



**HAL**  
open science

# Regularity theory and geometry of unbalanced optimal transport

Thomas Gallouët, Roberta Ghezzi, François-Xavier Vialard

► **To cite this version:**

Thomas Gallouët, Roberta Ghezzi, François-Xavier Vialard. Regularity theory and geometry of unbalanced optimal transport. 2021. hal-03498098v1

**HAL Id: hal-03498098**

**<https://hal.science/hal-03498098v1>**

Preprint submitted on 20 Dec 2021 (v1), last revised 27 Jun 2024 (v3)

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# REGULARITY THEORY AND GEOMETRY OF UNBALANCED OPTIMAL TRANSPORT

THOMAS GALLOUËT, ROBERTA GHEZZI, AND FRANÇOIS-XAVIER VIALARD

ABSTRACT. Using the dual formulation only, we show that regularity of unbalanced optimal transport also called entropy-transport inherits from regularity of standard optimal transport. We then provide detailed examples of Riemannian manifolds and costs for which unbalanced optimal transport is regular. Among all entropy-transport formulations, Wasserstein-Fisher-Rao metric, also called Hellinger-Kantorovich, stands out since it admits a dynamic formulation, which extends the Benamou-Brenier formulation of optimal transport. After demonstrating the equivalence between dynamic and static formulations on a closed Riemannian manifold, we prove a polar factorization theorem, similar to the one due to Brenier and Mc-Cann. As a byproduct, we formulate the Monge-Ampère equation associated with Wasserstein-Fisher-Rao metric, which also holds for more general costs.

## 1. INTRODUCTION

In the past few years, optimal transport has seen an impressive development mainly driven by applied fields in which real data require robust and largely applicable models. In many applications, data are modeled by probability distributions. To compare two such distributions, optimal transport (OT) provides a distance which is geometrically meaningful. Indeed, OT lifts a distance on the base space to the space of probability measures. In OT, the underlying idea consists in explaining variation of mass between measures via displacement, thereby having a global constraint of equal total mass for the two measures. The last constraint can easily be alleviated with global renormalization but the obtained model will not be able to account for possible local change of mass. Considering this shortcoming, it was natural to enrich the model using local change of mass as proposed by the last author and co-authors and independently by others in [7, 8, 20, 25].

When looking for a generalization of optimal transport to unnormalized measures, there are at least two possible directions. The first one consists in extending the Kantorovich formulation of optimal transport, which is static in contrast to the Benamou-Brenier formulation. This idea amounts to relax the marginal constraints using some divergence such as the relative entropy (Kullback-Leibler). By doing so, it is not trivial to know whether the resulting functional gives a proper distance between positive densities. The second one is to start by the dynamic formulation of Benamou and Brenier [3], which is of interest since it uncovers the Riemannian-like structure of the Wasserstein metric for the  $L^2$  cost. A natural Riemannian tensor on the space of densities which is one-homogeneous with respect to rescaling of mass is the Hessian of the entropy, known as the Fisher-Rao metric when restricted to the set of probability densities.

The latter idea was the starting point of the concurrent works [7, 8, 20, 25] that introduced what is now called *unbalanced optimal transport* and which has seen several applications in data sciences. Arguably, the most significant result on this model is the equivalence between the static formulation and the dynamic formulation [8, 25]. Importantly, the article [25] gives another characterization of unbalanced optimal transport as a standard optimal transport problem on the cone over the base manifold with second order moment constraints. This formulation was exploited in [18, 35] to reformulate the Camassa-Holm equation as a standard incompressible Euler equation on an extension of the cone. Then, generalized flows à la Brenier were studied in [17] for the Camassa-Holm equation and its higher-dimensional extension. Other interesting extensions and related works of the unbalanced framework include the projection of this distance to the set of probability measures using

homogeneity property [23] and gradient flows that retains more convexity than standard Wasserstein gradient flows [22, 21]. The dynamic formulation of unbalanced optimal transport has also drawn some interest [4, 2], also for defining new metrics between metric measure spaces [29, 33]. Applications of unbalanced optimal transport are numerous [38, 31, 32, 33, 14], in particular in data science and computer vision, since this model is more robust in some sense than standard optimal transport and computationally feasible using entropic regularization [9].

