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METRIC EXTRAPOLATION IN THE WASSERSTEIN SPACE

THOMAS O. GALLOUËT, ANDREA NATALE, AND GABRIELE TODESCHI

ABSTRACT. In this article we study a variational problem providing a way to extend for all times minimizing geodesics connecting two given probability measures, in the Wasserstein space. This is simply obtained by allowing for negative coefficients in the classical variational characterization of Wasserstein barycenters. We show that this problem admits two equivalent convex formulations: the first can be seen as a particular instance of Toland duality and the second is a barycentric optimal transport problem. We propose an efficient numerical scheme to solve this latter formulation based on entropic regularization and a variant of Sinkhorn algorithm.

1. INTRODUCTION

Given a metric space (X, d) , a globally minimizing geodesic on X defined on $[t_0, t_1] \subset \mathbb{R}$, with $t_1 > t_0$, is a curve $x : s \in [t_0, t_1] \rightarrow x(s) \in X$ verifying

$$(1.1) \quad d(x(s_0), x(s_1)) = \frac{|s_1 - s_0|}{|t_1 - t_0|} d(x(t_0), x(t_1)),$$

for all $s_0, s_1 \in [t_0, t_1]$. If such a curve exists, its points can be characterized as the minimizers of the following variational problem: for any $s \in [t_0, t_1]$

$$(1.2) \quad x(s) \in \operatorname{argmin}_{x \in X} \left\{ (s - t_0) \frac{d^2(x, x(t_1))}{2} + (t_1 - s) \frac{d^2(x, x(t_0))}{2} \right\}.$$

Let us consider problem (1.2) for $s \notin [t_0, t_1]$. Specifically, after a rescaling, we consider the following problem: given two points $x_0, x_1 \in X$ and $t > 1$, find $x \in X$ that solves

$$(1.3) \quad \inf_{x \in X} \left\{ \frac{d^2(x, x_1)}{2(t-1)} - \frac{d^2(x, x_0)}{2t} \right\}.$$

By triangular and Young's inequality, we always have that such infimum is larger than $-d^2(x_0, x_1)/2$. Moreover, if there exists a globally minimizing geodesic $x : s \in [0, t] \rightarrow x(s) \in X$ such that $x(0) = x_0$ and $x(1) = x_1$ then this lower bound is attained by $x(t)$, which is therefore a minimizer. In particular, in the case where $X = \mathbb{R}^d$, equipped with the Euclidean distance, one always has a unique minimizer

$$x(t) = x_0 + t(x_1 - x_0).$$

In general, problem (1.3) gives a variational definition of geodesic extrapolation even if no geodesic, connecting x_0 to x_1 on the interval $[0, 1]$, may be extended up to time $t > 1$ while staying globally length minimizing.

In this work, we consider a specific instance of problem (1.3) where (X, d) is $\mathcal{P}_2(\mathbb{R}^d)$, the set of probability measures with finite second moments, equipped with the L^2 -Wasserstein distance W_2 . This latter is defined as follows: for any $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$

$$(1.4) \quad W_2^2(\mu, \nu) := \min \left\{ \int |x - y|^2 d\gamma(x, y) ; \gamma \in \Gamma(\mu, \nu) \right\},$$

where $\Gamma(\mu, \nu) \subset \mathcal{P}_2(\mathbb{R}^d \times \mathbb{R}^d)$ is the set of couplings having μ and ν as first and second marginal, respectively. The problem we consider is therefore given by:

$$(\mathcal{P}) \quad \min_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \left\{ \frac{W_2^2(\mu, \nu_1)}{2(t-1)} - \frac{W_2^2(\mu, \nu_0)}{2t} \right\}.$$

By the derivation above, problem (\mathcal{P}) provides a natural notion for geodesic extrapolation in the Wasserstein space. This was named *metric extrapolation* in [15] and used for the construction of higher order time discretization of Wasserstein gradient flows. In contrast to the classical Wasserstein version of problem (1.2) introduced in [1], it was shown in [15] (see also Section 2.1) that problem (\mathcal{P}) always admits a unique minimizer even when there are multiple geodesics connecting ν_0 to ν_1 . This may be surprising given the lack of convexity of the problem with respect to the linear interpolation of probability measures, but is due to the fact that (\mathcal{P}) is strongly convex along particular curves known as generalized geodesics [2]. The goal of this paper is to provide a full characterization of the hidden convexity in problem (1.2) which is responsible for its well-posedness. More precisely, we show that it admits two different convex formulations, which can be seen as an instance of Toland duality and of weak optimal transport, respectively, and which we describe in general terms in this section. We will use such formulations to give a precise characterization of the minimizers of problem (1.2) and to construct an efficient numerical scheme to compute them.

1.1. Geodesics in the Wasserstein space. Consider the optimal transport problem (1.4) from ν_0 to ν_1 . If, for example, ν_0 is absolutely continuous then Brenier's theorem states that there exists a unique solution $\gamma^* \in \Gamma(\nu_0, \nu_1)$ to this problem which is furthermore induced by a transport map $\nabla u : \mathbb{R}^d \rightarrow \mathbb{R}^d$, where $u : \mathbb{R}^d \rightarrow \mathbb{R}$ is a convex function usually called the Brenier potential for the transport from ν_0 to ν_1 , i.e.

$$\gamma^* = (\text{Id}, \nabla u)_{\#} \nu_0.$$

Furthermore, in this case, there exists a uniquely defined geodesic on the interval $[0, 1]$ connecting ν_0 to ν_1 , which is given by McCann's interpolant [23]

$$(1.5) \quad \nu(s) = ((1-s)\text{Id} + s\nabla u)_{\#} \nu_0, \quad \forall s \in [0, 1].$$

This curve can be extended up to $s = t > 1$ while staying a length-minimizing geodesic if and only if $((1-t)\text{Id} + t\nabla u)$ is an optimal transport map, or equivalently

$$x \mapsto u(x) - \frac{t-1}{t} \frac{|x|^2}{2} \text{ is convex.}$$

However, this condition is not verified in general, since we may only expect u to be convex (and not strongly convex), which corresponds to the fact that the trajectories of the particles, induced by (1.5), may cross precisely at $t = 1$.

Note that in the following, for brevity, we will occasionally omit to specify “length-minimizing” when referring to Wasserstein geodesics, but we will always refer to curves that are globally length-minimizing.

1.2. Toland’s duality. Toland’s duality [31, 32] concerns the minimization of the difference of two convex, proper and lower semi-continuous functions $F, G : V \rightarrow (-\infty, \infty]$, where V is a normed vector space. Specifically, we have the equivalence

$$\inf_{x \in V} \{F(x) - G(x)\} = \inf_{p \in V^*} \{G^*(p) - F^*(p)\}$$

where V^* is the topological dual of V and F^* and G^* are the Legendre transforms of F and G respectively.

The idea of using Toland duality to deal with differences of Wasserstein distances stems from the work of Carlier [9], who considered a variant of problem (\mathcal{P}) where the coefficients multiplying the two distances are equal and \mathbb{R}^d is replaced by a compact convex set. In our case, F and G are replaced by the maps

$$\mu \in \mathcal{P}_2(\mathbb{R}^d) \mapsto \frac{W_2^2(\mu, \nu_1)}{2(t-1)} \quad \text{and} \quad \mu \in \mathcal{P}_2(\mathbb{R}^d) \mapsto \frac{W_2^2(\mu, \nu_0)}{2t}$$

Then, at least formally, one can check that the resulting dual problem is given by

$$(\mathcal{P}^*) \quad \inf \left\{ \int u^* d\nu_1 + \int u d\nu_0 : u - \frac{t-1}{t} \frac{|\cdot|^2}{2} \text{ is convex and l.s.c.} \right\}.$$

A detailed proof of this result is provided in Section 2.2. Remarkably, and differently from (\mathcal{P}) , this is a convex optimization problem in the usual sense. Also, we observe that requiring u to be only convex rather than strongly convex, one recovers one of the possible dual formulations of the quadratic optimal transport problem from ν_0 to ν_1 . In particular, in this case, any Brenier potential u is a solution and, if ν_1 is a.c., $\nabla u_{\#}^* \nu_1 = \nu_0$. On the other hand, if u is a solution to (\mathcal{P}^*) we show that $\bar{\nu}_0 := \nabla u_{\#}^* \nu_1$ may be different from ν_0 but is dominated by it in the convex order (see Lemma 2.4), i.e.

$$(1.6) \quad \int \varphi d\bar{\nu}_0 \leq \int \varphi d\nu_0$$

for all convex functions $\varphi : \mathbb{R}^d \rightarrow \mathbb{R}$. Moreover, we show that the (unique) solution to problem (\mathcal{P}) can be written as

$$(1.7) \quad \nu_t := ((1-t)\text{Id} + t\nabla u)_{\#} \bar{\nu}_0,$$

at least in the case where $\bar{\nu}_0$ is absolutely continuous (see Theorem 2.5 for the precise statement in the general case). Since u is strongly convex this means that the measure $\bar{\nu}_0$, defined via the solution of problem (\mathcal{P}^*) is such that the geodesic from $\bar{\nu}_0$ to ν_1 on the time interval $[0, 1]$ can be extended up to time t and the resulting extension is precisely the solution to (\mathcal{P}) .

1.3. Weak optimal transport formulation. The convex order relation between $\bar{\nu}_0 = \nabla u_{\#}^* \nu_1$ and ν_0 , with u solving (\mathcal{P}^*) , can be exploited to derive an equivalent formulation of problem (\mathcal{P}) which fits in the framework of weak (and in particular barycentric) optimal transport, a generalization of optimal transport introduced in [18]. This reads as follows:

$$(\mathcal{B}) \quad \inf_{\gamma \in \Gamma(\nu_0, \nu_1)} \int |tx_1 - (t-1)\text{bary}(\gamma_{x_1})|^2 d\nu_1(x_1), \quad \text{bary}(\gamma_{x_1}) = \int x_0 d\gamma_{x_1}(x_0),$$

where γ_{x_1} is the disintegration of γ with respect to the projection on the second marginal. On the other hand, by Strassen's theorem (see Lemma 3.1 and [30]), the convex order condition (1.6) implies the existence of a coupling $\theta \in \Gamma(\bar{\nu}_0, \nu_0)$ which is the law of a martingale, i.e. $d\theta(x, y) = d\theta_x(y) d\bar{\nu}_0(x)$ and

$$\int y d\theta_x(y) = x, \quad \text{for } \bar{\nu}_0\text{-a.e. } x \in \mathbb{R}^d,$$

where now θ_x is the disintegration of θ with respect to the projection on the first marginal. Thus, formally, the link between problem (\mathcal{P}^*) and (\mathcal{B}) can be stated as follows: u solves (\mathcal{P}^*) if and only if the coupling $\pi \in \Gamma(\nu_0, \nu_1)$ defined by

$$(1.8) \quad d\pi(x_0, x_1) = d\theta_{\nabla u^*(x_1)}(x_0) d\nu_1(x_1)$$

solves (\mathcal{B}) (see Theorem 3.3). Note that this gives a characterization of the minimizers of problem (\mathcal{B}) as the composition of a martingale and a sufficiently smooth transport plan. Such a characterization can also be derived as a slight modification of a result of Gozlan and Juillet [17]. Our proof shows that this can be alternatively obtained as a consequence of Strassen's theorem and Toland duality.

1.4. Related works. The problem of defining Wasserstein geodesic extensions has appeared in the literature in different contexts. Several approaches, different from the one discussed in this article, were proposed in [4] as a byproduct of different definitions for cubic splines in the Wasserstein space, with the aim of interpolating (and extrapolating) multiple measures by a single curve. A variant of problem (\mathcal{P}) was introduced in [22] in order to construct higher order versions of the JKO scheme for the numerical computation of Wasserstein gradient flows. The idea of using geodesic extensions is also proposed in [21] with the same purpose.

Problem (\mathcal{P}) has also a strong link with fluid dynamics. In one dimension, the curve $t \mapsto \nu_t$ defined by equation (1.7) yields a ‘‘sticky solution’’ of the pressureless Euler equation [7, 24]; see also Section 4.1. In general, the idea of modifying the initial conditions to retrieve the solution of a fluid dynamic model at the final time via convex optimization (as it occurs in our model; see equation (1.7)) was proposed by Brenier in [5] for the incompressible Euler equations, but it applies to a large class of models [6, 34].

From a computational perspective, the use of strongly convex Brenier potentials has been advocated in [27] to regularize standard optimal transport, but via a variational formulation that differs from ours and in particular is non-convex. On the other hand, problem (\mathcal{P}^*) , with additional constraint of L -smoothness on the potential, has been

recently considered in [33] to provide an estimator of the true Brenier potential between sampled measures. In our case, however, the equivalence with the barycentric problem (\mathcal{B}) enables us to propose an algorithm with similar performance as the well-known Sinkhorn method. Furthermore, the numerical scheme that we propose leverages Sinkhorn in a different way than related methods introduced in [26] for general weak optimal transport problems.

The variational formulation of the Wasserstein barycenters between multiple measures with negative coefficients appears naturally also in the context of nonlinear reduced basis models in the Wasserstein space, as in [12] for example, and for statistical regression [13]. However, in these works the non-convexity of the problem is not addressed directly. In particular, in [12] the authors use a simpler proxy for the W_2 distance which allows for an explicit characterization of the barycenters. In [13] instead, the problem is tackled numerically using a convex optimization approach, without convergence guarantees. We refer to Remark 3.4 for some considerations on the extension of our work to the setting with multiple measures.

Finally, we remark that a weak optimal transport version of Wasserstein barycenters (rather than extrapolation as in our case) has been recently introduced in [11].

1.5. Structure of the paper. The rest of the article is structured as follows. In section 2 we collect some well-posedness results for the metric extrapolation problem, and prove strong duality with problem (\mathcal{P}^*). In section 3, we prove the equivalence with the weak optimal transport formulation (\mathcal{B}). In section 4 we give a precise link of our problem with the H^1 projection on convex functions, via a Γ -convergence result. In section 5 we provide some exact solutions to the problem providing some intuition on the behavior of the metric extrapolation. Finally, in Section 6, we propose and analyze a variant of Sinkhorn algorithm to solve the problem in the case of atomic measures, and provide some numerical results.

2. MAIN PROPERTIES AND TOLAND DUALITY

In this section we collect some well-posedness results for problem (\mathcal{P}), i.e., existence and uniqueness of solutions and convexity of the problem along generalized geodesics, that were already proven in [15]. We further show that the problem admits a convex dual formulation given by problem (\mathcal{P}^*). This last result is inspired by the duality principle studied in [9] for the case where the transport costs are multiplied by the same coefficient with opposite signs, but it does not contain this latter since our proof requires the coefficients to be different in absolute value.

