensional optimization problem resulting from the discretization to directly obtain the discretized Kantorovich potential, the latter being the discretize-then-optimize approach. In this paper we have first laid the theoretical framework for the infinite-dimensional

Algorithm 1 Primal-dual based multi-agent optimal transport

Input: Target measure μ^* , Transport cost $c(x, y)$, Bound on step size ϵ , Time step τ

For each agent i at time instant k of transport:

- 1: Obtain: Positions $x_j(k)$ of neighbors within communication/sensing radius r ($r \leq \text{diam}(\Omega)$, large enough to cover Voronoi neighbors)
 - 2: Compute: Voronoi cell $\mathcal{V}_i(k)$, Mass of cell $\mu^*(\mathcal{V}_i(k))$, Voronoi neighbors $\mathcal{N}_i(k)$
 - 3: Initialize: $\phi^i \leftarrow \Phi_{k-1}^d(x_i(k))$, $\lambda_{ij} \leftarrow \lambda_{ij}(k-1)$ (with $\Phi_0^d = 0$, $\lambda_{ij}(0) = 0$)
 - 4: Implement n iterations of primal-dual algorithm (11) (synchronously, in communication with neighbors $j \in \mathcal{N}_i(k)$ to obtain $\phi^j(k)$, $\lambda_{ij}(k)$)
 - 5: Communicate with neighbors $j \in \mathcal{N}_i(k)$ to obtain $\phi^j(k)$, construct local estimate of Φ_k^d by multivariate interpolation
 - 6: Implement transport step (7) with local estimate of Φ_k^d (which approximates $\phi_{\mu_k \rightarrow \mu^*}$)
-

Kantorovich problem, which in principle represents the $N \rightarrow \infty$ limit. This allows for multi-agent algorithm design by either approach. It is worth noting that while the distributed primal-dual algorithm (11) is presented as solving the discretized finite-dimensional optimization problem (10), it can equivalently be viewed as computing the discretized solution of the PDE characterizing the first-order optimality in Theorem 1. In the limits $N \rightarrow \infty$ of the number of agents and $n \rightarrow \infty$ of the number of iterations of the primal-dual algorithm, i.e. as the discretization more closely approximates the Kantorovich potential, we expect the two approaches to be equivalent, although this analysis is outside the scope of this paper.

The primal-dual algorithm is scalable with respect to the number of agents, wherein the agents are only required to communicate with their spatial (Voronoi) neighbors, as seen from (11). Voronoi partition-based distributed algorithms have been widely developed in the literature and scalable implementations exist [9]. Complexity of internal iterations is explicitly controlled by the number of agents N , the number of iterations n of the distributed primal-dual algorithm (11) and computing $\mu^*(\mathcal{V}_i)$ across the Voronoi partition by the agents. The runtime of the outer optimization is controlled by the distance between μ_0 and μ^* , the bound ϵ on the transport step size and the conformal factor ξ , while every agent incurs a cost to implement the optimization involved in the transport step that is distributed across the agents.

4.2 Numerical experiments

We now present numerical results for multi-agent optimal transport in \mathbb{R}^2 , based on the the stochastic process (7) (with c being the Euclidean metric and $\epsilon = 0.02$), where the local estimates of the Kantorovich potential

are computed by the distributed online algorithm (11) with a step size $\tau = 1$, as outlined in Algorithm 1.

We chose as the target distribution the histogram of i.i.d. samples of a multimodal, bivariate Gaussian distribution (shown in grayscale in Figure 1), and $N = 100$ agents for the transport. Figure 1 shows the agents along with the corresponding Voronoi partition of the domain, at three different stages (time instants $k = 0, 50, 100, 300$) during the course of their transport. We observe that the agents are transported towards the target probability measure and that a quantization of the target measure is obtained. This is clarified further in Figure 2, as described below. As we had noted in the previous section, there exists a fundamental trade-off between optimality and an online implementation of the distributed optimal transport. We sought to investigate the extent of this trade-off in simulation by running multiple iterations n of the primal-dual algorithm (11) for every iteration of the transport (7). The underlying rationale is that the distributed computation is many times faster than the transport. Figure 2 shows the rate of convergence (w.r.t. the variance in target mass $\mu^*(\mathcal{V}_i)$ across the partition) for $n = 1, 10$. The randomness in Figure 2 (as seen by the variation across trials and the 95% confidence intervals) is partly due to the fact that the same initial distribution μ_0 results in different samples across the trials, and the fact that the transport step (7) doesn't yield a unique minimizer but the agents are allowed to sample any one of the minimizers within an ϵ -ball. The numerical experiments were implemented in MATLAB R2023b on an Intel(R) Xeon(R) Platinum 8375C 2.90GHz CPU with 16GB of RAM. The average runtime across 10 independent runs of the experiment, for $k = 400$ steps of the transport with $N = 100$ agents, was 9.9s. The average runtime for $n = 20$ iterations of the distributed online primal-dual algorithm was 0.015s.

5 Conclusion

We proposed a scalable, distributed iterative proximal point algorithm for large-scale optimal transport of multi-agent collectives. We obtained a dynamical formulation of optimal transport of agents, for metric transport costs that are conformal to the Euclidean distance. We proposed a distributed primal-dual algorithm to be implemented by the agents to obtain local estimates of the Kantorovich potential, which are then used to implement the multi-agent optimal transport. We studied the behavior of the transport in simulation and investigated the suboptimality of the online implementation. The analytic characterization of the extent of the trade-off between optimality and the online nature of the implementation is left for future work.

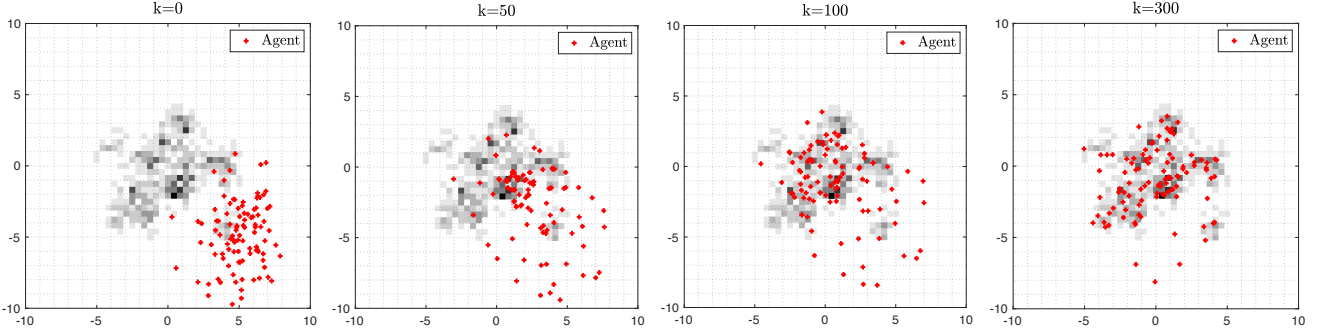


Fig. 1. Positions of agents at three different stages (time instants $k = 0, 50, 100, 300$) of transport by Algorithm 1, i.e., the iterative process (7) with local estimates of Kantorovich potential supplied by (11) (with $n = 1$ iterations of the primal-dual algorithm (11) for every transport step (11)); Target probability measure shown in grayscale with a darker shade indicating a region of higher target density; The plots show convergence in time of the agents to full coverage of the target coverage profile (represented by the target probability distribution).