An open question in this unbalanced framework is the issue of regularity. In the context of standard optimal transport, regularity appeared after Brenier stated the existence of an optimal transport map under mild conditions in Euclidean space. Since then, an “implicit” regularity of optimal transport was discovered in [6] and following works, see [12] for a recent overview. Regularity does not hold in general but it is observed when the underlying densities are regular and have convex support in Euclidean space. These results are based on Monge-Ampère equation and they have triggered a number of works concerned with extensions to Riemannian manifolds [27].

**Contributions and structure of the article.** In this paper, we address the question of regularity of unbalanced optimal transport. We focus on two important instances of the problem which give rise to a metric on the space of positive Radon measures, namely the Wasserstein-Fisher-Rao (or Hellinger-Kantorovich) and the Gaussian-Hellinger distances. Obviously, there is not just a single map as in standard optimal transport. However, the objects of interest are still encoded via optimal potentials, on which regularity can be studied or from the primal formulation which involves an optimal plan. Interestingly, a plan which minimizes the primal formulation of unbalanced optimal transport actually is an optimal transport plan between its marginals.

From the above remarks, it is expected that regularity of the potentials is inherited from regularity theory for optimal transport. This fact is proven in Section 2 in Theorem 4 by studying the dual formulation and in particular the first-order optimality condition which encodes optimal transport between the optimal marginals. Starting from the general formulation of [25], this theorem requires Lipschitz regularity of the optimal potentials. Existence of Lipschitz potentials is proven in Section 2.2, under geometric conditions on the measures. Under these conditions, we obtain our results for Gaussian-Hellinger and Wasserstein-Fisher-Rao in Section 2.3. In particular, Gaussian-Hellinger is regular on the sphere and the Euclidean space, whereas Wasserstein-Fisher-Rao is regular only on the sphere but not on the Euclidean space. We then focus in Section 3 on the Wasserstein-Fisher-Rao metric for which we show the equivalence between static and dynamic formulations on a closed Riemannian manifold. To derive our main contribution in this section, we take advantage of a geometric point of view to show a polar factorization [5, 27] theorem on a semi-direct product of groups, which is the natural extension of the diffeomorphism group to the unbalanced setting.

## 2. REGULARITY OF UNBALANCED OPTIMAL TRANSPORT

**2.1. From optimal transport regularity to unbalanced optimal transport regularity.** In what follows, we use the notation  $X, Y$  for two spaces that are either Euclidean spaces, bounded convex sets of Euclidean spaces, or Riemannian manifolds. In fact, results in this section apply to the more general setting of [25] but since we are interested in regularity theory, we choose to focus on the aforementioned cases.

We consider the general case of an entropy function, that replaces the relative entropy.

**Definition 1.** An *entropy function*  $F : \mathbb{R} \rightarrow [0, +\infty]$  is a convex, lower semi-continuous, nonnegative function such that  $F(1) = 0$  and  $F(x) = +\infty$  if  $x < 0$ . Its recession constant is  $F'_\infty = \lim_{r \rightarrow +\infty} \frac{F(r)}{r}$ .

**Proposition 1.** *The Legendre-Fenchel transform of  $F$ , denoted by  $F^*$ , has a domain of definition  $\text{dom}(F^*) = (-\infty, F'_\infty]$  and it satisfies*

$$(2.1) \quad \partial F^*(\text{dom}(F^*)) \subset \mathbb{R}_{\geq 0}.$$

Moreover, if  $\partial F(0) = +\infty$ , then  $\partial F^*(\text{dom}(F^*)) \subset \mathbb{R}_{> 0}$ .

**Remark 1.** The hypothesis  $\partial F(0) = +\infty$  is satisfied, for instance, by the choice  $F(x) = x \log(x) - x + 1$ , arguably the most important and most frequent entropy function used in unbalanced optimal transport. In this case, the Legendre-Fenchel transform is  $F^*(x) = e^x - 1$ .