2.1. Existence and uniqueness of solutions. Existence and uniqueness for solutions to problem (\mathcal{P}) follows from the fact that the functional

$$(2.1) \quad \mathcal{F}_t(\nu_0, \nu_1; \mu) := \frac{W_2^2(\mu, \nu_1)}{2(t-1)} - \frac{W_2^2(\mu, \nu_0)}{2t}$$

is bounded from below and is strongly convex along specific curves, known as generalized geodesics [2, Definition 9.1.1]. As for the lower bound, this can be found directly using

the notion of Wasserstein geodesic. In fact, if $\nu : s \in [0, t] \rightarrow \nu(s) \in \mathcal{P}_2(\mathbb{R}^d)$ is a geodesic from ν_0 to μ , we have

$$(2.2) \quad \begin{aligned} \frac{W_2^2(\mu, \nu_0)}{2t} &= \frac{W_2^2(\mu, \nu(1))}{2(t-1)} + \frac{W_2^2(\nu(1), \nu_0)}{2} \\ &\leq \frac{W_2^2(\mu, \nu_1)}{2(t-1)} + \frac{W_2^2(\nu_1, \nu_0)}{2} \end{aligned}$$

where we have used the variational characterization of globally minimizing geodesics in equation (1.2), and specifically the fact that

$$\nu(1) \in \operatorname{argmin}_{\nu \in \mathcal{P}_2(\mathbb{R}^d)} \left\{ \frac{W_2^2(\mu, \nu)}{2} + (t-1) \frac{W_2^2(\nu, \nu_0)}{2} \right\}$$

Then, equation (2.2) yields

$$(2.3) \quad \mathcal{F}_t(\nu_0, \nu_1; \mu) \geq -\frac{W_2^2(\nu_0, \nu_1)}{2}.$$

A precise statement for the strong convexity of $\mathcal{F}_t(\nu_0, \nu_1; \cdot)$ along generalized geodesics is contained in the following lemma:

Lemma 2.1 (Theorem 3.4 in [22]). *Let $\nu_0, \nu_1 \in \mathcal{P}_2(\mathbb{R}^d)$, and consider the functional $\mathcal{F}_t(\nu_0, \nu_1; \cdot) : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ defined in (2.1). For any $\mu_0, \mu_1 \in \mathcal{P}_2(\mathbb{R}^d)$, let $\mu : [0, 1] \rightarrow \mathcal{P}_2(\mathbb{R}^d)$, $\mu(0) = \mu_0, \mu(1) = \mu_1$, be a generalized geodesic based in ν_1 . Then, for all $0 \leq s \leq 1$ it holds*

$$(2.4) \quad \mathcal{F}_t(\nu_0, \nu_1; \mu(s)) \leq (1-s)\mathcal{F}_t(\nu_0, \nu_1; \mu_0) + s\mathcal{F}_t(\nu_0, \nu_1; \mu_1) - \frac{s(1-s)}{2} \frac{W_2^2(\mu_0, \mu_1)}{t(t-1)}.$$

Note that this Lemma can be viewed as a simple consequence of the fact that $\mathcal{F}_t(\nu_0, \nu_1; \cdot)$ is the sum of $W_2^2(\cdot, \nu_1)/(2t-2)$, which is $1/(t-1)$ -convex along generalized geodesics based at ν_1 [2, Lemma 9.2.1] (in the sense of equation (2.4)), and $-W_2^2(\cdot, \nu_1)/(2t)$, which is $-1/t$ -convex along *any* generalized geodesic [2, Proposition 9.3.12]. Therefore, the sum must be $(1/(t-1) - 1/t)$ -convex along generalized geodesics based at ν_1 .

Using the fact that the space $\mathcal{P}_2(\mathbb{R}^d)$ equipped with the Wasserstein distance is complete, one can show that Lemma 2.1 together with the lower bound (2.3) implies that problem (P) admits a unique solution. We refer to [15, Proposition 4.10] for the proof.

Remark 2.2 (Link with extrapolation). *Suppose that there exists a length-minimizing geodesic $s \in [0, t] \rightarrow \nu(s) \in \mathcal{P}_2(\mathbb{R}^d)$ such that $\nu(0) = \nu_0$ and $\nu(1) = \nu_1$, then $\nu(t)$ is the unique minimizer to problem (P), since*

$$\frac{W_2^2(\nu(t), \nu_1)}{2(t-1)} - \frac{W_2^2(\nu(t), \nu_0)}{2t} = -\frac{W_2^2(\nu_0, \nu_1)}{2}.$$

The converse is also true: if the unique minimizer μ realizes the lower bound, i.e. $\mathcal{F}_t(\nu_0, \nu_1; \mu) = -W_2^2(\nu_0, \nu_1)/2$, then the geodesic ν is well-defined and $\mu = \nu(t)$. In fact, equation (2.2) holds in this case with an equality instead of an inequality, which implies that ν_1 belongs to a globally minimizing geodesic connecting ν_0 and μ .

2.2. Dual formulation. Let us recall the classical dual Kantorovich formulation of the L^2 -optimal transport problem: for any $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ and $s > 0$

$$(2.5) \quad \frac{W_2^2(\mu, \nu)}{2s} = \sup \left\{ \int \phi \, d\mu + \int \phi_s^c \, d\nu \right\},$$

where the supremum is taken over any continuous bounded function $\phi \in C_b(\mathbb{R}^d)$ and $\phi_s^c \in C_b(\mathbb{R}^d)$ denotes the c -transform of ϕ associated with the l^2 cost rescaled by the factor $2s$, i.e.

$$\phi_s^c(y) := \inf_x \frac{|x - y|^2}{2s} - \phi(x).$$

We will denote the c -transform with respect to the cost $c(x, y) = |x - y|^2/2$ by $\phi^c := \phi_1^c$. In the following we will also use an alternative form of the dual formulation (2.5) written in terms of the Brenier potential. More precisely

$$(2.6) \quad \frac{W_2^2(\mu, \nu)}{2} = - \inf \left\{ \int u \, d\mu + \int u^* \, d\nu \right\} + \int \frac{|x|^2}{2} \, d\mu(x) + \int \frac{|x|^2}{2} \, d\nu(x)$$

where the infimum is computed over all convex functions $u : \mathbb{R}^d \rightarrow \mathbb{R}$ (or equivalently over all lower semi-continuous convex function $u : \mathbb{R}^d \rightarrow (-\infty, \infty]$). Note that this formulation can be obtained from (2.5) via the change of variable $u = |\cdot|^2/2 - \phi$. The problem on the right-hand side of (2.6) always admits a lower semi-continuous solution (which is not necessarily continuous). We refer to any such solution as an optimal Brenier potential for the transport from μ to ν .

By the dual formulation in equation (2.5), we have

$$(2.7) \quad \begin{aligned} (\mathcal{P}) &= \inf_{\mu, \varphi} \sup_{\psi} \left\{ \int (\psi - \varphi) \, d\mu + \int \psi_{t-1}^c \, d\nu_1 - \int \varphi_t^c \, d\nu_0 \right\} \\ &\geq \inf_{\varphi} \left\{ \int \varphi_{t-1}^c \, d\nu_1 - \int \varphi_t^c \, d\nu_0 \right\}, \end{aligned}$$

where the first equality is obtained by using the dual formulation for both Wasserstein distances, whereas the inequality follows by selecting $\psi = \varphi$ in the sup over ψ . Now, let us observe that

$$(2.8) \quad \begin{aligned} -[\varphi_t^c]^c(x) &= - \inf_y \left\{ \frac{|x - y|^2}{2} - \inf_z \left\{ \frac{|y - z|^2}{2t} - \varphi(z) \right\} \right\} \\ &\leq \inf_z \sup_y \left\{ -\frac{|x - y|^2}{2} + \frac{|y - z|^2}{2t} - \varphi(z) \right\} = \varphi_{t-1}^c(x) \end{aligned}$$

and therefore we have

$$(\mathcal{P}) \geq - \sup \left\{ \int \phi^c \, d\nu_1 + \int \phi \, d\nu_0 \right\},$$

where now $\phi \in C_b(\mathbb{R}^d)$, and with the constraint that there must exist a function $\varphi \in C_b(\mathbb{R}^d)$ such that

$$(2.9) \quad \phi(x) = \varphi_t^c(x) = \inf_y \left\{ \frac{|x - y|^2}{2t} - \varphi(y) \right\}.$$

Note that without this last constraint, we have precisely the dual formulation of the L^2 -optimal transport problem from ν_0 to ν_1 in equation (2.5), with $s = 1$. Making the change of variable $u = |\cdot|^2/2 - \phi$, which would correspond to the Brenier potential from ν_0 to ν_1 , the constraint (2.9) implies the existence of a function $\xi \in C(\mathbb{R}^d)$ given by $\xi = |\cdot|^2/2 - t\varphi$ such that

$$u(x) = \frac{t-1}{t} \frac{|x|^2}{2} + \frac{\xi^*(x)}{t},$$

where ξ^* is the convex function given by the Legendre transform of ξ . Hence, if we consider the following problem

$$(\mathcal{P}^*) \quad \inf \left\{ \int u^* d\nu_1 + \int u d\nu_0 : u - \frac{t-1}{t} \frac{|\cdot|^2}{2} \text{ is convex and l.s.c.} \right\},$$

where again u^* is the Legendre transform of u , we obtain

$$(2.10) \quad (\mathcal{P}) \geq (\mathcal{P}^*) - \int \frac{|x|^2}{2} d\nu_0(x) - \int \frac{|x|^2}{2} d\nu_1(x).$$

Problem (\mathcal{P}^*) is a convex optimization problem. It appeared already in [17], up to slight variations, as the dual of a barycentric optimal transport problem. For completeness, we provide a proof of existence of minimizers, which follows essentially the same lines as the one used in [27] to show existence of minimizers for the W_2 projection on measures obtained via push-forward by smooth and strongly convex Brenier potentials. The key property we will use is the fact that a lower semi-continuous proper convex function $u : \mathbb{R}^d \rightarrow (-\infty, \infty]$ is $1/L$ -strongly convex if and only if ∇u^* is L -Lipschitz; see, e.g., Theorem 18.15 in [3].

Lemma 2.3. *There exists a lower semi-continuous strongly convex function u solving (\mathcal{P}^*) .*

Proof. Since $u^{**} = u$, setting $v = u^*$ we obtain the equivalent problem

$$(2.11) \quad \inf \left\{ \int v d\nu_1 + \int v^* d\nu_0 : v \in C^1(\mathbb{R}^d) \text{ is convex, } \nabla v \text{ is } L\text{-Lipschitz} \right\},$$

where $L = t/(t-1)$. Note that for any admissible v , the functional minimized in (2.11) cannot take the value $-\infty$. In fact, on one hand v^* is bounded from below being strongly convex, and on the other $v(y) \geq \langle y, x_0 \rangle - v^*(x_0)$ for some $x_0 \in \mathbb{R}^d$ for which $v^*(x_0)$ is finite and ν_0 has finite first moment. We prove the existence of a minimizer for problem (2.11). Let $(v_n)_n$ be a minimizing sequence. We start by showing that up to a subsequence extraction this converges pointwise to a function \bar{v} which is admissible for problem (2.11). Since the problem is independent of the addition of a constant to v , without loss of generality we can assume $v_n(0) = 0$. Let $y_n = \nabla v_n(0)$, for any $p_n \in \partial v^*(y_n)$, the sub-differential of v^* at y_n , and for all $y \in \mathbb{R}^d$, we have

$$(2.12) \quad v_n^*(y) \geq v_n^*(y_n) + \langle p_n, y - y_n \rangle + \frac{1}{2L} |y - y_n|^2$$

and we can pick $p_n = 0$ since $y_n = \nabla v_n(0)$. Therefore we obtain, by Jensen's inequality,

$$\begin{aligned} \int v_n d\nu_1 + \int v_n^* d\nu_0 &\geq v_n(\text{bary}(\nu_1)) + v_n^*(y_n) + \frac{1}{2L} \int |y - y_n|^2 d\nu_0 \\ &\geq \langle \text{bary}(\nu_1), y_n \rangle + \frac{1}{2L} \int |y - y_n|^2 d\nu_0, \end{aligned}$$

where the second inequality is due to Fenchel–Young inequality, and where

$$\text{bary}(\nu_1) := \int x d\nu_1(x).$$

This implies that $y_n = \nabla v_n(0)$ is uniformly bounded, moreover for all $x \in \mathbb{R}^d$

$$|\nabla v_n(x)| \leq |\nabla v_n(x) - \nabla v_n(0)| + |\nabla v_n(0)| \leq L|x| + |\nabla v_n(0)|.$$

Therefore, by the Arzelà-Ascoli theorem $(\nabla v_n)_n$ converges uniformly on compact subsets (up to a subsequence extraction) to a function g which is L -Lipschitz. Since $v_n(0) = 0$, one can show that v_n converges pointwise (again, up to a subsequence extraction) to a convex function \bar{v} such that $\bar{v}(0) = 0$ and that $g = \nabla \bar{v}$. Indeed, we have that for all $n, m \geq 0$,

$$|v_n(x) - v_m(x)| = \left| \int_0^1 \langle \nabla v_n(sx) - \nabla v_m(sx), x \rangle ds \right| \leq |x| \int_0^1 |\nabla v_n(sx) - \nabla v_m(sx)| ds$$

and so the uniform convergence of ∇v_n on compact sets implies that $(v_n(x))_n$ is Cauchy for all $x \in \mathbb{R}^d$. Furthermore, since $\bar{v}(0) = 0$, for all $x, y \in \mathbb{R}^d$

$$\begin{aligned} (2.13) \quad v_n(x) - v_n(y) &= \int_0^1 \langle \nabla v_n(sy + (1-s)x), x - y \rangle ds \\ &\implies \bar{v}(y) - \bar{v}(x) = \int_0^1 \langle g(sy + (1-s)x), y - x \rangle ds, \end{aligned}$$

which in turn implies that \bar{v} is differentiable and $g = \nabla \bar{v}$.

Now, observe that by the definition of Legendre transform and the fact that $v_n(0) = 0$, we have $v_n^* \geq 0$. Therefore by Fatou's lemma,

$$\liminf_{n \rightarrow \infty} \int v_n^* d\nu_0 \geq \int \liminf_{n \rightarrow \infty} v_n^* d\nu_0 \geq \int \bar{v}^* d\nu_0.$$

On the other hand $v_n(x) - \langle y_n, x \rangle \geq 0$ for all $x \in \mathbb{R}^d$. Applying again Fatou's lemma with respect to the sequence of functions $x \mapsto v_n(x) - \langle y_n, x \rangle$, and using the fact that y_n converges to $\nabla \bar{v}(0)$, we obtain

$$\liminf_{n \rightarrow \infty} \int v_n d\nu_1 \geq \int \bar{v} d\nu_1.$$

Therefore \bar{v} solves (2.11) and \bar{v}^* solves (\mathcal{P}^*) . \square

Additionally, we have the following characterization of the minimizers, which will be useful to establish the strong duality between (\mathcal{P}) and (\mathcal{P}^*) . This is also contained in [17], but we include a sketch of the proof here for completeness. Before stating the

result, we remark that for any strongly convex function u , ∇u^* is Lipschitz continuous so $(\nabla u^*)_{\#}\nu_1$ is well-defined also when ν_1 is not absolutely continuous.