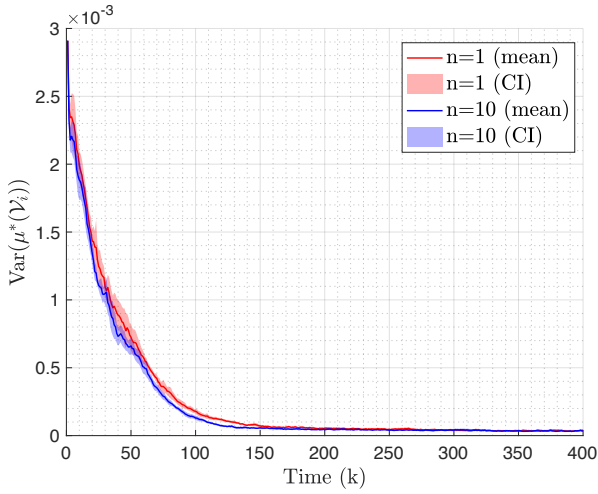


Fig. 2. Variance in target mass $\mu^*(V_i)$ across the partition vs time for iteration steps $n = 1, 10$ of the primal-dual algorithm (11) for every transport step (7). The plot shows the (empirical) mean along with 95% confidence bounds of the variance of $\mu^*(V_i)$ from 10 trials for each n from the same initial condition.

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A Proofs of Lemmas

A.1 Proof of Lemma 1

(a) This part of the proof employs similar arguments as the proof of the Kantorovich duality [35]. From (4), we have:

$$\begin{aligned}\phi(x) &= \inf_{y \in \Omega} \left(c(x, y) - \inf_{z \in \Omega} (c(z, y) - \phi(z)) \right) \\ &= \inf_{y \in \Omega} \sup_{z \in \Omega} \left(c(x, y) - c(z, y) + \phi(z) \right) \\ &\geq \inf_{y \in \Omega} \left(c(x, y) - c(z, y) + \phi(z) \right) \\ &= \inf_{y \in \Omega} \left(c(x, y) - c(z, y) \right) + \phi(z) \\ &\geq -c(x, z) + \phi(z),\end{aligned}$$

where we have used the fact that c is a metric to obtain the final inequality (for any y , we have $c(x, y) - c(z, y) = c(x, y) - c(y, z) \geq -c(x, z)$, which implies that $\inf_{y \in \Omega} (c(x, y) - c(z, y)) \geq -c(x, z)$). Moreover, since the above inequality holds for any $x, z \in \Omega$, we have $|\phi(x) - \phi(z)| \leq c(x, z)$.

Now, when $|\phi(x) - \phi(y)| \leq c(x, y)$, we have that $-\phi(x) \leq c(x, y) - \phi(y)$, which implies that $-\phi(x) \leq \inf_y (c(x, y) - \phi(y)) = \phi^c(x)$. Equivalently, we obtain the relation $\phi(x) \geq -\phi^c(x)$.

Similarly, from (4) $\phi^c(x) = \inf_y c(x, y) - \phi(y)$, we obtain $\phi^c(x) \leq c(x, y) - \phi(y)$. By setting $y = x$ in the above inequality, and using $c(x, x) = 0$ we get $\phi(x) \leq -\phi^c(x)$. In all, we have that $\phi^c(x) = -\phi(x)$ and $|\phi(x) - \phi(y)| \leq c(x, y)$.

(b) We now have that ϕ is Lipschitz continuous in Ω (since c is conformal to the Euclidean metric from and Ω is compact). It follows from Rademacher's theorem⁴ that ϕ is differentiable almost everywhere in Ω . Also, from Theorems 4 and 5, Chapter 5.8 in [18], we infer that $\phi \in W^{1, \infty}(\Omega)$ and that its (a.e.) gradient $\nabla \phi$ is equal to its weak gradient almost everywhere in Ω .

For any minimizing curve $\gamma \in C^1([0, 1]; \Omega)$ of (5), we have

$$\begin{aligned}\lim_{h \rightarrow 0^+} \frac{c(\gamma(h), \gamma(0))}{h} &= \lim_{h \rightarrow 0^+} \frac{1}{h} \int_0^h \xi(\gamma(t)) |\dot{\gamma}(t)| dt \\ &= \xi(\gamma(0)) |\dot{\gamma}(0)|\end{aligned}$$

⁴ **Rademacher's Theorem [24]:** Let $U \subset \mathbb{R}^d$ be open and bounded, and $f : U \rightarrow \mathbb{R}^m$ be locally Lipschitz continuous in U . Then f is differentiable at almost every $x \in U$.

Furthermore, note that for any $\psi \in C^1(\Omega)$ for which $|\psi(x) - \psi(y)| \leq c(x, y)$ for all $x, y \in \Omega$, we get

$$\begin{aligned}|\nabla \psi(\gamma(0)) \cdot \dot{\gamma}(0)| &= \left| \frac{d}{dh} \psi(\gamma(h)) \Big|_{h=0} \right| \\ &= \lim_{h \rightarrow 0^+} \frac{|\psi(\gamma(h)) - \psi(\gamma(0))|}{h} \\ &\leq \lim_{h \rightarrow 0^+} \frac{c(\gamma(h), \gamma(0))}{h} \\ &= \xi(\gamma(0)) |\dot{\gamma}(0)|.\end{aligned}$$

Since the above bound holds for any minimizing curve $\gamma \in C^1([0, 1]; \Omega)$ of (5), it follows that $|\nabla \psi(\gamma(0))| \leq \xi(\gamma(0))$. Now, applying the foregoing reasoning to the pointwise gradient of $\phi \in W^{1, \infty}(\Omega)$ satisfying $|\phi(x) - \phi(y)| \leq c(x, y)$ (which exists almost everywhere in Ω and is equal to its weak gradient), we get that the weak gradient (which we interchangeably denote as $\nabla \phi$) satisfies $|\nabla \phi(x)| \leq \xi(x)$ almost everywhere in Ω . The above formal reasoning involved the use of a C^1 test function ψ to define the derivative and carrying that over to the Lipschitz function ϕ wherever it is differentiable.