**Definition 2.** Let  $F$  be an entropy function and  $\mu, \nu$  be Radon measures on a Riemannian manifold  $M$ . The *Csiszàr divergence* associated with  $F$  is

$$(2.2) \quad D_F(\mu, \nu) = \int_M F\left(\frac{d\mu(x)}{d\nu(x)}\right) d\nu(x) + F'_\infty \int_M d\mu^\perp,$$

where  $\mu^\perp$  is the orthogonal part of the Lebesgue decomposition of  $\mu$  with respect to  $\nu$ .

One of the most important case is for  $F(x) = x \log(x) - x + 1$ ,  $D_F$  is also known as *Kullback-Leibler divergence* or *relative entropy*, which reads

$$(2.3) \quad \text{KL}(\mu, \nu) = \int \frac{d\mu}{d\nu} \log\left(\frac{d\mu}{d\nu}\right) d\nu + |\nu| - |\mu|.$$

Given  $F$ , the resulting divergence  $D_F$  is jointly convex and lower semi-continuous on the space of pairs of finite and positive Radon measures, see [25, Corollary 2.9]. We can now define the primal formulation of unbalanced optimal transport, which is similar to the Kantorovich formulation of optimal transport. We denote by  $\mathcal{M}_+(X)$  the space of finite and positive Radon measures on  $X$ .

**Definition 3.** Let  $(\rho_0, \rho_1) \in \mathcal{M}_+(X) \times \mathcal{M}_+(Y)$  and  $F_0, F_1$  be entropy functions. The *unbalanced optimal transport problem* is defined as

$$(2.4) \quad \text{UOT}(\rho_0, \rho_1) = \inf_{\gamma \in \mathcal{M}_+(X \times Y)} D_{F_0}(\gamma_0, \rho_0) + D_{F_1}(\gamma_1, \rho_1) + \int_{X \times Y} c(x, y) d\gamma(x, y),$$

where  $\gamma_0, \gamma_1$  are marginals of  $\gamma$ , and  $c : X \times Y \rightarrow \mathbb{R}$  is a cost function.

In this section, we rely on the dual formulation of (2.4) provided by Fenchel-Rockafellar theorem.

**Proposition 2.** The dual formulation of (2.4) is

$$(2.5) \quad \sup_{(z_0, z_1) \in C_b(X) \times C_b(Y)} - \int_X F_0^*(-z_0(x)) d\rho_0(x) - \int_Y F_1^*(-z_1(y)) d\rho_1(y)$$

under the constraint

$$(2.6) \quad z_0(x) + z_1(y) \leq c(x, y).$$

We denote by  $\mathcal{S}(z_0, z_1)$  the functional (2.5) above.

For a proof in the general case, see for instance [25, Proposition 4.3].

Our next goal is to show that regularity of unbalanced optimal transport follows from regularity of standard optimal transport for the cost  $c$ . This result can be expected since once the optimal marginals  $\gamma_0, \gamma_1$  are fixed in (2.4), optimizing on the plan  $\gamma$  (with fixed marginals) is indeed a standard optimal transport problem between  $\gamma_0$  and  $\gamma_1$  for the cost  $c$ .

**Lemma 3.** Assume that the entropy functions  $F_i$  are differentiable on their domain. Let  $(z_0^*, z_1^*) \in C_b(X) \times C_b(Y)$  be a pair of optimal potentials for the dual problem (2.5) satisfying  $\text{range}(-z_i^*) \subset \text{dom}(F_i^*)$ . Then  $(z_0^*, z_1^*)$  is a solution of the standard optimal transport problem

$$(2.7) \quad \sup_{(z_0, z_1) \in C_b(X) \times C_b(Y)} \int_X z_0(x) d\tilde{\rho}_0(x) + \int_Y z_1(y) d\tilde{\rho}_1(y)$$

under the constraint  $z_0(x) + z_1(y) \leq c(x, y)$  where  $\tilde{\rho}_i = F_i^{*'}(-z_i^*)\rho_i$  for  $i = 0, 1$ .