Lemma 2.4. *Define $\eta := (\nabla u^*)_{\#}\nu_1 - \nu_0$. Then, a $(t-1)/t$ -convex lower semi-continuous function u solves (\mathcal{P}^*) if and only if*

$$(2.14) \quad \int \left(u(x) - \frac{t-1}{t} \frac{|x|^2}{2} \right) d\eta(x) = 0 \quad \text{and} \quad \int \varphi(x) d\eta(x) \leq 0$$

for all lower semi-continuous convex functions $\varphi : \mathbb{R}^d \rightarrow (-\infty, \infty]$.

Proof. Equation (2.14) is equivalent to the optimality conditions of problem (\mathcal{P}^*) . In fact, if u is a lower semi-continuous function solving (\mathcal{P}^*) , given any lower semi-continuous function φ such that $u + \varphi$ is $(t-1)/t$ -convex, then $u + \varepsilon\varphi$ is $(t-1)/t$ -convex and lower semi-continuous for all $0 < \varepsilon \leq 1$ and it is therefore an admissible competitor for problem (\mathcal{P}^*) . Hence we find that

$$\int (u + \varepsilon\varphi)^* d\nu_1 + \int (u + \varepsilon\varphi) d\nu_0 \geq \int u^* d\nu_1 + \int u d\nu_0,$$

or equivalently

$$\int \frac{(u + \varepsilon\varphi)^* - u^*}{\varepsilon} d\nu_1 \geq - \int \varphi d\nu_0.$$

By Lemma 6.1 in [17], generalizing a result of Gangbo [16], if there exist $a, b \geq 0$ such that $\varphi(x) \geq -a|x| - b$ for all $x \in \mathbb{R}^d$ and φ is continuous, then the integrand on the left-hand side tends pointwise to $-\varphi \circ \nabla u^*$ as $\varepsilon \rightarrow 0^+$. Therefore for such functions φ , by Fatou's lemma,

$$\int \varphi d(\nabla u^*)_{\#}\nu_1 \leq \int \varphi d\nu_0.$$

In particular, the inequality holds for any lower semi-continuous convex function φ , since these may be approximated by Lipschitz functions, e.g., by setting $\varphi^n(x) = \inf_y \varphi(y) + n|x - y|$. Moreover, formally, taking $\varphi = \pm(u - |\cdot|^2(t-1)/(2t))$ we get the first condition in (2.14). Note however that even if $\varphi = -(u - |\cdot|^2(t-1)/(2t))$ is such that $u + \varphi$ is convex, it may itself be neither convex nor continuous so one needs an additional regularization argument to conclude the proof; see point (b) in the proof of Theorem 1.2 in [17].

On the other hand, given a lower semi-continuous $(t-1)/t$ -convex function u that satisfies (2.14), for any lower semi-continuous $(t-1)/t$ -convex function \tilde{u} ,

$$\int (\tilde{u} - u) d\eta = \int \left(\tilde{u}(x) - \frac{t-1}{t} \frac{|x|^2}{2} \right) d\eta(x) - \int \left(u(x) - \frac{t-1}{t} \frac{|x|^2}{2} \right) d\eta(x) \leq 0.$$

This implies that

$$\begin{aligned} \int u d\nu_0 + \int u^* d\nu_1 &= \int u d(\nabla u^*)_{\#}\nu_1 + \int u^* d\nu_1 - \int u d\eta \\ &\leq \int \tilde{u} d(\nabla u^*)_{\#}\nu_1 + \int \tilde{u}^* d\nu_1 - \int \tilde{u} d\eta \\ &= \int \tilde{u}^* d\nu_1 + \int \tilde{u} d\nu_0, \end{aligned}$$

where we also used the fact that u is an optimal Brenier potential for the transport from $\nabla u^*_{\#}\nu_1$ to ν_1 . \square

The following theorem establishes that strong duality holds between problems (\mathcal{P}) and (\mathcal{P}^*) .

Theorem 2.5. *We have*

$$(2.15) \quad (\mathcal{P}) = (\mathcal{P}^*) - \int \frac{|x|^2}{2} d\nu_0(x) - \int \frac{|x|^2}{2} d\nu_1(x).$$

Moreover,

(1) μ solves (\mathcal{P}) if and only if $\mu = T(t)_{\#}\nu_1$, where

$$T(t) := \nabla u^* + t(\text{Id} - \nabla u^*)$$

and u solves (\mathcal{P}^*) ;

(2) conversely, u solves (\mathcal{P}^*) if and only if $-(t-1)u^* + t|\cdot|^2/2$ and $tu - (t-1)|\cdot|^2/2$ are optimal Brenier potentials from ν_1 to μ and from ν_0 to μ , respectively, and μ solves (\mathcal{P}) .

Proof. Let u solve (\mathcal{P}^*) . By the optimality conditions in Lemma 2.4, and specifically the equality in (2.14), we have

$$(2.16) \quad \begin{aligned} (\mathcal{P}^*) &= \int (u(\nabla u^*(x)) + u^*(x)) d\nu_1(x) - \frac{t-1}{2t} \int |x|^2 d\eta(x) \\ &= \int \left(\langle \nabla u^*(x), x \rangle - \frac{t-1}{2t} |\nabla u^*(x)|^2 \right) d\nu_1(x) + \frac{t-1}{2t} \int |x|^2 d\nu_0(x). \end{aligned}$$

Define

$$\mu := (\nabla u^* + t(\text{Id} - \nabla u^*))_{\#}\nu_1 \quad \text{and} \quad \bar{\nu}_0 := (\nabla u^*)_{\#}\nu_1.$$

By the optimality conditions for u , and denoting $w := tu - (t-1)|\cdot|^2/2$ (which is convex due to the strong convexity of u), we deduce that

$$(2.17) \quad \begin{aligned} -\frac{W_2^2(\mu, \nu_0)}{2t} &= \frac{1}{t} \inf_{v \text{ convex}} \left\{ \int v d\nu_0 + \int v^* d\mu \right\} - \int \frac{|x|^2}{2t} d\nu_0(x) - \int \frac{|x|^2}{2t} d\mu(x) \\ &\leq \frac{1}{t} \left[\int w d\bar{\nu}_0 + \int w^* d\mu \right] - \int \frac{|x|^2}{2t} d\nu_0(x) - \int \frac{|x|^2}{2t} d\mu(x) \\ &= \frac{1}{t} \int [w(\nabla u^*(x)) + w^*(\nabla u^*(x) + t(x - \nabla u^*(x)))] d\nu_1(x) \\ &\quad - \int \frac{|x|^2}{2t} d\nu_0(x) - \int \frac{|x|^2}{2t} d\mu(x), \end{aligned}$$

where for the first equality we used the dual formulation in (2.6). Since $x \in \partial u(\nabla u^*(x))$, the subdifferential of u at $\nabla u^*(x)$, and given that w is convex, we have that $\nabla u^*(x) +$

$t(x - \nabla u^*(x)) \in \partial w(\nabla u^*(x))$, the subdifferential of w at $\nabla u^*(x)$. Therefore, we obtain

$$(2.18) \quad -\frac{W_2^2(\mu, \nu_0)}{2t} \leq \frac{1}{t} \int \langle \nabla u^*(x), \nabla u^*(x) + t(x - \nabla u^*(x)) \rangle d\nu_1(x) \\ - \int \frac{|x|^2}{2t} d\nu_0(x) - \int \frac{|\nabla u^*(x) + t(x - \nabla u^*(x))|^2}{2t} d\nu_1(x).$$

Consider now the coupling:

$$\gamma := (\text{Id}, \nabla u^* + t(\text{Id} - \nabla u^*))_{\#} \nu_1 \in \Gamma(\nu_1, \mu).$$

Since γ is an admissible coupling for the transport from ν_1 to μ ,

$$(2.19) \quad (\mathcal{P}) \leq \int \frac{|x - x_1|^2}{2(t-1)} d\gamma(x_1, x) - \frac{W_2^2(\mu, \nu_0)}{2t} \\ \leq - \int \frac{|tx - (t-1)\nabla u^*(x)|^2}{2t(t-1)} d\nu_1(x) + \int \frac{|x|^2}{2(t-1)} d\nu_1(x) - \int \frac{|x|^2}{2t} d\nu_0(x),$$

where the second inequality can be obtained by using (2.18) and the definition of γ , and rearranging terms. Developing the square and comparing the result with equation (2.16) we get

$$(\mathcal{P}) \leq (\mathcal{P}^*) - \int \frac{|x|^2}{2} d\nu_0(x) - \int \frac{|x|^2}{2} d\nu_1(x).$$

Recalling (2.10), this implies the equality.

The reasoning above implies a posteriori that given u optimal for (\mathcal{P}^*) , $\mu = (\nabla u^* + t(\text{Id} - \nabla u^*))_{\#} \nu_1$ is necessarily the unique minimizer of problem (\mathcal{P}) . This implies point (1) in the theorem.

For the only if part of point (2), in view of (2.15) and the inequalities (2.18) and (2.19), we just need to check that $(1-t)u^* + t|\cdot|^2/2$ is convex if u is $(t-1)/t$ -strongly convex. Observe that if ∇u^* is $t/(t-1)$ -Lipschitz, for all $x, y \in \mathbb{R}^d$,

$$(2.20) \quad u^*(y) \leq u^*(x) + \langle \nabla u^*(x), y - x \rangle + \frac{t}{t-1} \frac{|y-x|^2}{2}.$$

Then, since $t > 1$, this is equivalent to

$$(1-t)u^*(y) + t \frac{|y|^2}{2} \geq (1-t)u^*(x) + (1-t)\langle \nabla u^*(x), y - x \rangle - t \frac{|y-x|^2}{2} + t \frac{|y|^2}{2} \\ = (1-t)u^*(x) + t \frac{|x|^2}{2} + \langle (1-t)\nabla u^*(x) + tx, y - x \rangle,$$

which in turn is equivalent to the convexity of $(1-t)u^* + t|\cdot|^2/2$.

Finally, to show the if part in point (2) of the theorem we follow the same steps to show (2.10). Specifically, let μ solve (\mathcal{P}) and $tu + (1-t)|\cdot|^2/2$ be an optimal Brenier potential from ν_0 to μ . Then u is admissible for problem (\mathcal{P}^*) . Moreover, proceeding as in equation (2.7),

$$(2.21) \quad (\mathcal{P}) \geq \int \varphi_{t-1}^c d\nu_1 - \int \varphi_t^c d\nu_0,$$

where φ is an optimal Kantorovich potential for the transport from μ to ν_0 (i.e., an optimal potential for the dual formulation in equation (2.5) with $s = t$). By direct calculation, $\varphi_t^c = -u + |\cdot|^2/2$ and $\varphi_{t-1}^c \geq -[\varphi_t^c]^c = u^* - |\cdot|^2/2$, by equation (2.8). Reinserting this in (2.21) and using the equality (2.15), we deduce that u solves (\mathcal{P}^*) . \square

From the proof of Theorem 2.5, one can also deduce that given u solving (\mathcal{P}^*) then $tu + (1-t)|\cdot|^2/2$ is an optimal Brenier potential for the transport not only from ν_0 to μ but also from $\bar{\nu}_0$ to μ . In particular, if ν_0 and $\bar{\nu}_0$ are absolutely continuous, one has that the solution μ to (\mathcal{P}) verifies

$$\mu = (t\nabla u + (1-t)\text{Id})_{\#}\bar{\nu}_0 = (t\nabla u + (1-t)\text{Id})_{\#}\nu_0.$$

Theorem 2.5 confirms the observation in Remark 2.2. In particular, the optimal Brenier potential u from ν_0 to ν_1 is $(t-1)/t$ -convex if and only if there exists a length-minimizing geodesic $s \in [0, t] \mapsto \nu(s) \in \mathcal{P}_2(\mathbb{R}^d)$ such that $\nu(0) = \nu_0$ and $\nu(1) = \nu_1$. In this case u solves (\mathcal{P}^*) , and the solution to (\mathcal{P}) is $\nu(t)$. If on the contrary the optimal Brenier potential from ν_0 to ν_1 is not sufficiently convex, problem (\mathcal{P}^*) still selects a potential u which is sufficiently convex to trace a geodesic connecting ν_0 at time 0 to the extrapolation μ at time t . However, by the optimality conditions (2.14), ∇u^* pushes ν_1 to $\bar{\nu}_0 \preceq_C \nu_0$: the mass at the initial time is reorganized to guarantee the existence of a length-minimising geodesic up to time t passing through ν_1 at time 1.

Remark 2.6 (Toland's duality). *The strong duality established in Theorem 2.5 can be partly seen as an instance of Toland's duality [31, 32], just as for the case studied in [9]. Given two convex, proper and lower semi-continuous functions $F, G : V \rightarrow (\infty, \infty]$, where V is a normed vector space, Toland's duality yields the equivalence*

$$\inf_{x \in V} \{F(x) - G(x)\} = \inf_{p \in V^*} \{G^*(p) - F^*(p)\}$$

where V^* is the topological dual of V and F^* and G^* are the Legendre transforms of F and G respectively. In our case, F and G are replaced by the maps

$$\mu \in \mathcal{P}_2(\mathbb{R}^d) \mapsto \frac{W_2^2(\mu, \nu_1)}{2(t-1)} \quad \text{and} \quad \mu \in \mathcal{P}_2(\mathbb{R}^d) \mapsto \frac{W_2^2(\mu, \nu_0)}{2t},$$

respectively, whereas F^* and G^* are replaced by

$$\varphi \in C_b(\mathbb{R}^d) \mapsto - \int \varphi_{t-1}^c d\nu_1 \quad \text{and} \quad \varphi \in C_b(\mathbb{R}^d) \mapsto - \int \varphi_t^c d\nu_0,$$

respectively. Then, at least formally, the Toland dual is the problem appearing on the right-hand side in (2.7). Note, however, that this is not a convex problem and one needs a further change of variable to recover (\mathcal{P}^*) .

3. BARYCENTRIC OPTIMAL TRANSPORT FORMULATION

In this section we provide yet another equivalent formulation of problem (\mathcal{P}) , which turns out to coincide to a specific type of barycentric optimal transport given by

$$(\mathcal{B}) \quad \inf_{\pi \in \Gamma(\nu_0, \nu_1)} \int |tx_1 - (t-1)\text{bary}(\pi_{x_1})|^2 d\nu_1(x_1),$$

where

$$\text{bary}(\pi_{x_1}) := \int x_0 \, d\pi_{x_1}(x_0).$$

This is a specific instance of a weak optimal transport problem as studied in [18, 17]. This equivalence is not surprising given that the dual formulation (\mathcal{P}^*) coincides up to minor modifications to that derived for the barycentric optimal transport problem in [18]. We give here a direct proof of the equivalence between (\mathcal{P}) and (\mathcal{B}): this can also be seen as an alternative way to prove the dual formulation (\mathcal{P}^*) for problem (\mathcal{B}) via Toland's duality. As a byproduct, it also yields the same type of characterization for the minimizers of problem (\mathcal{B}) as the one proved in [17] for a slight variant of our problem.