A.2 Proof of Lemma 2

The statement of Lemma 2 is a consequence of the metric property of C (Chapter 6, [35]), which can be established using the triangle inequality for c along minimum-length geodesics within the Monge formulation (1). From the Monge formulation (1), we have:

$$C(\mu, \mu^*) = \inf_{\substack{T \in \mathcal{T}(\Omega) \\ T_{\#} \mu = \mu^*}} \int_{\Omega} c(x, T(x)) d\mu(x),$$

where $\mathcal{T}(\Omega)$ is the set of measurable maps over Ω . For any measurable map $T : \Omega \rightarrow \Omega$ such that $T_{\#} \mu_0 = \mu^*$ and any $x, z \in \Omega$, we have:

$$c(x, T(x)) \leq c(x, z) + c(z, T(x)).$$

Moreover, we have:

$$c(x, T(x)) = \inf_{z \in \Omega} c(x, z) + c(z, T(x)),$$

where the minimum is attained when z lies on the minimum-length geodesic from x to $T(x)$ (the existence of minimum-length geodesics follows from the Hopf-Rinow Theorem). Since the above holds for any $x \in \Omega$, it then follows that:

$$\begin{aligned}C(\mu, \mu^*) &= \inf_{\substack{T \in \mathcal{T}(\Omega) \\ T_{\#} \mu = \mu^*}} \int_{\Omega} c(x, T(x)) d\mu(x) \\ &= \inf_{\substack{T \in \mathcal{T}(\Omega) \\ T_{\#} \mu = \mu^*}} \int_{\Omega} \inf_{z \in \Omega} [c(x, z) + c(z, T(x))] d\mu(x)\end{aligned}$$

$$\begin{aligned}
&\stackrel{(a)}{=} \inf_{\substack{T \in \mathcal{T}(\Omega) \\ T_{\#}\mu = \mu^*}} \inf_{\tilde{T} \in \mathcal{T}(\Omega)} \int_{\Omega} \left[c(x, \tilde{T}(x)) + c(\tilde{T}(x), T(x)) \right] d\mu(x) \\
&= \inf_{\substack{T \in \mathcal{T}(\Omega) \\ T_{\#}\mu = \mu^*}} \inf_{\tilde{T} \in \mathcal{T}(\Omega)} \left[\int_{\Omega} c(x, \tilde{T}(x)) d\mu(x) \right. \\
&\quad \left. + \int_{\Omega} c(x, T \circ \tilde{T}^{-1}(x)) d\tilde{T}_{\#}\mu(x) \right] \\
&= \inf_{\tilde{T} \in \mathcal{T}(\Omega)} \left[\int_{\Omega} c(x, \tilde{T}(x)) d\mu(x) \right. \\
&\quad \left. + \inf_{\substack{T \in \mathcal{T}(\Omega) \\ T_{\#}\mu = \mu^*}} \int_{\Omega} c(x, T \circ \tilde{T}^{-1}(x)) d\tilde{T}_{\#}\mu(x) \right] \\
&= \inf_{\nu \in \mathcal{P}(\Omega)} \left[\inf_{\substack{\tilde{T}^{(1)} \in \mathcal{T}(\Omega) \\ \tilde{T}_{\#}^{(1)}\mu = \nu}} \int_{\Omega} c(x, \tilde{T}^{(1)}(x)) d\mu(x) \right. \\
&\quad \left. + \inf_{\substack{\tilde{T}^{(2)} \in \mathcal{T}(\Omega) \\ \tilde{T}_{\#}^{(2)}\nu = \mu^*}} \int_{\Omega} c(x, \tilde{T}^{(2)}(x)) d\nu(x) \right] \\
&= \inf_{\nu \in \mathcal{P}(\Omega)} C(\mu, \nu) + C(\nu, \mu^*),
\end{aligned}$$

where the equality (a) follows from an application of Theorem 3A in [31]. We note that there clearly exists at least one minimizer ν above (the choices $\nu = \mu^*$ and $\nu = \mu$ trivially minimize the cost). We therefore conclude that $C(\mu, \mu^*) = \min_{\nu \in \mathcal{P}(\Omega)} C(\mu, \nu) + C(\nu, \mu^*)$.

B Proofs of Theorems

B.1 Proof of Theorem 1

(i) *Existence of Kantorovich potential ϕ* : We first rewrite the Kantorovich duality (6) as

$$\begin{aligned}
C(\mu, \mu^*) &= - \inf_{\phi \in W^{1,\infty}(\Omega, \mu)} \mathbb{E}_{\mu^*}[\phi] - \mathbb{E}_{\mu}[\phi], \\
&\quad \text{s.t. } |\nabla\phi| \leq \xi, \mu - \text{a.e.}
\end{aligned}$$

We note that the objective functional above is such that for any $p \in \mathbb{R}$ and any $\phi \in W^{1,\infty}(\Omega, \mu)$ with $|\nabla\phi| \leq \xi$, we have $-\mathbb{E}_{\mu}[\phi+p] + \mathbb{E}_{\mu^*}[\phi+p] = -\mathbb{E}_{\mu}[\phi] + \mathbb{E}_{\mu^*}[\phi]$. Furthermore, the constraint is such that $|\nabla(\phi+p)| = |\nabla\phi| \leq \xi$. It follows that the objective functional and constraint in the above optimization problem are invariant to constant vertical shifts $\phi \mapsto \phi+p$. In particular, for $\phi \mapsto \phi - \mathbb{E}_{\mu}[\phi]$, we can rewrite the above as

$$C(\mu, \mu^*) = - \inf_{\phi \in W^{1,\infty}(\Omega, \mu)} \underbrace{\mathbb{E}_{\mu^*}[\phi]}_{\triangleq L_{\mu^*}(\phi)},$$

$$\text{s.t. } \begin{cases} \mathbb{E}_{\mu}[\phi] = 0, \\ |\nabla\phi| \leq \xi, \mu - \text{a.e.} \end{cases}$$

To see the invariance under the transformation, recall that the dual problem is given by

$$\begin{aligned}
C(\mu, \mu^*) &= \sup_{\phi \in W^{1,\infty}(\Omega, \mu)} \int_{\Omega} \phi \left(1 - \frac{d\mu^*}{d\mu} \right) d\mu, \\
&\quad \text{s.t. } |\nabla\phi| \leq \xi, \mu - \text{a.e. in } \Omega,
\end{aligned}$$

which, for absolutely continuous probability measures $\mu, \mu^* \in \mathcal{P}(\Omega)$, we can rewrite as

$$\begin{aligned}
C(\mu, \mu^*) &= \sup_{\phi \in W^{1,\infty}(\Omega, \mu)} J(\phi) \triangleq \mathbb{E}_{\mu}[\phi] - \mathbb{E}_{\mu^*}[\phi], \\
&\quad \text{s.t. } |\nabla\phi| \leq \xi, \mu - \text{a.e. in } \Omega.
\end{aligned}$$