*Proof.* Given some potentials  $(z_0, z_1) \in C_b(X) \times C_b(Y)$ , one can differentiate the dual functional to get

$$\int_X \delta z_0(x) F_0^{*'}(-z_0(x)) d\rho_0(x) + \int_Y \delta z_1(y) F_1^{*'}(-z_1(y)) d\rho_1(y),$$

where  $(\delta z_0, \delta z_1) \in C_b(X) \times C_b(Y)$  denote the first order variations of  $z_0, z_1$ . Such linearization must satisfy the inequality constraint  $z_0(x) + \delta z_0(x) + z_1(y) + \delta z_1(y) \leq c(x, y)$  to give admissible variations. Up to an additive constant, the linearized dual problem can be rewritten as

$$(2.8) \quad \sup_{(z_0, z_1) \in C_b(X) \times C_b(Y)} \int_X \delta z_0(x) d\tilde{\rho}_0(x) + \int_Y \delta z_1(y) d\tilde{\rho}_1(y)$$

under the constraint  $\delta z_0(x) + \delta z_1(y) \leq c(x, y)$ . Whenever  $(z_0^*, z_1^*)$  is optimal for (2.5), the linearized dual problem is nonpositive at  $(z_0^*, z_1^*)$ , because of standard first-order optimality condition, which implies that the linearized formulation (2.8) achieves its optimum at  $(z_0^*, z_1^*)$ .  $\square$

**Remark 2.** *An immediate consequence of this proof is that the corresponding Radon measures  $\tilde{\rho}_i$  have the same total mass. Indeed, given a pair of potentials  $(z_0, z_1)$  satisfying (2.6), for every  $\lambda \in \mathbb{R}$  the pair  $(z_0 + \lambda, z_1 - \lambda)$  still satisfies (2.6). However, the linearized objective functional differs with the term  $\lambda(|\tilde{\rho}_0| - |\tilde{\rho}_1|)$  where  $|\cdot|$  denotes total mass. This term can be made arbitrarily large unless  $|\tilde{\rho}_0| = |\tilde{\rho}_1|$ , thus contradicting the fact that the linearization is bounded.*

The following definition is useful to state the main result of this section.

**Definition 4.** Let  $(\rho_0, \rho_1) \in \mathcal{M}_+(X) \times \mathcal{M}_+(Y)$  be two measures which are absolutely continuous with respect to a reference volume with densities  $(\rho_0, \rho_1) \in C^{k, \alpha}(X) \times C^{k, \alpha}(Y)$  for a given non-negative integer  $k$ ,  $\alpha \in (0, 1)$ . We say that  $(\rho_0, \rho_1)$  is a *k-regular pair of measures* if, for every  $0 \leq l \leq k$  and every pair  $(\lambda_0, \lambda_1) \in C^{l, \alpha}(X) \times C^{l, \alpha}(Y)$  of positive functions bounded away from zero and infinity, the optimal potentials for the pair  $\tilde{\rho}_0 = \lambda_0 \rho_0 / |\lambda_0 \rho_0|$  and  $\tilde{\rho}_1 = \lambda_1 \rho_1 / |\lambda_1 \rho_1|$  are of class  $C^{l+2, \alpha}$ .

This definition/assumption encapsulates the regularity of balanced optimal transport needed for its extension to the unbalanced setting. This condition is realized in [11, Theorem 3.3] for  $C^k$  positive densities whose support is a convex domain and which are bounded away from zero and infinity. More generally, this definition fits well with the regularity theory developed for Monge-Ampère equation. Indeed, there is often geometric assumptions on the support of the measures, for instance convexity in the Euclidean case, which are left unchanged under pointwise multiplication with a positive function.

We now state the main result of this section which says that unbalanced optimal transport inherits the regularity of standard optimal transport associated with the cost  $c$ .