Our main tool will be Strassen's theorem [30]. Before stating it, let us recall that given $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$ and a coupling $\theta \in \Gamma(\mu, \nu)$, we can always represent θ in the following disintegrated form (with respect to the projection on the first marginal):

$$d\theta(x, y) = d\theta_x(y) d\mu(x)$$

where we can interpret θ_x as a probability measure on \mathbb{R}^d for all x (which is uniquely defined μ -a.e.). We will use a similar notation for couplings with multiple marginals. Furthermore, we say that $\mu, \nu \in \mathcal{P}_1(\mathbb{R}^d)$ are in the convex order $\mu \preceq_C \nu$ if and only if

$$\int \varphi d\mu \leq \int \varphi d\nu$$

for all (continuous) convex functions $\varphi : \mathbb{R}^d \rightarrow \mathbb{R}$.

Lemma 3.1 (Strassen's theorem). *Let $\mu, \nu \in \mathcal{P}_1(\mathbb{R}^d)$ then $\mu \preceq_C \nu$ if and only if there exists a coupling $\theta \in \Gamma(\mu, \nu)$ such that $d\theta(x, y) = d\theta_x(y) d\mu(x)$ and*

$$(3.1) \quad \int y d\theta_x(y) = x \quad \text{for } \mu\text{-a.e. } x \in \mathbb{R}^d.$$

Remark 3.2. *In probabilistic terms, the condition on θ in equation (3.1) is equivalent to the existence of a martingale (X, Y) , where X and Y are random variables with laws μ and ν , respectively. Then, θ is the law of the martingale (X, Y) .*

Let us go back to showing the equivalence of problems (\mathcal{P}) and (\mathcal{B}). We start by rewriting problem (\mathcal{P}) as follows, using the definition of the Wasserstein distance in (1.4),

$$(3.2) \quad \begin{aligned} (\mathcal{P}) &= \inf_{\mu} \left[\inf_{\gamma_1 \in \Gamma(\nu_1, \mu)} \int \frac{|x_1 - x|^2}{2(t-1)} d\gamma_1(x_1, x) - \inf_{\gamma_0 \in \Gamma(\nu_0, \mu)} \int \frac{|x_0 - x|^2}{2t} d\gamma_0(x_0, x) \right] \\ &= \inf_{\mu} \left[\inf_{\gamma_1 \in \Gamma(\nu_1, \mu)} \int \frac{|x_1 - x|^2}{2(t-1)} d\gamma_1(x_1, x) - \inf_{\eta \in \Gamma(\nu_0, \nu_1, \mu)} \int \frac{|x_0 - x|^2}{2t} d\eta(x_0, x_1, x) \right]. \end{aligned}$$

Given a $\pi \in \Gamma(\nu_0, \nu_1)$, which can be disintegrated as follows

$$d\pi(x_0, x_1) = d\pi_{x_1}(x_0) d\nu_1(x_1),$$

one can construct a coupling η by setting

$$d\eta(x_0, x_1, x) = d\pi_{x_1}(x_0) d\gamma_1(x_1, x).$$

It is easy to check that $\eta \in \Gamma(\nu_0, \nu_1, \mu)$. If we restrict η in (3.2) to belong to this specific class of couplings we get the following lower bound:

$$\begin{aligned} (\mathcal{P}) &\geq \inf_{\mu} \inf_{\gamma_1 \in \Gamma(\nu_1, \mu)} \sup_{\pi \in \Gamma(\nu_0, \nu_1)} \left[\int \frac{|x_1 - x|^2}{2(t-1)} d\gamma_1(x_1, x) - \int \int \frac{|x_0 - x|^2}{2t} d\pi_{x_1}(x_0) d\gamma_1(x_1, x) \right] \\ &\geq \sup_{\pi \in \Gamma(\nu_0, \nu_1)} \inf_{\gamma_1 \in \Gamma(\nu_1, \mu)} \left[\int \frac{|x_1 - x|^2}{2(t-1)} d\gamma_1(x_1, x) - \int \int \frac{|x_0 - x|^2}{2t} d\pi_{x_1}(x_0) d\gamma_1(x_1, x) \right] \end{aligned}$$

where the second inequality is due to the exchange of inf and sup. We can obtain a further lower bound by minimising the whole integrand with respect to x , i.e.

$$\begin{aligned} (\mathcal{P}) &\geq \sup_{\pi \in \Gamma(\nu_0, \nu_1)} \inf_{\gamma_1 \in \Gamma(\nu_1, \mu)} \int \inf_x \left[\frac{|x_1 - x|^2}{2(t-1)} - \int \frac{|x_0 - x|^2}{2t} d\pi_{x_1}(x_0) \right] d\gamma_1(x_1, x) \\ &= \sup_{\pi \in \Gamma(\nu_0, \nu_1)} \int \inf_x \left[\frac{|x_1 - x|^2}{2(t-1)} - \int \frac{|x_0 - x|^2}{2t} d\pi_{x_1}(x_0) \right] d\nu_1(x_1). \end{aligned}$$

Expanding the squares and using the fact that $\pi \in \Gamma(\nu_0, \nu_1)$ we obtain

$$\begin{aligned} (\mathcal{P}) &\geq -\frac{1}{2t(t-1)} \inf_{\pi \in \Gamma(\nu_0, \nu_1)} \int |tx_1 - (t-1)\text{bary}(\pi_{x_1})|^2 d\nu_1(x_1) \\ &\quad + \frac{1}{2(t-1)} \int |x|^2 d\nu_1(x) - \frac{1}{2t} \int |x|^2 d\nu_0(x). \end{aligned}$$

Hence we have

$$(\mathcal{P}) \geq -\frac{1}{2t(t-1)} (\mathcal{B}) + \frac{1}{2(t-1)} \int |x|^2 d\nu_1(x) - \frac{1}{2t} \int |x|^2 d\nu_0(x).$$

The fact that the inequality we obtained between (\mathcal{P}) and (\mathcal{B}) is in fact an equality is a direct consequence of Strassen's theorem. Specifically, if u solves (\mathcal{P}^*) , then by Lemma 2.4, we have that $\bar{\nu}_0 := \nabla u_{\#}^* \nu_1 \preceq_C \nu_0$, and therefore by Strassen's theorem, there exists a coupling $\theta \in \Gamma(\bar{\nu}_0, \nu_0)$ with $d\theta(x, y) = d\theta_x(y) d\bar{\nu}_0(x)$ and

$$(3.3) \quad \int y d\theta_x(y) = x, \quad \text{for } \bar{\nu}_0\text{-a.e. } x \in \mathbb{R}^d.$$

This can be used to show the following result:

Theorem 3.3. *The following equality holds:*

$$(3.4) \quad (\mathcal{P}) = -\frac{1}{2t(t-1)} (\mathcal{B}) + \frac{1}{2(t-1)} \int |x|^2 d\nu_1(x) - \frac{1}{2t} \int |x|^2 d\nu_0(x)$$

Moreover,

(1) π solves (\mathcal{B}) if and only if

$$(3.5) \quad \nabla u^*(x_1) = \text{bary}(\pi_{x_1}), \quad \text{for } \nu_1\text{-a.e. } x \in \mathbb{R}^d,$$

and u solves (\mathcal{P}^*) ;

(2) conversely, u solves (\mathcal{P}^*) if and only if (3.5) holds and π solves (\mathcal{B}) ;

Proof. Let u solve (\mathcal{P}^*) . Reasoning as in the the proof of Theorem 2.5 we get the bound in equation (2.19), i.e.

$$(\mathcal{P}) \leq - \int \frac{|tx - (t-1)\nabla u^*(x)|^2}{2t(t-1)} d\nu_1(x) + \frac{1}{2(t-1)} \int |x|^2 d\nu_1(x) - \frac{1}{2t} \int |x|^2 d\nu_0(x).$$

By Strassen's theorem, there exists a coupling $\theta \in \Gamma(\bar{\nu}_0, \nu_0)$ verifying (3.3). Therefore, we can define a coupling $\pi \in \Gamma(\nu_0, \nu_1)$ as follows

$$(3.6) \quad d\pi(x_0, x_1) = d\theta_{\nabla u^*(x_1)}(x_0) d\nu_1(x_1)$$

which is equivalent to (3.5). Then the inequality (2.19) is equivalent to

$$(\mathcal{P}) \leq - \frac{1}{2t(t-1)} \int \left| tx_1 - (t-1) \int x_0 d\pi_{x_1}(x_0) \right|^2 d\nu_1(x_1) + \frac{1}{2(t-1)} \int |x|^2 d\nu_1(x) - \frac{1}{2t} \int |x|^2 d\nu_0(x).$$

This shows that π is optimal for (\mathcal{B}) and directly implies equation (3.4).

In order to conclude the proof, we just need to observe that the function minimized in problem (\mathcal{B}) is strongly convex when viewed as a function of $\text{bary}(\pi_{x_1})$. This means that any minimizer of problem (\mathcal{B}) must satisfy (3.5) with u solving (\mathcal{P}^*) . \square

Remark 3.4 (Generalizations). *It is natural to ask to what extent the study presented in this and the previous sections applies to other variants of problem (\mathcal{P}) . The most natural scenarios are the case where the l^2 cost is replaced by a general cost function, and the case with multiple measures. For the first one, when using a general cost one needs to at least require convexity along generalized geodesics, which is guaranteed upon some conditions on the cost, and namely the so-called non-negative cross curvature condition [20, 14]. The case with multiple measures would consist in considering the problem:*

$$\inf_{\mu} \left\{ \sum_{i=1}^{K^+} \lambda_i^+ W_2^2(\mu, \nu_i^+) - \sum_{j=1}^{K^-} \lambda_j^- W_2^2(\mu, \nu_j^-) \right\},$$

where $K^-, K^+ \geq 1$, $\nu_i^+, \nu_j^- \in \mathcal{P}_2(\mathbb{R}^d)$ and $\lambda_i^+, \lambda_j^- > 0$ for all i, j , $\sum_i \lambda_i^+ > \sum_j \lambda_j^-$. In the particular case where $K^+ = 1$, the functional is still strongly convex along generalized geodesics based at ν_1^+ , and we expect that one can derive an equivalent version of problem (\mathcal{P}^*) and (\mathcal{B}) . In the general case, however, the picture is much less clear, and although one can still apply Toland duality, it is not trivial to check that the resulting problem is convex in appropriate variables and to derive an associated weak optimal transport problem. We reserve to study these issues in future works.

4. RELATION WITH THE H^1 PROJECTION ON CONVEX FUNCTIONS

In this section we show that problem (\mathcal{P}) is strongly linked to the problem of computing the \dot{H}^1 projection of an appropriate potential on the set of convex functions. This also allows us to further justify the interpretation of problem (\mathcal{P}) as a notion of geodesic extrapolation.

4.1. One-dimensional setting. Let us consider the specific case where $d = 1$. Given $\mu \in \mathcal{P}_2(\mathbb{R})$, let us denote by $F_\mu : \mathbb{R} \rightarrow [0, 1]$ the right-continuous non-decreasing function given by the cumulative distribution of μ , i.e. $F_\mu(x) := \mu((-\infty, x])$, and denote by $F_\mu^{[-1]} : [0, 1] \rightarrow \overline{\mathbb{R}}$ its (left-continuous) pseudo-inverse defined by

$$F_\mu^{[-1]}(a) = \inf\{x \in \mathbb{R} : F_\mu(x) \geq a\}$$

with the usual convention $\inf \emptyset = +\infty$, which is also known as the quantile function associated with μ .

The optimal transport plan between two measures in $\mathcal{P}_2(\mathbb{R})$ for the l^2 cost is given by the monotone rearrangement plan [29, Theorem 2.9]. As a consequence we can reformulate the minimization problem (\mathcal{P}) as follows

$$\inf \left\{ \frac{1}{2(t-1)} \int_0^1 |F_\mu^{[-1]}(x) - F_{\nu_1}^{[-1]}(x)|^2 dx - \frac{1}{2t} \int_0^1 |F_\mu^{[-1]}(x) - F_{\nu_0}^{[-1]}(x)|^2 dx \right\},$$

where the infimum is taken over any quantile function $F_\mu^{[-1]}$. Rearranging the squares, the minimizers of this problem are the solutions to

$$(4.1) \quad \inf \int_0^1 |F_\mu^{[-1]}(x) - (tF_{\nu_1}^{[-1]}(x) - (t-1)F_{\nu_0}^{[-1]}(x))|^2 dx.$$

Suppose that ν_0 is absolutely continuous, then the optimal transport map from ν_0 to ν_1 is $T_0 := F_{\nu_1}^{[-1]} \circ F_{\nu_0}$ and the problem above is equivalent to

$$(4.2) \quad \inf_T \int_0^1 |T - (tT_0(x) - (t-1)x)|^2 d\nu_0(x),$$

where $T \in L^2_{\nu_0}(\mathbb{R})$ is required to be non-decreasing, and given a minimizer T we can retrieve the minimizer μ of the original problem by

$$\mu = T_{\#}\nu_0.$$

This is just the L^2 projection on the space of monotone functions of the map

$$x \mapsto x + t(T_0(x) - x).$$

Remark 4.1 (Equivalence with pressureless fluids). *Suppose still that ν_0 is absolutely continuous and let $T_0(x) = x + \partial_x \phi_0$, where $x \mapsto |x|^2/2 + \phi_0(x)$ is the Brenier potential for the transport from ν_0 and ν_1 . The solutions to the minimization problem (4.2) can be related to the particular solutions of the pressureless Euler system, $\mu : [0, \infty) \rightarrow \mathcal{P}_2(\mathbb{R})$, $v : [0, \infty) \rightarrow L^2(\mu(t); \mathbb{R})$, solving*

$$(4.3) \quad \begin{cases} \partial_t \mu + \partial_x(\mu v) = 0, \\ \partial_t(\mu v) + \partial_x(\mu v^2) = 0, \end{cases}$$

with initial conditions given by

$$\mu(0) = \nu_0, \quad v(0, \cdot) = \nabla \phi_0(\cdot),$$

and satisfying the sticky collision condition, which consists in requiring particles to share the same position after collision. Brenier and Grenier [7] constructed sticky solutions to problem (4.3) for which the evolution of μ is expressed explicitly by the curve

$$\mu(t) = \tilde{X}(t, \cdot) \# \nu_0,$$

with

$$(4.4) \quad \tilde{X}(t, x) := (\partial_x \text{co} \psi(t, \cdot)) \circ F_0(x), \quad \psi(t, s) := \int_0^s X(t, F_{\nu_0}^{[-1]}(s')) ds',$$

and $X(t, x) = x + t \nabla \phi_0(x)$. Note that as long as the geodesic can be extended $\psi(t, \cdot)$ stays convex (as it is the integral of a monotone function) and therefore $\tilde{X} = X$. It is easy to check that $\tilde{X}(t, \cdot)$ and $\mu(t)$ are precisely the solutions to (4.2) and (P), respectively.