Let $\psi = \phi - \mathbb{E}_{\mu}[\phi]$. First see that $\phi \in W^{1,\infty}(\Omega, \mu)$ if and only if $\psi \in W^{1,\infty}(\Omega, \mu)$. The objective function, evaluated at ψ , is given by

$$\begin{aligned}
J(\psi) &= \mathbb{E}_{\mu}[\psi] - \mathbb{E}_{\mu^*}[\psi] \\
&= \mathbb{E}_{\mu}[\phi - \mathbb{E}_{\mu}[\phi]] - \mathbb{E}_{\mu^*}[\phi - \mathbb{E}_{\mu}[\phi]] \\
&= \mathbb{E}_{\mu}[\phi] - \mathbb{E}_{\mu}[\mathbb{E}_{\mu}[\phi]] - \mathbb{E}_{\mu^*}[\phi] + \mathbb{E}_{\mu^*}[\mathbb{E}_{\mu}[\phi]] \\
&= \mathbb{E}_{\mu}[\phi] - \mathbb{E}_{\mu^*}[\phi] - \mathbb{E}_{\mu}[\mathbb{E}_{\mu}[\phi]] + \mathbb{E}_{\mu^*}[\mathbb{E}_{\mu}[\phi]]
\end{aligned}$$

Observe that $\mathbb{E}_{\mu}[\mathbb{E}_{\mu}[\phi]] = \mathbb{E}_{\mu^*}[\mathbb{E}_{\mu}[\phi]] = \mathbb{E}_{\mu}[\phi]$ as μ and μ^* are probability measures. Therefore, it follows that

$$J(\psi) = \mathbb{E}_{\mu}[\phi] - \mathbb{E}_{\mu^*}[\phi] = J(\phi)$$

Furthermore, note that $\nabla\psi = \nabla(\phi - \mathbb{E}_{\mu}[\phi]) = \nabla\phi - \nabla(\mathbb{E}_{\mu}[\phi]) = \nabla\phi$, since $\nabla(\mathbb{E}_{\mu}[\phi]) = 0$ (this is due to the fact that $\mathbb{E}_{\mu}[\phi] = \int_{\Omega} \phi(x) d\mu(x)$, the average value of ϕ over Ω , is a constant w.r.t $x \in \Omega$).

Note that $\mathcal{L}(\Omega, \mu) = \{\phi \in W^{1,\infty}(\Omega, \mu) \mid \mathbb{E}_{\mu}[\phi] = 0, |\nabla\phi| \leq \xi, \mu - \text{a.e.}\}$ is closed, convex and bounded. Boundedness of $\mathcal{L}(\Omega, \mu)$ follows from the compactness of $\mathbb{Y} = \cup_{\phi \in \mathcal{L}(\Omega, \mu)} \phi(\Omega)$ which implies that there exists an $M \in \mathbb{R}_{\geq 0}$ such that $\mathbb{Y} \subset B_M(0)$. It follows that for any $\phi \in \mathcal{L}(\Omega, \mu)$, we have $\|\phi\|_{L^\infty(\Omega, \mu)} \leq M$. Moreover, we have $\|\nabla\phi\|_{L^\infty(\Omega, \mu)} \leq \|\xi\|_{L^\infty(\Omega, \mu)}$. Therefore, $\|\phi\|_{W^{1,\infty}(\Omega, \mu)} = \|\phi\|_{L^\infty(\Omega, \mu)} + \|\nabla\phi\|_{L^\infty(\Omega, \mu)} \leq M + \|\xi\|_{L^\infty(\Omega, \mu)} < \infty$ for any $\phi \in \mathcal{L}(\Omega, \mu)$.

The objective functional L_{μ^*} is convex and lower semicontinuous (in fact, it is (Gateaux) differentiable [32] as seen earlier for absolutely continuous μ^*). Let $\{\phi_n\}_{n \in \mathbb{N}}$ be a minimizing sequence in $\mathcal{L}(\Omega, \mu)$ for L_{μ^*} , such that $\phi_n \in \mathcal{L}(\Omega, \mu)$ and $\lim_{n \rightarrow \infty} L_{\mu^*}(\phi_n) = \inf_{\phi \in \mathcal{L}(\Omega, \mu)} L_{\mu^*}(\phi)$. Clearly, the sequence $\{\phi_n\}_{n \in \mathbb{N}}$ is uniformly bounded since $\|\phi_n\|_{W^{1,\infty}(\Omega, \mu)} \leq M + \sup_{x \in \Omega} |\xi|$. It is also uniformly equicontinuous, since $|\phi_n(x_1) - \phi_n(x_2)| \leq (\sup_{x \in \Omega} |\xi|) |x_1 - x_2|$ for all $n \in \mathbb{N}$.

Therefore, by the Arzelà-Ascoli Theorem [32], there exists a uniformly convergent subsequence $\{\phi_{n_j}\}_{j \in \mathbb{N}}$, with the limit $\phi^* \in \mathcal{L}(\Omega, \mu)$. Furthermore, by the continuity of L_{μ^*} , we get $\lim_{j \rightarrow \infty} L_{\sigma}(\phi_{n_j}) = L_{\mu^*}(\phi^*) = \min_{\phi \in \mathcal{L}(\Omega, \mu)} L_{\mu^*}(\phi)$. By the convexity of the loss L_{μ^*} , we get that ϕ^* is a global minimizer of L_{μ^*} .

(ii) *Saddle points of Lagrangian functional L* : The set $\mathcal{L}(\Omega)$ in the above problem can be expressed as $\mathcal{L}(\Omega) = \{\phi \in W^{1,\infty}(\Omega) \mid G(\phi) \in (-\infty, 0]\}$, where the functional $G(\phi) = \text{ess sup} |\nabla \phi|^2 - \xi^2$, and we have the constraint qualification:

$$0 \in \text{int} \{G(W^{1,\infty}(\Omega)) - (-\infty, 0]\},$$

where $G(W^{1,\infty}(\Omega)) - (-\infty, 0] = G(W^{1,\infty}(\Omega)) + [0, \infty)$, and the operation $+$ denotes the Minkowski sum. This allows us to apply Theorem 3.6 in [7] to infer that the set of Lagrange multipliers corresponding to the minimizer $\bar{\phi}$ is a non-empty, convex, bounded and weakly- $*$ compact subset of $L^\infty(\Omega)_{\geq 0}^*$, and the set of Lagrange multipliers is the same for any minimizer $\bar{\phi}$. Moreover, we note that $(-\infty, 0]$ is a closed convex cone, and it follows from Theorem 3.4-(iii) in [7] that for any Lagrange multiplier $\bar{\lambda}$, the pair $(\bar{\phi}, \bar{\lambda})$ is a saddle point of the Lagrangian functional L .