4.2. A Γ -convergence result. In this section we elucidate the link between problem (P) and a generalization of the projection onto monotone maps (4.2) in the multi-dimensional setting. For the sake of clarity, from now on we focus on the case ν_0 absolutely continuous. Consider a function $\phi_0 : \mathbb{R}^d \rightarrow \mathbb{R}$ such that $x \mapsto |x|^2 + 2\bar{\varepsilon}\phi_0(x)$ is convex for some $\bar{\varepsilon} \geq 1$, and such that $\nabla \phi_0$ is L -Lipschitz. For $0 < \varepsilon \leq \bar{\varepsilon}$, we consider the functionals defined by

$$\mathcal{G}_\varepsilon(\mu) := \frac{t(t - \varepsilon)}{\varepsilon} \left[\frac{W_2^2(\mu, \nu_\varepsilon)}{t - \varepsilon} - \frac{W_2^2(\mu, \nu_0)}{t} \right]$$

where

$$\nu_\varepsilon := (\text{Id} + \varepsilon \nabla \phi_0) \# \nu_0.$$

We investigate here the limit $\varepsilon \rightarrow 0^+$ which, loosely speaking and up to multiplicative factors, corresponds to the case where ν_1 tends to ν_0 in (P) along the geodesic connecting the two.

Proposition 4.2. *The functionals \mathcal{G}_ε , as $\varepsilon \rightarrow 0^+$, Γ -converge on $(\mathcal{P}_2(\mathbb{R}^d), W_2)$ towards the functional $\mathcal{G} : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ defined by*

$$(4.5) \quad \mathcal{G}(\mu) := \int |\nabla u(x) - (x + t \nabla \phi_0(x))|^2 d\nu_0(x) - t^2 W_2^2(\nu_0, \nu_1)$$

where $u : \mathbb{R}^d \rightarrow \mathbb{R}$ is the unique convex function such that $(\nabla u) \# \nu_0 = \mu$.

Proof. First of all, we rewrite \mathcal{G}_ε as follows

$$\mathcal{G}_\varepsilon(\mu) = t \mathcal{H}_\varepsilon(\mu) + W_2^2(\mu, \nu_0), \quad \mathcal{H}_\varepsilon(\mu) := \frac{W_2^2(\mu, \nu_\varepsilon) - W_2^2(\mu, \nu_0)}{\varepsilon}.$$

We prove that \mathcal{H}_ε Γ -converge towards

$$(4.6) \quad \mathcal{H}(\mu) = -2 \int \langle \nabla u(x) - x, \nabla \phi_0(x) \rangle d\nu_0(x),$$

which implies the result directly. For this, observe that

$$\mathcal{H}_\varepsilon(\mu) \leq \frac{1}{\varepsilon} \left[\int |\nabla u - (x + \varepsilon \nabla \phi_0(x))|^2 d\nu_0 - \int |\nabla u - x|^2 d\nu_0 \right] = \mathcal{H}(\mu) + \varepsilon W_2^2(\nu_0, \nu_1)$$

where we used the fact that $(\nabla u, \text{Id} + \varepsilon \nabla \phi_0) \# \nu_0$ is an admissible coupling for the transport from μ to ν_ε . This implies directly the Γ -lim sup. For the Γ -lim inf, let

$(\mu_\varepsilon)_\varepsilon \subset \mathcal{P}_2(\mathbb{R}^d)$ be such that $\mu_\varepsilon \rightarrow \mu$ in W_2 as $\varepsilon \rightarrow 0^+$. Let $\gamma_\varepsilon \in \Gamma(\mu_\varepsilon, \nu_\varepsilon)$ be an optimal coupling and denote

$$u_\varepsilon(x) := \frac{|x|^2}{2} + \varepsilon\phi_0(x),$$

which is convex by hypothesis. Note that $(\nabla u_\varepsilon^*)_{\#}\nu_\varepsilon = \nu_0$. We have

$$\begin{aligned} \mathcal{H}_\varepsilon(\mu_\varepsilon) &\geq \frac{1}{\varepsilon} \left[\int |z - y|^2 d\gamma_\varepsilon(z, y) - \int |\nabla u_\varepsilon^*(y) - z|^2 d\gamma_\varepsilon(z, y) \right] \\ &= -\frac{1}{\varepsilon} \int |\nabla u_\varepsilon^*(y) - y|^2 d\nu_\varepsilon(y) + \frac{2}{\varepsilon} \int \langle \nabla u_\varepsilon^*(y) - y, z - y \rangle d\gamma_\varepsilon(z, y) \\ &= -\varepsilon \int |\nabla \phi_0(x)|^2 d\nu_0(x) - 2 \int \langle \nabla \phi_0(\nabla u_\varepsilon^*(y)), z - y \rangle d\gamma_\varepsilon(z, y). \end{aligned}$$

Recalling that L is the Lipschitz constant of $\nabla \phi_0$, we obtain

$$\begin{aligned} \mathcal{H}_\varepsilon(\mu_\varepsilon) &\geq -\varepsilon W_2^2(\nu_0, \nu_1) - 2 \int \langle \nabla \phi_0(\nabla u_\varepsilon^*(y)) - \nabla \phi_0(y) + \nabla \phi_0(y), z - y \rangle d\gamma_\varepsilon(z, y) \\ &\geq -\varepsilon W_2^2(\nu_0, \nu_1) - 2L\varepsilon W_2(\nu_0, \nu_1)W_2(\mu_\varepsilon, \nu_\varepsilon) - 2 \int \langle \nabla \phi_0(y), z - y \rangle d\gamma_\varepsilon(z, y). \end{aligned}$$

By the stability of optimal transport maps, as $\varepsilon \rightarrow 0^+$, γ_ε converges in W_2 towards the optimal map γ from ν_0 to μ (since it converges weakly and its 2-moments converge towards those of γ), therefore we get

$$\liminf_{\varepsilon \rightarrow 0^+} \mathcal{H}_\varepsilon(\mu_\varepsilon) \geq \mathcal{H}(\mu).$$

□

Remark 4.3. *The functional \mathcal{G} defined in (4.5) is 2-convex along generalized geodesics based at ν_0 , which is expected since it is the Γ -limit of the functionals \mathcal{G}_ε which are 2-convex along generalized geodesics based at ν_ε .*

5. PARTICULAR SOLUTIONS

When there is no geodesic from ν_0 to ν_1 that stays length-minimizing when extended up to time t , the solution to problem (\mathcal{P}) is not trivial in general. Nonetheless, in this section, we construct some explicit solutions corresponding to specific choices for the measures ν_0 and ν_1 .

5.1. Extrapolation when ν_1 is a Dirac mass. We suppose $\nu_1 = \delta_{x_1}$ with $x_1 \in \mathbb{R}^d$ fixed. As before, for any $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, we denote by $\text{bary}(\mu) \in \mathbb{R}^d$ its barycenter

$$\text{bary}(\mu) := \int x d\mu(x).$$

By Jensen's inequality

$$\begin{aligned} W_2^2(\mu, \nu_0) &= \int |x|^2 d\mu(x) + \int |x|^2 d\nu_0(x) - 2 \inf \left\{ \int u d\nu_0 + \int u^* d\mu; u \text{ convex} \right\} \\ &\leq \int |x|^2 d\mu(x) + \int |x|^2 d\nu_0(x) - 2 \inf \left\{ \int u d\nu_0 + u^*(\text{bary}(\mu)); u \text{ convex} \right\} \\ &\leq \int |x|^2 d\mu(x) - |\text{bary}(\mu)|^2 + W_2^2(\delta_{\text{bary}(\mu)}, \nu_0). \end{aligned}$$

On the other hand,

$$\begin{aligned} W_2^2(\mu, \nu_1) &= \int |x - x_1|^2 d\mu(x) = \int |x|^2 d\mu(x) + |x_1|^2 - 2\langle \text{bary}(\mu), x_1 \rangle \\ &= \int |x|^2 d\mu(x) - |\text{bary}(\mu)|^2 + W_2^2(\delta_{\text{bary}(\mu)}, \nu_1). \end{aligned}$$

This implies that

$$(5.1) \quad \frac{W_2^2(\mu, \nu_1)}{t-1} - \frac{W_2^2(\mu, \nu_0)}{t} \geq \frac{1}{t(t-1)} \left(\int |x|^2 d\mu(x) - |\text{bary}(\mu)|^2 \right) + \frac{W_2^2(\delta_{\text{bary}(\mu)}, \nu_1)}{t-1} - \frac{W_2^2(\delta_{\text{bary}(\mu)}, \nu_0)}{t}.$$

Applying again Jensen's inequality, the first term on the right-hand side of (5.1) is non-negative. Hence μ must be a Dirac mass, and in particular

$$\mu = \delta_{x_t} \quad \text{where} \quad x_t = \text{bary}(\nu_0) + t(x_1 - \text{bary}(\nu_0)).$$

Remark 5.1. *In this specific setting, the extrapolation is consistent with a sticky particle interaction. In particular after collapsing at a single point all particles move together while the total momentum is preserved.*

5.2. Difference with locally minimizing geodesics. We detail here an example highlighting the difference between the metric extrapolation and locally minimizing geodesics.

The setting we consider is represented in Figure 1. In this example, $d = 2$ and $\nu_0 = \nu_0^+ + \nu_0^-$ and $\nu_1 = \nu_1^+ + \nu_1^-$ are each the sum of two Dirac masses:

$$\nu_0^+ = \frac{1}{2}\delta_{(-2,1)}, \quad \nu_0^- = \frac{1}{2}\delta_{(2,-1)}, \quad \nu_1^+ = \frac{1}{2}\delta_{(-1,1)}, \quad \nu_1^- = \frac{1}{2}\delta_{(1,-1)}.$$

Note that the curve

$$s \in \mathbb{R} \mapsto \nu(s) = \frac{1}{2}\delta_{(-2+s,1)} + \frac{1}{2}\delta_{(2-s,-1)}$$

is a locally length-minimizing geodesic such that $\nu(0) = \nu_0$ and $\nu(1) = \nu_1$. However we now show that for t sufficiently large the minimizer of (\mathcal{P}) is not $\nu(t)$.

First of all we observe that in this case any minimizer μ of (\mathcal{P}) must be symmetric with respect to the origin. Furthermore it must be contained in the set $\{y \geq \max(-x/2, 2x)\} \cup \{y \leq \min(-x/2, 2x)\}$ (shaded in the figure). In fact, if this was not the case, we could always reflect the part of μ which is not contained in that

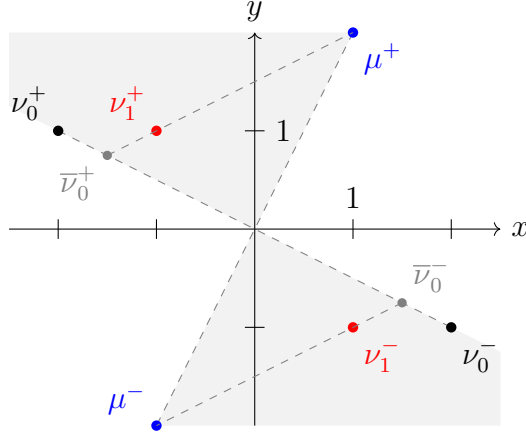


FIGURE 1. An example in which locally length-minimizing geodesic passing by $\nu_0 = \nu_0^+ + \nu_0^-$ and $\nu_1 = \nu_1^+ + \nu_1^-$ exists for all times but the metric extrapolation does not coincide with it.

area with respect to the axis $y = 2x$ or $y = -x/2$ to get a measure $\bar{\mu}$ satisfying $W_2(\mu, \nu_0) = W_2(\bar{\mu}, \nu_0)$ and $W_2(\mu, \nu_1) \geq W_2(\bar{\mu}, \nu_1)$, leading to a contradiction.

Hence, we can write $\mu = \mu^+ + \mu^-$ where μ^+ and μ^- have equal mass and solve

$$\begin{aligned} \mu^+ &= \operatorname{argmin}_{\mu} \frac{W^2(\mu, \nu_1^+)}{2(t-1)} - \frac{W^2(\mu, \nu_0^+)}{2t}, \\ \mu^- &= \operatorname{argmin}_{\mu} \frac{W^2(\mu, \nu_1^-)}{2(t-1)} - \frac{W^2(\mu, \nu_0^-)}{2t}, \end{aligned}$$

subject to the constraint that the support of μ^+ is contained in $\{y \geq \max(-x/2, 2x)\}$, whereas the support of μ^- is contained in $\{y \leq \min(-x/2, 2x)\}$. Proceeding like in the previous example, we deduce that $\mu^+ = \delta_{(x^+, y^+)}/2$ and $\mu^- = \delta_{(x^-, y^-)}/2$ are Dirac masses. Therefore, the minimization becomes explicit and we find

$$(x^+, y^+) = \begin{cases} (-2 + t, 1) & \text{if } t \leq \frac{5}{2}, \\ (\frac{1}{2}, 1) + (t - \frac{5}{2})(1, 2) & \text{if } t > \frac{5}{2}, \end{cases}$$

and $(x^-, y^-) = -(x^+, y^+)$.

Note that we can obtain the same result in an alternative way which highlights the link with the barycentric formulation. Specifically, using the symmetry of the solution with respect to the axis $y = -x/2$ we have

$$W_2^2(\mu, \nu_0) = \min_{s \in [0,1]} W_2^2(\mu^+, (1-s)\nu_0^+ + s\nu_0^-) + W_2^2(\mu^-, s\nu_0^+ + (1-s)\nu_0^-)$$

Replacing this in the original problem we obtain

$$(5.2) \quad \mu^+ = \operatorname{argmin}_{\mu} \max_{s \in [0,1]} \frac{W^2(\mu, \nu_1^+)}{2(t-1)} - \frac{W^2(\mu, s\nu_0^+ + (1-s)\nu_0^-)}{2t},$$

$$(5.3) \quad \mu^- = \operatorname{argmin}_{\mu} \max_{s \in [0,1]} \frac{W^2(\mu, \nu_1^-)}{2(t-1)} - \frac{W^2(\mu, (1-s)\nu_0^+ + s\nu_0^-)}{2t},$$

where now the minimizations are unconstrained. For a fixed s we are in the setting of the previous section, and in particular μ^+ (respectively μ^-) is the extrapolation up to time t from $\bar{\nu}_0^+$ to ν_1^+ (respectively, from $\bar{\nu}_0^-$ to ν_1^-), where

$$\bar{\nu}_0^+ := \operatorname{bary}(s\nu_0^+ + (1-s)\nu_0^-), \quad \bar{\nu}_0^- := \operatorname{bary}((1-s)\nu_0^+ + s\nu_0^-),$$

as shown in Figure 1. The optimal s can be determined by swapping the min and max in (5.2) and (5.3), leading to the same cost as in the barycentric problem (B).