We now evaluate the Gateaux derivative of L_λ ⁵ in the space $W^{1,\infty}(\Omega)$. For $\phi \in W^{1,\infty}(\Omega)$ and a variation $\eta \in W^{1,\infty}(\Omega)$, the directional derivative of L_λ at ϕ along η is given by:

$$\begin{aligned} L'_\lambda(\phi, \eta) &= \lim_{\epsilon \rightarrow 0^+} \frac{1}{\epsilon} \int_{\Omega} (\phi + \epsilon \eta - \phi)(-\rho + \rho^*) \, \text{dvol} \\ &\quad + \frac{1}{2\epsilon} \int_{\Omega} (|\nabla \phi + \epsilon \nabla \eta|^2 - |\xi|^2 - |\nabla \phi|^2 + |\xi|^2) \, d\lambda, \end{aligned}$$

which simplifies to:

$$\begin{aligned} L'_\lambda(\phi, \eta) &= \lim_{\epsilon \rightarrow 0^+} \frac{1}{\epsilon} \int_{\Omega} \epsilon \eta (-\rho + \rho^*) \, \text{dvol} \\ &\quad + \frac{1}{2\epsilon} \int_{\Omega} (\epsilon^2 |\nabla \eta|^2 + 2\epsilon \nabla \phi \cdot \nabla \eta) \, d\lambda \\ &= - \int_{\Omega} \eta (\rho - \rho^*) \, \text{dvol} + \int_{\Omega} \nabla \phi \cdot \nabla \eta \, d\lambda, \end{aligned}$$

where the dominated convergence theorem is applied in order to calculate the previous limit which exists for every $\eta \in W^{1,\infty}(\Omega)$.

By the Minimax theorem and since $(\bar{\phi}, \bar{\lambda})$ is a saddle point for the Lagrangian L , we have $L(\bar{\phi}, \bar{\lambda}) = \sup_{\lambda} \inf_{\phi} L(\phi, \lambda) = \inf_{\phi} \sup_{\lambda} L(\phi, \lambda)$. Moreover, for any feasible $\bar{\phi}$ and $\lambda \geq 0$, we note that $L(\bar{\phi}, \lambda) \leq L(\bar{\phi}, 0) <$

⁵ We adopt the notation $L_\lambda(\phi) = L(\phi, \lambda)$.

$+\infty$ and which implies that $\sup_{\lambda} L(\bar{\phi}, \lambda) \leq L(\bar{\phi}, 0)$. This implies $\sup_{\lambda} \inf_{\phi} L(\phi, \lambda) = \inf_{\phi} \sup_{\lambda} L(\phi, \lambda) \leq L(\bar{\phi}, 0) < +\infty$. Thus, for *feasibility* we must have $\int_{\Omega} (|\nabla \bar{\phi}|^2 - |\xi|^2) \, d\bar{\lambda} \leq 0$, from which it follows that $|\nabla \bar{\phi}|^2 \leq |\xi|^2$ a.e. in Ω as $\bar{\lambda} \in \text{ba}(\Omega)_{\geq 0}$ (since if $\bar{\phi}$ does not satisfy $|\nabla \bar{\phi}|^2 \leq |\xi|^2$ a.e. in Ω , we would have that $\sup_{\lambda} L(\bar{\phi}, \lambda) = +\infty$, violating the finite upper bound). We also have:

$$\begin{aligned} L(\bar{\phi}, 0) &= - \int_{\Omega} \bar{\phi}(\rho - \rho^*) \, \text{dvol} \leq L(\bar{\phi}, \bar{\lambda}) = \min_{\phi} L(\phi, \bar{\lambda}) \\ &\leq L(\bar{\phi}, \bar{\lambda}) = - \int_{\Omega} \bar{\phi}(\rho - \rho^*) \, \text{dvol} + \int_{\Omega} (|\nabla \bar{\phi}|^2 - |\xi|^2) \, d\bar{\lambda} \\ &\leq - \int_{\Omega} \bar{\phi}(\rho - \rho^*) \, \text{dvol}, \end{aligned}$$

where the first inequality is due to the saddle point definition, the second equality follows from the Minimax theorem, the last inequality from the fact that $\bar{\phi}$ is a feasible solution. All inequalities are indeed equalities, and we therefore see that *complementary slackness* holds in the form $\int_{\Omega} (|\nabla \bar{\phi}|^2 - |\xi|^2) \, d\bar{\lambda} = 0$.

Since the pair $(\bar{\phi}, \bar{\lambda})$ is a saddle point of L , it is also a stationary point of L and we have $L'_\lambda(\bar{\phi}, \eta) = 0$ for any $\eta \in W^{1,\infty}(\Omega)$, and we get the *stationarity* condition $\int_{\Omega} \eta (\rho - \rho^*) \, \text{dvol} = \int_{\Omega} \nabla \bar{\phi} \cdot \nabla \eta \, d\bar{\lambda}$.

(iii) *Improved regularity of Lagrange multipliers*: We now establish stronger regularity for the Lagrange multipliers $\bar{\lambda}$. We have that the Lagrange multipliers $\bar{\lambda} \in L^\infty(\Omega)_{\geq 0}^*$, which are finitely additive measures absolutely continuous w.r.t. the Lebesgue measure, are also linear continuous functionals on $L^\infty(\Omega)$ and must therefore vanish on sets of Lebesgue measure zero (i.e., $\bar{\lambda}(A) = 0$ for $A \subset \Omega$ with $\text{vol}(A) = 0$). Moreover, from Theorem 1.24 in [36], we can decompose $\bar{\lambda} = \bar{\lambda}_c + \bar{\lambda}_p$, where $\bar{\lambda}_c$ is a non-negative countably additive measure and $\bar{\lambda}_p$ is non-negative and purely finitely additive. By the Radon-Nikodym theorem, we get that there exists a function $h_c \in L^1(\Omega)$ such that the countably additive and absolutely continuous measure λ_c satisfies $d\bar{\lambda}_c = h_c \, \text{dvol}$. By substitution in the stationarity condition, we get $\int_{\Omega} \eta (\rho - \rho^*) \, \text{dvol} = \int_{\Omega} (\nabla \bar{\phi} \cdot \nabla \eta) \, h_c \, \text{dvol} + \int_{\Omega} \nabla \bar{\phi} \cdot \nabla \eta \, d\bar{\lambda}_p$. We now consider a set $D_\delta = \{x \in \Omega \mid -\delta \leq |\nabla \phi(x)|^2 - \xi^2(x) \leq 0\}$, with $0 < \delta < \min_{x \in \Omega} \xi^2(x)$. By complementary slackness, we note that $\bar{\lambda}(\Omega \setminus D_\delta) = 0$. Since $\bar{\lambda}_p$ is purely finitely additive, it implies that there must exist a collection of nonempty sets $\{E_n\}_{n \in \mathbb{N}}$ with $E_{n+1} \subset E_n$ and $\lim_{n \rightarrow \infty} E_n = \emptyset$, such that $\lim_{n \rightarrow \infty} \bar{\lambda}_p(E_n) > 0$ ⁶. Since