6. A NUMERICAL SCHEME FOR ATOMIC MEASURES

In this section we focus on the case where ν_0 and ν_1 are both atomic measures, i.e.

$$\nu_0 = \sum_{i=1}^M a_i \delta_{x_i}, \quad \nu_1 = \sum_{j=1}^N b_j \delta_{y_j},$$

for $(x_i)_{i=1}^M =: X, (y_j)_{j=1}^N =: Y \subset \mathbb{R}^d$ and $(a_i)_{i=1}^M, (b_j)_{j=1}^N \subset \mathbb{R}_+$, with $\sum_{i=1}^M a_i = 1$ and $\sum_{j=1}^N b_j = 1$. Any coupling $\pi \in \Gamma(\nu_0, \nu_1)$ is of the form

$$\pi = \sum_{i=1}^M \sum_{j=1}^N P_{ij} \delta_{(x_i, y_j)}$$

where

$$P \in G(a, b) := \left\{ P \in \mathbb{R}_+^{M \times N} : \sum_j P_{ij} = a_i, \sum_i P_{ij} = b_j \right\}.$$

The barycentric problem (B) in this setting can be written as follows:

$$(6.1) \quad \min_P \{g(P) : P \in G(a, b)\}$$

where

$$g(P) = \frac{1}{2t(t-1)} \sum_{j=1}^N \left| ty_j - (t-1) \operatorname{bary}_j(P) \right|^2 b_j,$$

with $\operatorname{bary}_j(P) = \sum_i x_i \frac{P_{ij}}{b_j}$, for $1 \leq j \leq N$. As already pointed out, this is a quadratic but not strictly convex optimization problem, due to the possible kernel of the barycenter operator. Following the discussion in Section 3, from a solution P one can recover the extrapolation from ν_0 to ν_1 at time t as

$$\nu_t = \sum_j b_j \delta_{z_j}, \quad \text{where } z_j = ty_j - (t-1) \sum_i x_i \frac{P_{ij}}{b_j}.$$

From the marginal constraints on P , $z_j \in ty_j - (t-1)\operatorname{conv}(X)$ for every $1 \leq j \leq N$, where conv denotes the convex hull.

Entropic regularization is a popular approach for solving optimal transport in this fully discrete setting [28]. It consists in adding the entropy of the transport plan as a barrier function, in order to smoothen the problem and enforce at the same time the nonnegativity constraint. The approach is particularly attractive as one can explicitly

write the dual problem as an unconstrained minimization problem and solve it via the Sinkhorn algorithm. However, since problem (6.1) is quadratic and not linear as the standard optimal transport problem, one cannot rely on the Sinkhorn algorithm directly. Following [10], we consider a variant of Sinkhorn algorithm, alternating the Sinkhorn iterations with a gradient descent step on an appropriate auxiliary variable, with similar complexity and a linear convergence guarantee. We will provide a detailed proof of this last result following the same strategy as in [10], but with some adaptations to deal with the specific form of our cost, and to ensure that the gradient descent step-size can scale linearly with ε . This was not a concern in [10] but it is crucial in our case since we are mainly interested in the limit $\varepsilon \rightarrow 0$.

6.1. Sinkhorn algorithm with an additional gradient descent step. For $\varepsilon > 0$, the entropic barycentric problem is

$$(6.2) \quad \min_P \left\{ g(P) + \varepsilon \sum_{ij} P_{ij} \left(\log \left(\frac{P_{ij}}{a_i b_j} \right) - 1 \right) : \sum_j P_{ij} = a_i, \sum_i P_{ij} = b_j \right\},$$

where the regularization term is the relative entropy of P with respect to the coupling $(a_i b_j)_{i=1, j=1}^{M, N} \in G(a, b)$. The entropy is by definition equal to $+\infty$ for any negative value, thereby automatically ensuring the non-negativity of any finite candidate coupling. The following proposition collects useful facts for problem (6.2). Importantly, this admits an unconstrained dual formulation, as the standard entropic optimal transport problem.

Proposition 6.1. *The following holds:*

- i) there exists a unique solution P^ε to (6.2) and $P^\varepsilon \rightarrow P$ for $\varepsilon \rightarrow 0$, where P is the maximal entropy solution to (6.1);
- ii) (6.2) is equal, up to a constant term and a sign change, to

$$(6.3) \quad \min_{\phi, \psi, Z} f(\phi, \psi, Z)$$

where $\phi = (\phi_i)_{i=1}^M, \psi = (\psi_j)_{j=1}^N \subset \mathbb{R}, Z = (z_j)_{j=1}^N \subset \mathbb{R}^d$ and

$$(6.4) \quad f(\phi, \psi, Z) = \varepsilon \sum_{ij} a_i b_j \left[\exp \left(\frac{-C_{ij}^t(Z) + \phi_i + \psi_j}{\varepsilon} \right) - \frac{\phi_i + \psi_j}{\varepsilon} \right] + \frac{1}{2(t-1)} \sum_j |z_j - y_j|^2 b_j$$

- for $C_{ij}^t(Z) = \frac{1}{2t} |z_j - x_i|^2$;
- iii) $\nu_t^\varepsilon := \sum_{j=1}^N b_j \delta_{z_j^\varepsilon} \rightharpoonup \sum_{j=1}^N b_j \delta_{z_j} = \nu_t$, for $\varepsilon \rightarrow 0$, where Z^ε solves (6.3).

Proof. i) Existence and uniqueness is evident since the function to be minimized is strictly convex and coercive and the feasible set is convex and not empty. The convergence towards the unregularized problem can be easily obtained adapting the proof in [28, Proposition 4.1] to the quadratic case.

ii) Notice that, as done in Section 3, the function $g(P)$ can be rewritten as

$$(6.5) \quad g(P) = \max_Z \sum_{ij} C_{ij}^t(Z) P_{ij} - \frac{1}{2(t-1)} \sum_j |z_j - y_j|^2 b_j + C,$$

for any $P \in G(a, b)$, where the constant term is

$$C = -\frac{1}{2t} \sum_{ij} |x_i|^2 P_{ij} + \frac{1}{2(t-1)} |y_j|^2 b_j = -\frac{1}{2t} \sum_i |x_i|^2 a_i + \frac{1}{2(t-1)} \sum_j |y_j|^2 b_j.$$

Enforcing the mass constraints with the Lagrange multiplier ϕ and ψ , and exchanging inf and sup by a standard duality argument, we obtain the dual problem

$$\begin{aligned} \max_{\phi, \psi, Z} \min_P \sum_{ij} C_{ij}^t(Z) P_{ij} - \frac{1}{2(t-1)} \sum_j |z_j - y_j|^2 b_j + \varepsilon \sum_{ij} P_{ij} \left(\log \left(\frac{P_{ij}}{a_i b_j} \right) - 1 \right) \\ + \sum_i \phi_i a_i + \sum_j \psi_j b_j, \end{aligned}$$

up to the constant term. The optimization in P provides

$$P_{ij} = a_i b_j \exp \left(\frac{-C_{ij}^t(Z) + \phi_i + \psi_j}{\varepsilon} \right), \quad 1 \leq i \leq M, 1 \leq j \leq N.$$

Plugging this in the dual problem and switching sign, we obtain (6.3).

iii) By the optimality, $P^\varepsilon \in G(a, b)$ and

$$z_j^\varepsilon = t y_j - (t-1) \text{bary}_j(P^\varepsilon), \quad 1 \leq j \leq N.$$

The convergence of $\nu_t^\varepsilon \rightarrow \nu_t$ is therefore an immediate consequence of i). \square

A similar entropic optimal transport problem with non-fixed cost matrix has been considered in the recent paper [10]. The authors introduced a novel iterative procedure, called SISTA, alternating between the phase of exact minimization over the potentials and a phase of proximal gradient descent over the parameters defining the transport cost. We follow the same approach for (6.3), performing a gradient descent step with respect to Z . Notice that the potentials are defined up to a common constant, as $(\phi + c, \psi - c)$ attain the same value in (6.3) as (ϕ, ψ) for any $c \in \mathbb{R}$. We fix this constant by setting $\phi_M^n = 0$ for any $n \geq 0$. Then, starting from ψ^0 and Z^0 , the ϕ and ψ updates are

$$(6.6) \quad \phi_i^{n+1} = -\varepsilon \log \sum_{j=1}^N b_j \exp \left(\frac{-C_{ij}^t(Z^n) + \psi_j^n}{\varepsilon} \right), \quad 1 \leq i \leq M-1,$$

$$\phi_M^{n+1} = 0,$$

$$(6.7) \quad \psi_j^{n+1} = -\varepsilon \log \sum_{i=1}^M a_i \exp \left(\frac{-C_{ij}^t(Z^n) + \phi_i^{n+1}}{\varepsilon} \right), \quad 1 \leq j \leq N,$$

whereas for $\tau > 0$ the gradient descent step writes for $1 \leq j \leq N$ as

$$(6.8) \quad z_j^{n+1} = z_j^n - \tau \left[\frac{z_j^n - y_j}{t-1} b_j - \sum_{i=1}^M \frac{z_j^n - x_i}{t} a_i b_j \exp \left(\frac{-C_{ij}^t(Z^n) + \phi_i^{n+1} + \psi_j^{n+1}}{\varepsilon} \right) \right].$$

Note that the first two steps coincide with the classical Sinkhorn algorithm, but we perform a gradient step with respect to Z instead of an exact minimization since this latter would lead to a nonlinear system to be solved at each iteration.

6.2. Convergence analysis. Let us denote $x^n = (\phi^n, \psi^n, Z^n) \in \mathbb{R}^{M+(1+d)N}$ and

$$x^{n+\frac{1}{3}} = (\phi^{n+1}, \psi^n, Z^n), \quad x^{n+\frac{2}{3}} = (\phi^{n+1}, \psi^{n+1}, Z^n), \quad x^{n+1} = (\phi^{n+1}, \psi^{n+1}, Z^{n+1}).$$

To perform the convergence analysis, we will consider the norm $|\cdot|_S$, and its dual, defined as

$$|x|_S^2 := |\phi|_\infty^2 + |\psi|_\infty^2 + |Z|_2^2, \quad |p|_{S^*}^2 = |p_\phi|_1^2 + |p_\psi|_1^2 + |p_Z|_2^2,$$

for $x = (\phi, \psi, Z)$ and $p = (p_\phi, p_\psi, p_Z)$. Note, in particular, that the l^∞ norm for the discrete potentials is the natural counterpart for the supremum norm, and it will simplify some of the necessary estimates in the proof. We define:

$$(6.9) \quad L_\phi := \sup_{n \geq 0} \max_{s \in [0,1]} \max_{\substack{|h_\phi|_\infty = 1 \\ (h_\phi)_M = 0}} \nabla_\phi^2 f((1-s)x^{n+\frac{1}{3}} + sx^{n+1}) h_\phi \cdot h_\phi,$$

$$(6.10) \quad L_\psi := \sup_{n \geq 0} \max_{s \in [0,1]} \max_{|h_\psi|_\infty = 1} \nabla_\psi^2 f((1-s)x^{n+\frac{2}{3}} + sx^{n+1}) h_\psi \cdot h_\psi,$$

$$(6.11) \quad L_Z := \sup_{n \geq 0} \max_{s \in [0,1]} \max_{|h_Z|_2 = 1} \nabla_Z^2 f((1-s)x^{n+\frac{2}{3}} + sx^{n+1}) h_Z \cdot h_Z.$$

These constants quantify the smoothness of f , with respect to the $|\cdot|_S$ norm, restricted along linear interpolations between consecutive iterations of the algorithm.

The following lemmas show that the iterates Z^n stay bounded upon a step restriction independent of ε , and as a consequence the constants above scale linearly with $1/\varepsilon$. In the following we will denote

$$D := \max_{ij} |x_i - y_j|.$$

Lemma 6.2. *Assume $z_j^0 \in ty_j - (t-1)\text{conv}(X)$, for all j , and $\tau \leq \frac{t(t-1)}{|b|_\infty}$. Then, for all $n \geq 0$ and all j , $z_j^n \in ty_j - (t-1)\text{conv}(X)$, and in particular,*

$$|z_j - y_j| \leq (t-1)D, \quad |z_j - x_i| \leq tD.$$

Proof. The gradient descent update on Z^n can be written as

$$z_j^{n+1} = \left(1 - \frac{b_j \tau}{t(t-1)}\right) z_j^n + \frac{b_j \tau}{t(t-1)} \sum_i (ty_j - (t-1)x_i) \frac{P_{ij}^n}{b_j}, \quad 1 \leq j \leq N.$$

Since by assumption $\frac{b_j \tau}{t(t-1)} \leq 1$, we deduce recursively that at each step $z_j^{n+1} \in ty_j - (t-1)\text{conv}(X)$. \square

Lemma 6.3. *Assume $z_j^0 \in ty_j - (t-1)\text{conv}(X)$, for all j , and $\tau \leq \frac{t(t-1)}{|b|_\infty}$. Then,*

$$L_\phi \leq \frac{C}{\varepsilon}, \quad L_\psi \leq \frac{C}{\varepsilon}, \quad L_Z \leq |b|_\infty \left(\frac{(t-1)C + t}{t(t-1)} + \frac{CD^2}{\varepsilon} \right),$$

where $C := \exp(2\lambda D^2 |b|_\infty)$ and $\lambda := \tau/\varepsilon$.

Proof. Notice first that from the updates on ϕ and ψ , we have

$$(6.12) \quad \sum_{j=1}^N b_j \exp \left(\frac{-C_{ij}^t(Z^n) + \phi_i^{n+1} + \psi_j^n}{\varepsilon} \right) = 1, \quad 1 \leq i \leq M-1,$$

$$(6.13) \quad \sum_{i=1}^M a_i \exp \left(\frac{-C_{ij}^t(Z^n) + \phi_i^{n+1} + \psi_j^{n+1}}{\varepsilon} \right) = 1, \quad 1 \leq j \leq N.$$

Then, the second non-mixed derivatives of the objective function along the iterations of the algorithm are, for all $1 \leq i \leq M-1$ and $1 \leq j \leq N$,

$$\begin{aligned} \partial_{\phi_i}^2 f(x^{n+\frac{1}{3}}) &= \frac{a_i}{\varepsilon} \sum_{j=1}^N b_j \exp \left(\frac{-C_{ij}^t(Z^n) + \phi_i^{n+1} + \psi_j^n}{\varepsilon} \right) = \frac{a_i}{\varepsilon}, \\ \partial_{\psi_j}^2 f(x^{n+\frac{2}{3}}) &= \frac{b_j}{\varepsilon} \sum_{i=1}^M a_i \exp \left(\frac{-C_{ij}^t(Z^n) + \phi_i^{n+1} + \psi_j^{n+1}}{\varepsilon} \right) = \frac{b_j}{\varepsilon}, \\ \nabla_{z_j}^2 f(x^{n+\frac{2}{3}}) &= \frac{b_j}{t-1} \text{Id}_d - \frac{1}{t} \sum_{i=1}^M a_i b_j \exp \left(\frac{-C_{ij}^t(Z^n) + \phi_i^{n+1} + \psi_j^{n+1}}{\varepsilon} \right) \text{Id}_d \\ &\quad + \frac{1}{\varepsilon t^2} \sum_{i=1}^M (z_j^n - x_i) \otimes (z_j^n - x_i) a_i b_j \exp \left(\frac{-C_{ij}^t(Z^n) + \phi_i^{n+1} + \psi_j^{n+1}}{\varepsilon} \right) \\ &= \frac{b_j}{t(t-1)} \text{Id}_d + \frac{1}{\varepsilon t^2} \sum_{i=1}^M (z_j^n - x_i) \otimes (z_j^n - x_i) a_i b_j \exp \left(\frac{-C_{ij}^t(Z^n) + \phi_i^{n+1} + \psi_j^{n+1}}{\varepsilon} \right), \end{aligned}$$

where Id_d is the identity matrix on \mathbb{R}^d . Moreover, $\nabla_\phi^2 f(x)$ and $\nabla_\psi^2 f(x)$ are diagonal matrices with nonnegative components, whereas $\nabla_Z f(x)$ is block-diagonal for any x . It follows that

$$\begin{aligned} \max_{\substack{|h_\phi|_\infty=1 \\ (h_\phi)_M=0}} \nabla_\phi^2 f(x) h_\phi \cdot h_\phi &= \sum_{i=1}^{M-1} \partial_{\phi_i}^2 f(x), \\ \max_{|h_\psi|_\infty=1} \nabla_\psi^2 f(x) h_\psi \cdot h_\psi &= \sum_{j=1}^N \partial_{\psi_j}^2 f(x), \\ \max_{|h_Z|_2=1} \nabla_Z^2 f(x) h_Z \cdot h_Z &= \max_j \max_{|h_{z_j}|_2=1} \nabla_{z_j}^2 f(x) h_{z_j} \cdot h_{z_j}. \end{aligned}$$

By Lemma 6.2, for all $n \geq 0$ and all $1 \leq j \leq N$, $z_j^n \in ty_j - (t-1)\text{conv}(X)$ and

$$|\nabla_{z_j} f(x^{n+\frac{2}{3}})| \leq b_j \left(\frac{1}{t} \max_i |z_j^n - x_i| + \frac{1}{t-1} |z_j^n - y_j| \right) \leq 2Db_j,$$

Therefore, using the gradient descent update (6.8),

$$\begin{aligned} -C_{ij}^t(Z^n + s(Z^{n+1} - Z^n)) &\leq -C_{ij}^t(Z^n) + s\tau D |\nabla_{z_j} f(\phi^{n+1}, \psi^{n+1}, Z^n)| \\ &\leq -C_{ij}^t(Z^n) + s\tau 2D^2 |b|_\infty. \end{aligned}$$

Then, by convexity of the exponential function and using (6.12)-(6.13), we can bound L_ϕ and L_ψ as

$$\begin{aligned} L_\phi &\leq \sup_n \max_{s \in [0,1]} \exp(s\lambda 2D^2 |b|_\infty) \left((1-s) \sum_{i=1}^{M-1} \partial_{\phi_i}^2 f(x^{n+\frac{1}{3}}) + s \sum_{i=1}^{M-1} \partial_{\phi_i}^2 f(x^{n+\frac{2}{3}}) \right) \\ &\leq \max_{s \in [0,1]} \frac{\exp(s\lambda 2D^2 |b|_\infty)}{\varepsilon} \left((1-s) \sum_{i=1}^M a_i + s \sum_{j=1}^N b_j \right) \leq \frac{C}{\varepsilon}, \\ L_\psi &\leq \sup_n \max_{s \in [0,1]} \exp(s\lambda 2D^2 |b|_\infty) \left(\sum_{j=1}^N \partial_{\psi_j}^2 f(x^{n+\frac{2}{3}}) \right) \\ &= \max_{s \in [0,1]} \frac{\exp(s\lambda 2D^2 |b|_\infty)}{\varepsilon} \sum_{j=1}^N b_j \leq \frac{C}{\varepsilon}. \end{aligned}$$

Finally, using again (6.2) and (6.13),

$$\begin{aligned} \max_{|h_{z_j}|_2=1} \nabla_{z_j}^2 f((1-s)x^{n+\frac{2}{3}} + sx^{n+1}) h_{z_j} \cdot h_{z_j} &\leq \\ &\leq \frac{b_j}{t-1} + \frac{Cb_j}{t} + \frac{Cb_j}{\varepsilon t^2} \max_i \max_{|h_{z_j}|_2=1} [(z_j^n - x_i) \otimes (z_j^n - x_i)] h_{z_j} \cdot h_{z_j} \\ &\leq b_j \left(\frac{(t-1)C + t}{t(t-1)} + \frac{CD^2}{\varepsilon} \right) \end{aligned}$$

and the last estimate follows. \square

Lemma 6.3 suggests that if τ scales linearly with ε , L_Z scales as $1/\varepsilon$ and therefore $L_Z \leq 1/\tau$ for τ sufficiently small. This is made precise in the following Lemma:

Lemma 6.4. *Assuming $\varepsilon \leq 1$, there exists $K > 0$ only depending on t , $|b|_\infty$ and D , such that if $\tau \leq K\varepsilon$ then $\tau \leq \min\left(\frac{t(t-1)}{|b|_\infty}, \frac{1}{L_Z}\right)$.*

Proof. One needs to find K such that

$$\begin{cases} K\varepsilon \leq \frac{t(t-1)}{|b|_\infty}, \\ K \exp(K)(A\varepsilon + B) + \frac{K\varepsilon}{t-1} \leq \frac{1}{|b|_\infty}, \end{cases}$$

where $A = \exp(2D^2 |b|_\infty)/t$ and $B = \exp(2D^2 |b|_\infty)D^2$. In particular, one can take $K = \min\left(\frac{t(t-1)}{|b|_\infty}, \bar{K}\right)$ where \bar{K} solves

$$\bar{K} \exp(\bar{K}) + \frac{\bar{K}}{t-1} = \frac{1}{(A+B)|b|_\infty}.$$

□

The following proof of convergence of iterations (6.6)-(6.7)-(6.8) is an adaptation from [10]. Before stating it, let us recall that f being μ -convex and L -smooth on a set S with respect to the norm $|\cdot|$ means that, $\forall x, y \in S$,

$$(6.14) \quad f(x) \geq f(y) + \nabla f(y) \cdot (x - y) + \frac{\mu}{2}|x - y|^2,$$

$$(6.15) \quad f(x) \leq f(y) + \nabla f(y) \cdot (x - y) + \frac{L}{2}|x - y|^2.$$

Moreover, the gradient of f is L -Lipschitz, that is

$$|\nabla f(x) - \nabla f(y)|_* \leq L|x - y|$$

$\forall x, y \in S$, where $|\cdot|_*$ is the dual norm with respect to $|\cdot|$.

See for example [25, 8] for more details on strong convexity and smoothness in convex optimization.

Proposition 6.5. *Suppose $\tau \leq K\varepsilon$, with K as in Lemma 6.4. Then, iterations (6.6)-(6.7)-(6.8) converge with linear rate, i.e. there exists $0 < \eta < 1$ such that*

$$f(x^{n+1}) - f(x^*) \leq \eta(f(x^n) - f(x^*)), \quad \forall n \geq 0,$$

where x^* is the unique solution of problem (6.3).

Proof. First of all, the objective function is decreasing monotonically along iterations of the algorithm, i.e.

$$(6.16) \quad f(x^{n+1}) \leq f(x^{n+\frac{2}{3}}) \leq f(x^{n+\frac{1}{3}}) \leq f(x^n), \quad \forall n \geq 0.$$

The first two inequalities come directly by definition of alternate minimization. Concerning the third inequality, since f is L_Z -smooth along $(1-s)x^{n+\frac{2}{3}} + sx^{n+1}$, $\forall n \geq 0$, and $L_Z \leq 1/\tau$ by Lemma 6.4,

$$(6.17) \quad \begin{aligned} f(x^{n+1}) &\leq f(x^{n+\frac{2}{3}}) + \nabla f(x^{n+\frac{2}{3}}) \cdot (x^{n+1} - x^{n+\frac{2}{3}}) + \frac{1}{2\tau}|x^{n+1} - x^{n+\frac{2}{3}}|_S^2 \\ &= f(x^{n+\frac{2}{3}}) - \frac{1}{\tau}|x^{n+1} - x^{n+\frac{2}{3}}|_S^2 + \frac{1}{2\tau}|x^{n+1} - x^{n+\frac{2}{3}}|_S^2 \\ &= f(x^{n+\frac{2}{3}}) - \frac{1}{2\tau}|x^{n+1} - x^{n+\frac{2}{3}}|_S^2, \end{aligned}$$

where we used the definition of gradient descent step in the first equality.

Consider

$$g(\phi, \psi) := \varepsilon \sum_{ij} a_i b_j \left[\exp\left(\frac{\phi_i + \psi_j}{\varepsilon} - \frac{tD^2}{2\varepsilon}\right) - \left(\frac{\phi_i + \psi_j}{\varepsilon} - \frac{tD^2}{2\varepsilon}\right) \right] - \frac{tD^2}{2},$$

and notice that $f(\phi, \psi, Z) \geq g(\phi, \psi)$ for any Z such that $z_j \in ty_j - (t-1)\text{conv}(X)$, $\forall j$. Since $f(x^n)$ is decreasing,

$$g(\phi^n, \psi^n) \leq f(x^n) \leq f(x^0), \quad \forall n \geq 0.$$

Using $\exp^x - x \geq |x|$, we obtain

$$|\phi_i^n + \psi_j^n| \leq f(x^0) + tD^2 =: \frac{C}{2}, \quad \forall (i, j),$$

which in turn provides, using $\phi_M^n = 0$ for any n , $|\phi^n|_\infty \leq C$ and $|\psi^n|_\infty \leq C$. Therefore, the iterates of the algorithm are uniformly bounded and belong to

$$S := \{(\phi, \psi, Z) \in \mathbb{R}^{M+(1+d)N} : |\phi|_\infty \leq C, |\psi|_\infty \leq C, z_j \in ty_j - (t-1)\text{conv}(X)\}.$$

The strictly convex function f is furthermore μ -convex on the compact set S , with

$$\mu := \min_{x \in S} \min_{|h|_S=1} \nabla^2 f(x) h \cdot h.$$

Hence, at each step n , by definition of the alternate minimization, which provides $\nabla_\phi f(x^{n+\frac{1}{3}}) = 0$ and $\nabla_\psi f(x^{n+\frac{2}{3}}) = 0$, and using (6.14) with respect to the norm $|\cdot|_S$, it holds

$$\begin{aligned} f(x^n) &\geq f(x^{n+\frac{1}{3}}) + \frac{\mu}{2} |x^{n+\frac{1}{3}} - x^n|_S^2, \\ f(x^{n+\frac{1}{3}}) &\geq f(x^{n+\frac{2}{3}}) + \frac{\mu}{2} |x^{n+\frac{2}{3}} - x^{n+\frac{1}{3}}|_S^2. \end{aligned}$$

Combing these with (6.17) we obtain

(6.18)

$$\begin{aligned} (f(x^n) - f(x^*)) - (f(x^{n+1}) - f(x^*)) &\geq \frac{\mu}{2} (|x^{n+\frac{1}{3}} - x^n|_S^2 + |x^{n+\frac{2}{3}} - x^{n+\frac{1}{3}}|_S^2) + \frac{1}{2\tau} |x^{n+1} - x^{n+\frac{2}{3}}|_S^2 \\ &\geq \frac{\mu}{2} |x^{n+1} - x^n|_S^2, \end{aligned}$$

since $\mu \leq L_Z \leq \frac{1}{\tau}$. Again by (6.14),

$$f(x^*) \geq f(x^{n+1}) + \nabla f(x^{n+1}) \cdot (x^* - x^{n+1}) + \frac{\mu}{2} |x^* - x^{n+1}|_S^2$$

and using further $x \cdot y + \frac{\mu}{2} |y|_S^2 \geq -\frac{1}{2\mu} |x|_{S^*}^2$, we can write

$$f(x^{n+1}) - f(x^*) \leq \frac{1}{2\mu} |\nabla f(x^{n+1})|_{S^*}^2.$$

Since f is L_ϕ -smooth along $(1-s)x^{n+\frac{1}{3}} + sx^{n+1}$, L_ψ -smooth along $(1-s)x^{n+\frac{2}{3}} + sx^{n+1}$, and L_Z -smooth along $(1-s)x^{n+\frac{2}{3}} + sx^{n+1}$, $\forall n \geq 0$ and for $s \in [0, 1]$, using again $\nabla_\phi f(x^{n+\frac{1}{3}}) = 0$ and $\nabla_\psi f(x^{n+\frac{2}{3}}) = 0$,

$$\begin{aligned} |\nabla_\phi f(x^{n+1})|_1^2 &= |\nabla_\phi f(x^{n+1}) - \nabla_\phi f(x^{n+\frac{1}{3}})|_1^2 \leq L_\phi^2 |x^{n+1} - x^{n+\frac{1}{3}}|_S^2, \\ |\nabla_\psi f(x^{n+1})|_1^2 &= |\nabla_\psi f(x^{n+1}) - \nabla_\psi f(x^{n+\frac{2}{3}})|_1^2 \leq L_\psi^2 |x^{n+1} - x^{n+\frac{2}{3}}|_S^2, \\ |\nabla_Z f(x^{n+1})|_2^2 &= |\nabla_Z f(x^{n+1}) - \nabla_Z f(x^{n+\frac{2}{3}})|_2^2 + \frac{1}{\tau} (Z^n - Z^{n+1})|_2^2 \\ &= |\nabla_Z f(x^{n+1}) - \nabla_Z f(x^{n+\frac{2}{3}})|_2^2 + \frac{1}{\tau^2} |(Z^n - Z^{n+1})|_2^2 \\ &\quad + \frac{2}{\tau} (Z^n - Z^{n+1}) \cdot (\nabla_Z f(x^{n+1}) - \nabla_Z f(x^{n+\frac{2}{3}})) \\ &\leq (L_Z^2 + \frac{1}{\tau^2}) |x^{n+1} - x^{n+\frac{2}{3}}|_S^2, \end{aligned}$$

where in the last inequality we also used the gradient descent step and the convexity of f with respect to Z . This provides

$$f(x^{n+1}) - f(x^*) \leq \frac{\hat{L}^2 + \tau^{-2}}{2\mu} |x^{n+1} - x^n|_S^2,$$

where $\hat{L}^2 = L_\phi^2 + L_\psi^2 + L_Z^2$, and combining this with (6.18) we finally get

$$f(x^{n+1}) - f(x^*) \leq \frac{\hat{L}^2 \tau^2 + 1}{\hat{L}^2 \tau^2 + 1 + \mu^2 \tau^2} (f(x^n) - f(x^*)).$$

□

Remark 6.6. *From the proof of Proposition 6.5, since the iterates are uniformly bounded with respect to ε , one can infer that $\mu \rightarrow 0$ exponentially fast for $\varepsilon \rightarrow 0$. Notice that on the compact set S the function f is furthermore L -smooth with*

$$L := \max_{x \in S} \max_{|h|_S=1} \nabla^2 f(x) h \cdot h,$$

and similarly, $L \rightarrow \infty$ exponentially fast for $\varepsilon \rightarrow 0$. Since the constant of smoothness is related to the maximal stepsize τ , this motivates our choice of working with the local smoothness constants (6.9)-(6.10)-(6.11), which scale only linearly with respect to $1/\varepsilon$, contrary to the global constant L . In the end, for $\tau = K\varepsilon$, we have

$$\eta \leq \frac{1}{1 + C_1 \exp(-C_2/\varepsilon)}$$

for some positive constants C_1, C_2 independent of ε , so that we obtain the same exponential dependency on ε of the linear convergence rate as in the classical Sinkhorn algorithm.