⁶ For a countably additive measure ν that is absolutely continuous w.r.t. the Lebesgue measure, and any collection of nonempty sets $\{E_n\}_{n \in \mathbb{N}}$ with $E_{n+1} \subset E_n$ and $\lim_{n \rightarrow \infty} E_n = \emptyset$, we have $\lim_{n \rightarrow \infty} \nu(E_n) = 0$ [36].

$\bar{\lambda}(\Omega \setminus D_\delta) = 0$, we can suppose without loss of generality that $E_0 \subset D_\delta$. We also consider another collection of nonempty sets $\{E'_n\}_{n \in \mathbb{N}}$, with the same properties (with $E'_0 \subset D_\delta$, $E'_{n+1} \subset E'_n$ and $\lim_{n \rightarrow \infty} E'_n = \emptyset$), such that $E_n \subset E'_n$ for all $n \in \mathbb{N}$. We note that for $x \in D_\delta$, we have $0 < \xi^2(x) - \delta \leq |\nabla \phi(x)|^2 \leq \xi^2(x)$, which implies that $\nabla \phi$ does not vanish on E'_n for any $n \in \mathbb{N}$. We now consider a family of variations $\eta_n \in W^{1,\infty}(\Omega)$ for $n \in \mathbb{N}$ such that η_n and $\nabla \eta_n$ are supported in E'_n , $\nabla \phi \cdot \nabla \eta_n \geq 0$ in E'_n and $\nabla \phi \cdot \nabla \eta_n \geq \epsilon$ in E_n (uniformly). The stationarity condition would now yield, for $n \in \mathbb{N}$:

$$\begin{aligned} & \int_{E'_n} \eta_n (\rho - \rho^*) \, \text{dvol} \\ &= \int_{E'_n} (\nabla \bar{\phi} \cdot \nabla \eta_n) h_c \, \text{dvol} + \int_{E'_n} \nabla \bar{\phi} \cdot \nabla \eta_n \, d\bar{\lambda}_p \\ &\geq \int_{E'_n} (\nabla \bar{\phi} \cdot \nabla \eta_n) h_c \, \text{dvol} + \epsilon \int_{E_n} d\bar{\lambda}_p. \end{aligned}$$

In the limit $n \rightarrow 0$, we have $\lim_{n \rightarrow \infty} \int_{E'_n} \eta_n (\rho - \rho^*) \, \text{dvol} = 0$ and $\lim_{n \rightarrow \infty} \int_{E'_n} (\nabla \bar{\phi} \cdot \nabla \eta_n) h_c \, \text{dvol} = 0$, which implies that $0 \leq \lim_{n \rightarrow \infty} \epsilon \int_{E_n} d\bar{\lambda}_p \leq 0$, and we get $\lim_{n \rightarrow \infty} \bar{\lambda}_p(E_n) = 0$, i.e., the measure $\bar{\lambda}$ does not have a purely finitely additive component. Therefore, the measure $\bar{\lambda}$ is countably additive (and absolutely continuous) and possesses a Radon-Nikodym derivative w.r.t. the Lebesgue measure, in $L^1(\Omega)$. For ease of notation, we henceforth let $\bar{\lambda} \in L^1(\Omega)$ also denote its density function. Moreover, we note that since $\bar{\lambda} \in L^1(\Omega)_{\geq 0}$ and $|\nabla \bar{\phi}|^2 - |\xi|^2 \leq 0$ a.e. in Ω , we can now indeed state the complementary slackness condition as $\bar{\lambda}(|\nabla \bar{\phi}|^2 - |\xi|^2) = 0$ a.e. in Ω , which implies that $\bar{\lambda}(|\nabla \bar{\phi}| - |\xi|) = 0$ a.e. in Ω . We also see that $\bar{\phi} \in W^{1,\infty}(\Omega)$.

We recall from the stationarity condition that for any variation $\eta \in W^{1,\infty}(\Omega)$ at $\bar{\phi}$, we have $\int_\Omega \eta (\rho - \rho^*) \, \text{dvol} = \int_\Omega \nabla \bar{\phi} \cdot \nabla \eta \, d\bar{\lambda} = \int_\Omega \bar{\lambda} \nabla \bar{\phi} \cdot \nabla \eta \, \text{dvol}$. Under stronger regularity of the saddle point $(\bar{\phi}, \bar{\lambda})$, the stationarity condition can be expressed as:

$$\begin{aligned} & \int_\Omega (\rho - \rho^*) \eta \, \text{dvol} = \int_\Omega \bar{\lambda} \nabla \bar{\phi} \cdot \nabla \eta \, \text{dvol} \\ &= - \int_\Omega \nabla \cdot (\bar{\lambda} \nabla \bar{\phi}) \eta \, \text{dvol} + \int_{\partial\Omega} \bar{\lambda} \nabla \bar{\phi} \cdot \mathbf{n} \eta \, dS \end{aligned}$$

where we have used the divergence theorem to obtain the final equality, with S as the surface measure on $\partial\Omega$. As the above holds for any variation $\eta \in W^{1,\infty}(\Omega)$, it must follow that $-\nabla \cdot (\bar{\lambda} \nabla \bar{\phi}) = \rho - \rho^*$ in Ω and $\bar{\lambda} \nabla \bar{\phi} \cdot \mathbf{n} = 0$ on $\partial\Omega$, and if we do not suppose stronger regularity of the saddle point $(\bar{\phi}, \bar{\lambda})$, the equations must be hold weakly. Therefore, the saddle point $(\bar{\phi}, \bar{\lambda})$ weakly satisfies $-\nabla \cdot (\bar{\lambda} \nabla \bar{\phi}) = \rho - \rho^*$ in Ω and $\bar{\lambda} \nabla \bar{\phi} \cdot \mathbf{n} = 0$ on $\partial\Omega$.

The above correspond to the necessary KKT conditions.

Conversely, any solution pair $(\bar{\phi}, \bar{\lambda})$ which satisfies the above KKT conditions results in a saddle point for the Lagrangian and it is a solution to the original optimization problem.

B.2 Proof of Theorem 2

(a) *Process (7) achieves (8)*. We recall from (4) and Lemma 1 that for the transport $\mu_k \rightarrow \mu^*$, and for any $x \in \Omega$, we have:

$$\phi_{\mu_k \rightarrow \mu^*}(x) = \inf_{y \in \Omega} c(x, y) + \phi_{\mu_k \rightarrow \mu^*}(y). \quad (12)$$

Clearly, for any $x, y \in \Omega$, we have the inequality $\phi_{\mu_k \rightarrow \mu^*}(x) \leq c(x, y) + \phi_{\mu_k \rightarrow \mu^*}(y)$. Now, since $c(x, y) = c(x, z) + c(z, y)$ for any (and only) z on a minimum-length geodesic from x to y , we have that the following holds μ_k -a.e.:

$$\begin{aligned} 0 = & \inf_{\substack{y \in \Omega, \\ z \in \bar{\gamma}_{x \rightarrow y}([0,1])}} [-\phi_{\mu_k \rightarrow \mu^*}(x) + \phi_{\mu_k \rightarrow \mu^*}(z) - \phi_{\mu_k \rightarrow \mu^*}(z) \\ & + \phi_{\mu_k \rightarrow \mu^*}(y) + c(x, z) + c(z, y)], \end{aligned}$$

where $\bar{\gamma}_{x \rightarrow y} : [0, 1] \rightarrow \Omega$ is a length-minimizing geodesic from x to y . Rearranging the above, it follows that the following holds μ_k -a.e.:

$$\begin{aligned} 0 = & \inf_{\substack{y \in \Omega, \\ z \in \bar{\gamma}_{x \rightarrow y}([0,1])}} [-\phi_{\mu_k \rightarrow \mu^*}(x) + \phi_{\mu_k \rightarrow \mu^*}(z) + c(x, z)] \\ & + [-\phi_{\mu_k \rightarrow \mu^*}(z) + \phi_{\mu_k \rightarrow \mu^*}(y) + c(z, y)]. \end{aligned}$$

Moreover, since the expressions (within the infimum) above are each non-negative, and their sum attains an infimum value of zero, we infer that they individually attain zero. Thus, for any minimizer y^* in (12), we get that every point on a length-minimizing geodesic from x to y^* is also a minimizer. We note that the set of minimizers $\mathcal{M}_{\mu_k}^\epsilon(x)$ in (7) therefore correspond to the segments of the length-minimizing geodesics (from the current iterate to the minimizers of (12)) contained in the ϵ -ball B_ϵ^c centered at the current iterate. Moreover, since $\phi_{\mu_k \rightarrow \mu^*}$ is differentiable μ_k -almost everywhere, it follows that the set of minimizers $\mathcal{M}_{\mu_k}^\epsilon(x)$ are one-dimensional and are segments of geodesics from (almost every) $x \in \Omega$. It is known from Theorem 5.10 in [35] that the optimal transport plans $\pi_k \in \mathcal{P}(\Omega \times \Omega)$ (with μ_k and μ^* as the marginals) are supported in the set:

$$\Gamma = \{(x, y) \in \Omega \times \Omega \mid \phi_{\mu_k \rightarrow \mu^*}(x) - \phi_{\mu_k \rightarrow \mu^*}(y) = c(x, y)\}.$$

Let $\Gamma_x = \{y \in \Omega \mid (x, y) \in \Gamma\}$ and $\Gamma_x^\epsilon = \Gamma_x \cap B_\epsilon^c(x)$ for all $x \in \Omega$ where $\phi_{\mu_k \rightarrow \mu^*}$ is differentiable (since this is the case almost everywhere in Ω , we ignore the set of zero measure where $\phi_{\mu_k \rightarrow \mu^*}$ is not differentiable in the rest of this proof). We see that Γ_x^ϵ is the set of minimizers $\mathcal{M}_{\mu_k}^\epsilon(x)$ in (7).

Now, for any transport map \tilde{T}_k from μ_k to μ^* , we get $\phi_{\mu_k \rightarrow \mu^*}(x) \leq c(x, \tilde{T}_k(x)) + \phi_{\mu_k \rightarrow \mu^*}(\tilde{T}_k(x))$. It then follows that:

$$\begin{aligned} & \int_{\Omega} \left(\phi_{\mu_k \rightarrow \mu^*}(x) - \phi_{\mu_k \rightarrow \mu^*}(\tilde{T}_k(x)) \right) d\mu_k(x) \\ &= \int_{\Omega} \phi_{\mu_k \rightarrow \mu^*} d\mu_k - \int_{\Omega} \phi_{\mu_k \rightarrow \mu^*} d\mu^* \\ &\leq \int_{\Omega} c(x, \tilde{T}_k(x)) d\mu_k(x). \end{aligned}$$

We see that the LHS is the optimal transport cost obtained from the Kantorovich dual formulation, while an infimum over the RHS w.r.t. \tilde{T}_k would again yield the optimal transport cost from the Monge formulation and an equality would then be attained. From Theorem 1 in [19], we get that the Monge problem attains a minimum, and let \tilde{T}_k^* be an optimal transport map from μ_k to μ^* . Thus, we infer that $-\phi_{\mu_k \rightarrow \mu^*}(x) + \phi_{\mu_k \rightarrow \mu^*}(\tilde{T}_k^*(x)) + c(x, \tilde{T}_k^*(x)) = 0$, μ_k -almost everywhere in Ω , and $\tilde{T}_k^*(x) \in \Gamma_x$. Moreover, the set Γ_x^c , which is obtained as minimizers $\mathcal{M}_{\mu_k}^c(x)$ in (7), is precisely the segment of the geodesic (of length ϵ) from x to $\tilde{T}_k^*(x)$ for μ_k -almost every $x \in \Omega$. From this correspondence between the Monge problem and the process (7), and from the proof of Lemma 2, it follows that the optimal transport cost $C(\mu_k, \mu^*)$ can be decomposed as in (8) by the process (7).