6.3. Numerical tests.

6.3.1. *Extrapolation of shapes.* Figure 2 illustrates some examples of extrapolations obtained using the algorithm discussed in this section. The data ν_0 and ν_1 are given by a collection of Dirac masses with equal weights, whose location is chosen to provide an optimal quantization in the W_2 sense of two uniformly distributed densities. For all test cases in this figure $\varepsilon = 10^{-3}$.

6.3.2. *Gradient flow of the opposite Wasserstein distance.* Let us consider the curve $\nu_{\text{gf}} : [1, \infty) \rightarrow \mathcal{P}_2(\mathbb{R}^d)$ obtained as the W_2 gradient flow of the time dependent energy:

$$(6.19) \quad \mathcal{E}(t, \mu) := -\frac{W_2^2(\nu_0, \mu)}{2t}$$

for $t \geq 1$ and initial conditions $\nu_{\text{gf}}(1) = \nu_1$. This is a well-defined flow as discussed in [2], and moreover if there exists a length-minimizing geodesic on $[0, t]$ passing through ν_0 at time 0 and ν_1 at time 1, ν coincides with it on the interval $[1, t]$ [2, Theorem 11.2.10] (note that differently from [2] we use a time-dependent energy to avoid rescaling time when comparing the gradient flow with geodesics). Our framework provides a natural

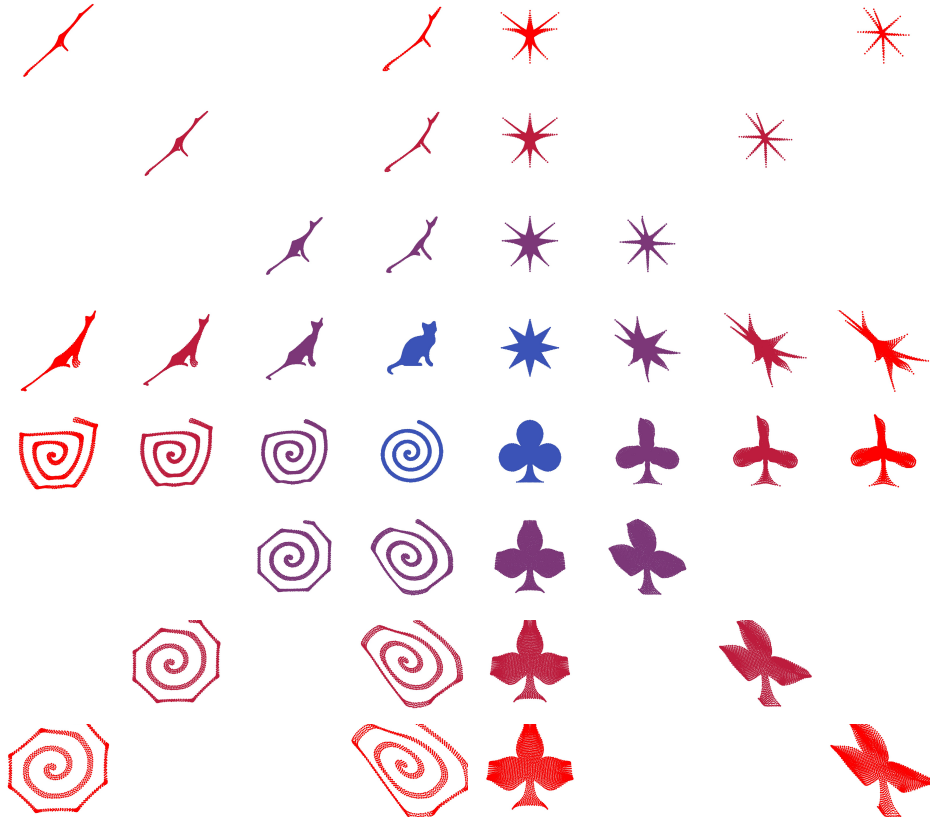


FIGURE 2. Example of extrapolation. The four images in the center are pairwise extrapolated in both positive and negative direction, from $t = 1$ (blue) to $t = 3$ (red).

way to discretize this flow. As a matter of fact, the JKO scheme [19] with time step $h > 0$ yields the following minimization problem, for all $n \geq 0$,

$$(6.20) \quad \nu_{\text{gf}}^{n+1} = \operatorname{argmin}_{\mu \in \mathcal{P}_2(\mathbb{R}^d)} \frac{W_2^2(\nu_{\text{gf}}^n, \mu)}{2h} - \frac{W_2^2(\nu_0, \mu)}{2t^{n+1}}$$

where we set $\nu_{\text{gf}}^0 = \nu_1$ and $t^n = 1 + nh$, which is a metric extrapolation problem. Remarkably, in one dimension $\nu_{\text{gf}}(t) = \nu_t$, the metric extrapolation from ν_0 to ν_1 at time t , and it also yields a sticky solution to the pressureless Euler equations (see [24] and Remark 4.1). In higher dimension, however, in general $\nu_{\text{gf}}(t) \neq \nu_t$, as it could be expected since only in one dimension the L^2 transport cost is equivalent to an L^2 distance on quantile functions. Note also that the metric extrapolation coincides with one single JKO step for the energy (6.19) up to the final time. A simple scenario where one can observe the difference between the two flows is provided in Figure 3, where ν_0 and ν_1 are a sum of Dirac measures with equal masses:

$$\nu_0 = \frac{1}{3} \sum_{i=1}^3 \delta_{x_i}, \quad \nu_1 = \frac{1}{2} \sum_{j=1}^2 \delta_{y_j}$$

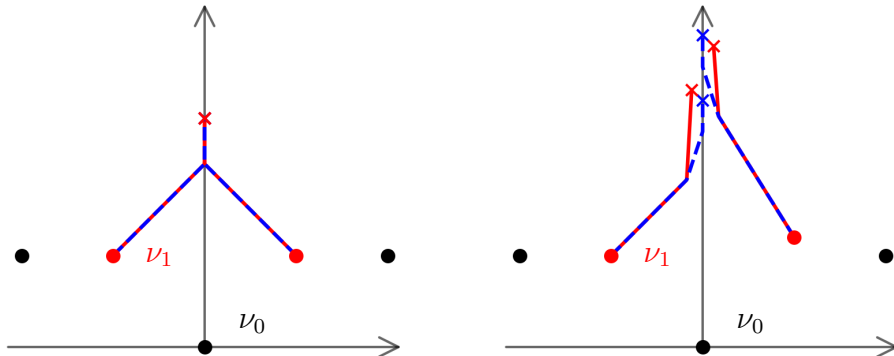


FIGURE 3. A comparison between the gradient flow ν_{gf} (dashed blue line) and metric extrapolation ν_t (solid red line) on the same time interval, for the same ν_0 and two different initial conditions for ν_1 .

where $x_1 = (-2, 1)$, $x_2 = (2, 1)$, $x_3 = (0, 0)$, and $y_1 = (-1, 1)$, $y_2 = (1, 1)$ on the left, and $y_2 = (1, 1.2)$ on the right. The two flows are represented on the time interval $[1, 5.5]$ and with time step $h = 4.5 \cdot 10^{-3}$. Note that when the mass is distributed symmetrically with respect to the y axis the two flows coincide (the same happens for the explicit examples of Section 5). However for a slightly perturbed ν_1 we obtain two different curves for the metric extrapolation and the gradient flow. Note that these results were obtained using an interior point scheme to solve the quadratic program (6.1) with high precision, but one obtains the same picture using the entropic scheme of this section for sufficiently small ε .

In Figure 4 we show another example of gradient flow of the opposite Wasserstein distance. As in the examples of Figure 2, the measures ν_0 and $\nu_{\text{gf}}(1) = \nu_1$ are obtained as optimal quantization in the W_2 sense of two uniformly distributed densities. The flow is approximated on the time interval $[1, 4]$ using the JKO scheme (6.20) and the entropic scheme presented in this section, for $h = 0.1$ and $\varepsilon = 10^{-3}$. The evolution is compared with the metric extrapolation ν_t .

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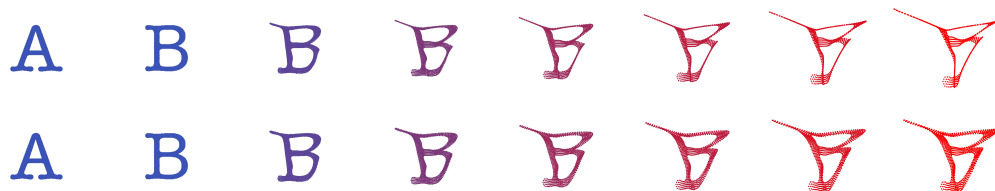


FIGURE 4. Example of gradient flow of the opposite Wasserstein distance (top row) from ν_0 (first column from the left) with initial condition ν_1 (second column from the left) and comparison with the metric extrapolation (bottom row). Time grows from left to right, from $t = 1$ (blue) to $t = 4$ (red).

REFERENCES

- [1] Martial Agueh and Guillaume Carlier. Barycenters in the Wasserstein space. *SIAM Journal on Mathematical Analysis*, 43(2):904–924, 2011.
- [2] Luigi Ambrosio, Nicola Gigli, and Giuseppe Savaré. *Gradient flows: in metric spaces and in the space of probability measures*. Springer Science & Business Media, 2008.
- [3] Combettes P. L. Bauschke, H. H. *Convex Analysis and Monotone Operators Theory in Hilbert Spaces*. CMS Books in Mathematics. Springer-Verlag, second edition, 2017.
- [4] Jean-David Benamou, Thomas O Gallouët, and François-Xavier Vialard. Second-order models for optimal transport and cubic splines on the Wasserstein space. *Foundations of Computational Mathematics*, 19:1113–1143, 2019.
- [5] Yann Brenier. The initial value problem for the euler equations of incompressible fluids viewed as a concave maximization problem. *Communications in Mathematical Physics*, 364:579–605, 2018.
- [6] Yann Brenier. Examples of hidden convexity in nonlinear PDEs. 2020.
- [7] Yann Brenier and Emmanuel Grenier. Sticky particles and scalar conservation laws. *SIAM Journal on Numerical Analysis*, 35(6):2317–2328, 1998.
- [8] Sébastien Bubeck et al. Convex optimization: Algorithms and complexity. *Foundations and Trends® in Machine Learning*, 8(3-4):231–357, 2015.
- [9] Guillaume Carlier. Remarks on Toland’s duality, convexity constraint and optimal transport. 2008.
- [10] Guillaume Carlier, Arnaud Dupuy, Alfred Galichon, and Yifei Sun. Sista: learning optimal transport costs under sparsity constraints. *Communications on Pure and Applied Mathematics*, 76(9):1659–1677, 2023.
- [11] Elsa Cazelles, Felipe Tobar, and Joaquin Fontbona. A novel notion of barycenter for probability distributions based on optimal weak mass transport. *Advances in Neural Information Processing Systems*, 34:13575–13586, 2021.
- [12] Maxime Dalery, Geneviève Dusson, Virginie Ehrlacher, and Alexei Lozinski. Nonlinear reduced basis using mixture Wasserstein barycenters: application to an eigenvalue problem inspired from quantum chemistry. *arXiv preprint arXiv:2307.15423*, 2023.
- [13] Jianing Fan and Hans-Georg Müller. Conditional Wasserstein barycenters and interpolation/extrapolation of distributions. *arXiv preprint arXiv:2107.09218*, 2021.
- [14] Alessio Figalli, Young-Heon Kim, and Robert J McCann. When is multidimensional screening a convex program? *Journal of Economic Theory*, 146(2):454–478, 2011.
- [15] Thomas Gallouët, Andrea Natale, and Gabriele Todeschi. From geodesic extrapolation to a variational bdf2 scheme for wasserstein gradient flows. *Mathematics of Computation*, 2024.
- [16] Wilfrid Gangbo. An elementary proof of the polar factorization of vector-valued functions. *Archive for rational mechanics and analysis*, 128:381–399, 1994.

- [17] Nathael Gozlan and Nicolas Juillet. On a mixture of Brenier and Strassen theorems. *Proceedings of the London Mathematical Society*, 120(3):434–463, 2020.
- [18] Nathael Gozlan, Cyril Roberto, Paul-Marie Samson, and Prasad Tetali. Kantorovich duality for general transport costs and applications. *Journal of Functional Analysis*, 273(11):3327–3405, 2017.
- [19] Richard Jordan, David Kinderlehrer, and Felix Otto. The variational formulation of the Fokker–Planck equation. *SIAM journal on mathematical analysis*, 29(1):1–17, 1998.
- [20] Young-Heon Kim and Robert J McCann. Continuity, curvature, and the general covariance of optimal transportation. *Journal of the European Mathematical Society*, 12(4):1009–1040, 2010.
- [21] Guillaume Legendre and Gabriel Turinici. Second-order in time schemes for gradient flows in Wasserstein and geodesic metric spaces. *Comptes Rendus Mathématique*, 355:345–353, 03 2017.
- [22] Daniel Matthes and Simon Plazotta. A variational formulation of the BDF2 method for metric gradient flows. *ESAIM: Mathematical Modelling and Numerical Analysis*, 53(1):145–172, 2019.
- [23] Robert J McCann. A convexity principle for interacting gases. *Advances in mathematics*, 128(1):153–179, 1997.
- [24] Luca Natile and Giuseppe Savaré. A Wasserstein approach to the one-dimensional sticky particle system. *SIAM journal on mathematical analysis*, 41(4):1340–1365, 2009.
- [25] Yurii Nesterov et al. *Lectures on convex optimization*, volume 137. Springer.
- [26] François-Pierre Paty, Philippe Choné, and Francis Kramarz. Algorithms for weak optimal transport with an application to economics. *arXiv preprint arXiv:2205.09825*, 2022.
- [27] François-Pierre Paty, Alexandre d’Aspremont, and Marco Cuturi. Regularity as regularization: Smooth and strongly convex brenier potentials in optimal transport. In *International Conference on Artificial Intelligence and Statistics*, pages 1222–1232. PMLR, 2020.
- [28] Gabriel Peyré and Marco Cuturi. Computational optimal transport, 2020.
- [29] Filippo Santambrogio. Optimal transport for applied mathematicians. *Birkhäuser*, NY, pages 99–102, 2015.
- [30] Volker Strassen. The existence of probability measures with given marginals. *The Annals of Mathematical Statistics*, 36(2):423–439, 1965.
- [31] John F Toland. Duality in nonconvex optimization. *Journal of Mathematical Analysis and Applications*, 66(2):399–415, 1978.
- [32] John F Toland. A duality principle for non-convex optimisation and the calculus of variations. *Archive for Rational Mechanics and Analysis*, 71:1432–0673, 1978.
- [33] Adrien Vacher and François-Xavier Vialard. Semi-dual unbalanced quadratic optimal transport: fast statistical rates and convergent algorithm. In *International Conference on Machine Learning*, pages 34734–34758. PMLR, 2023.
- [34] Dmitry Vorotnikov. Partial differential equations with quadratic nonlinearities viewed as matrix-valued optimal ballistic transport problems. *Archive for Rational Mechanics and Analysis*, 243(3):1653–1698, 2022.

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