(b) *Process (7) achieves convergence $C(\mu_k, \mu^*) \rightarrow 0$.* We now consider a single update step of the process $\{X(k)\}_{k \in \mathbb{N}}$. For simplicity of notation, let X be a random variable such that $X \sim \mu$ for some $\mu \in \mathcal{P}(\Omega)$ and let $x \in \Omega$ be a sample of X . Let x^+ be a sample drawn uniformly at random from the set of minimizers $\arg \min_{z \in B_{\epsilon}^c(x)} c(x, z) + \phi_{\mu \rightarrow \mu^*}(z) = \arg \min_{z \in B_{\epsilon}^c(x)} c(x, z) + c(z, T_{\mu \rightarrow \mu^*}(x))$. Note that any such x^+ satisfies $c(x^+, T_{\mu \rightarrow \mu^*}(x)) \leq c(x, T_{\mu \rightarrow \mu^*}(x))$. Since this holds for any sample x of X , we get that the random variable X^+ obtained from the single update of X , with $X^+ \sim \mu^+$, is such that $C(\mu^+, \mu^*) \leq C(\mu, \mu^*)$. Therefore, the sequence of measures $\{\mu_k\}_{k \in \mathbb{N}}$ corresponding to the process $\{X_k\}_{k \in \mathbb{N}}$ satisfies $C(\mu_{k+1}, \mu^*) \leq C(\mu_k, \mu^*)$ for all $k \in \mathbb{N}$, and applying the monotone convergence theorem, we get that $C(\mu_k, \mu^*) \rightarrow \bar{C}$. By Prokhorov's Theorem [35], from which we get that $\mathcal{P}(\Omega)$ is compact w.r.t. the topology of weak convergence, and the fact that μ_k lies on the (unique) geodesic between μ_0 and μ^* , it follows that there exists an accumulation point $\bar{\mu}$ on the geodesic between μ_0 and μ^* such that $\mu_k \rightarrow \bar{\mu}$. This implies that $C(\bar{\mu}, \bar{\mu}^+) = 0$, where $\bar{\mu}^+ \in \mathcal{P}(\Omega)$ is obtained from a one step update of $\bar{X} \sim \bar{\mu}$. Furthermore, we have

$$C(\bar{\mu}, \bar{\mu}^+) = \min_{\sigma \in \Pi(\bar{\mu}, \bar{\mu}^+)} \int_{\Omega \times \Omega} c(x, z) d\sigma(x, z).$$

From Section (a) of the proof, it follows that the process (7) results in optimal transport from $\bar{\mu}$ to $\bar{\mu}^+$. With π as the transition probability for the process (7), we get

$$\begin{aligned} C(\bar{\mu}, \bar{\mu}^+) &= \min_{\sigma \in \Pi(\bar{\mu}, \bar{\mu}^+)} \int_{\Omega \times \Omega} c(x, z) d\sigma(x, z) \\ &= \int_{x \in \Omega} \int_{z \in \Omega} c(x, z) d\pi(z | x) d\bar{\mu}(x) \\ &= \int_{x \in \Omega} \frac{1}{\ell(\mathcal{M}_{\bar{\mu}}^c(x))} \int_{z \in \mathcal{M}_{\bar{\mu}}^c(x)} c(x, z) d\ell(z) d\bar{\mu}(x). \end{aligned}$$

Suppose that $C(\bar{\mu}, \mu^*) = \eta > 0$. First note that for every $x \in \Omega$, the following holds

$$c(x, T_{\mu \rightarrow \mu^*}(x)) = \min_{z \in B_{\epsilon}^c(x)} c(x, z) + c(z, T_{\mu \rightarrow \mu^*}(x)),$$

owing to the triangle inequality being an equality along the c -geodesic. Furthermore, note that for any minimizer z above, i.e. for $z \in \mathcal{M}_{\bar{\mu}}^c(x)$ we have $c(z, T_{\mu \rightarrow \mu^*}(x)) \leq c(x, T_{\mu \rightarrow \mu^*}(x))$. We then have

$$\begin{aligned} \eta &= C(\bar{\mu}, \mu^*) = \int_{\Omega} c(x, T_{\bar{\mu} \rightarrow \mu^*}(x)) d\bar{\mu}(x) \\ &= \int_{\Omega} \min_{z \in B_{\epsilon}^c(x)} [c(x, z) + c(z, T_{\mu \rightarrow \mu^*}(x))] d\bar{\mu}(x) \\ &= \int_{\Omega} \frac{1}{\ell(\mathcal{M}_{\bar{\mu}}^c(x))} \int_{z \in \mathcal{M}_{\bar{\mu}}^c(x)} [c(x, z) \\ &\quad + c(z, T_{\mu \rightarrow \mu^*}(x))] d\ell(z) d\bar{\mu}(x) \\ &= C(\bar{\mu}, \bar{\mu}^+) \\ &\quad + \int_{\Omega} \frac{1}{\ell(\mathcal{M}_{\bar{\mu}}^c(x))} \int_{z \in \mathcal{M}_{\bar{\mu}}^c(x)} c(z, T_{\mu \rightarrow \mu^*}(x)) d\ell(z) d\bar{\mu}(x) \end{aligned}$$

From $C(\bar{\mu}, \bar{\mu}^+) = 0$ (since $\bar{\mu}$ is an accumulation point), we get

$$\int_{\Omega} \frac{1}{\ell(\mathcal{M}_{\bar{\mu}}^c(x))} \int_{z \in \mathcal{M}_{\bar{\mu}}^c(x)} c(z, T_{\mu \rightarrow \mu^*}(x)) d\ell(z) d\bar{\mu}(x) = \eta$$

which implies that $\bar{\mu}$ -a.e. in Ω

$$c(x, T_{\bar{\mu} \rightarrow \mu^*}(x)) = \frac{1}{\ell(\mathcal{M}_{\bar{\mu}}^c(x))} \int_{z \in \mathcal{M}_{\bar{\mu}}^c(x)} c(z, T_{\mu \rightarrow \mu^*}(x)) d\ell(z).$$

Since for $z \in \mathcal{M}_{\bar{\mu}}^c(x)$ we have $c(z, T_{\mu \rightarrow \mu^*}(x)) \leq c(x, T_{\mu \rightarrow \mu^*}(x))$, it follows that $\mathcal{M}_{\bar{\mu}}^c(x) = \{x\}$, $\bar{\mu}$ -a.e. in Ω , which is the case if and only if $T_{\bar{\mu} \rightarrow \mu^*}(x) = x$, i.e., $C(\bar{\mu}, \mu^*) = 0$, and we get a contradiction. Therefore, it follows that μ^* is the only accumulation point and the sequence $\{\mu_k\}_{k \in \mathbb{N}}$ converges to μ^* as $k \rightarrow \infty$ w.r.t. the topology of weak convergence in $\mathcal{P}(\Omega)$, i.e., $C(\mu_k, \mu^*) \rightarrow 0$.