**Theorem 4** (Reduction to standard optimal transport). *Assume that*

- (1) *the Fenchel-Legendre transform of the entropy functions have domain  $[0, +\infty)$ , are  $C^{k+1}$  on  $(0, \infty)$  and  $\partial F_i(0) = +\infty$ ,  $i = 0, 1$ ;*
  - (2) *the pair of measures  $(\rho_0, \rho_1)$  is k-regular;*
  - (3) *the optimal potentials for unbalanced optimal transport  $(z_0^*, z_1^*)$  are Lipschitz continuous.*
- Then, the optimal pair  $(z_0^*, z_1^*)$  is of class  $C^{k+2, \alpha}(X) \times C^{k+2, \alpha}(Y)$ .*

*Proof.* The proof is a straightforward bootstrap argument based on Lemma 3. Since the optimal potentials are Lipschitz, Lemma 3 gives that these potentials are optimal for a new pair of densities which inherits smoothness from the potentials and the initial densities, namely  $\tilde{\rho}_i = F_i^{*'}(-z_i^*)\rho_i$ . Hypothesis (1) gives that  $F_i^{*'}(-z_i^*)$  is  $C^l$  if  $z_i \in C^l$  for  $l \leq k$ . It implies that the regularity of  $\tilde{\rho}_i$  is given by that of  $z_i$ . At the initialization step of the bootstrap, they are only Lipschitz, and applying the Lemma, the optimal potentials gain in regularity to be  $C^{3,1}$ . Then, in turn, we obtain that the marginals are  $C^{\min(k,3)}$ . Iterating this bootstrap argument gives the result, the optimal potentials are  $C^{k+2, \alpha}$  and the optimal marginals  $\tilde{\rho}_i$  are  $C^{k, \alpha}$ .  $\square$

Note that assumption (1) ensures that the resulting marginals are sufficiently smooth and with unchanged support, i.e., the multiplicative term  $F_i^{*'}(-z_i^*)$  does not vanish. Existence of Lipschitz potentials is in general a consequence of Lipschitz continuity of the cost. However, for unbounded costs, it requires more assumptions, as detailed in the next section for the Wasserstein-Fisher-Rao metric.

**2.2. Existence of Lipschitz potentials for unbounded costs.** The choice of cost  $c$  in formulation (2.4) may vary. For instance, in usual applications outside mathematics, the Euclidean squared distance is often used. From the mathematical point of view, the case of

$$(2.9) \quad c(x, y) = -\log \left( \cos^2 \left( d(x, y) \wedge \frac{\pi}{2} \right) \right)$$

stands out since it appears in the static formulation of the Wasserstein-Fisher-Rao metric. Importantly, this cost is unbounded as well as its gradients, since it blows up when  $d(x, y)$  is close to  $\pi/2$ . In this section we prove existence of Lipschitz potential for the maximization problem in (2.5), (2.6) for unbounded costs under an admissibility assumption on the source and target measure. Such condition may be interpreted by saying that pure creation/destruction of mass is forbidden or, in other words, mass transport must be performed between the source and target measure on the whole supports.

For simplicity, we consider the case where  $M$  is either a compact Riemannian manifold or a convex and compact domain in Euclidean space. Let us recall the notion of conjugate function. Let  $c : M \times M \rightarrow \mathbb{R} \cup \{\pm\infty\}$  be a continuous function. The  $c$ -conjugate of a function  $z : M \rightarrow \mathbb{R}$  is defined by

$$\hat{z}(x) = \inf_{y \in M} c(x, y) - z(y).$$

We now define a class of functions that will be considered in this section as costs. In particular, such costs can be unbounded.

**Definition 5.** A function  $c : M \times M \rightarrow \mathbb{R} \cup \{\pm\infty\}$  is a *cost function* if it is bounded below and if, for every  $L \in \mathbb{R}$ , the restriction of  $c$  on the sub-level  $c^{-1}((-\infty, L])$  is Lipschitz.

Obviously, the Lipschitz constant on a sub-level may depend on the chosen  $L$ .

**Definition 6** (Admissible measures). A pair of Radon positive measures  $(\rho_1, \rho_2)$  is *admissible* if, denoting  $K_i = \text{Supp}(\rho_i)$ ,  $K_i \neq \emptyset$   $i = 1, 2$ , and there holds

$$(2.10) \quad \max \left( \sup_{x \in K_1} \inf_{y \in K_2} c(x, y), \sup_{y \in K_2} \inf_{x \in K_1} c(x, y) \right) < \infty.$$

We denote this finite number by  $c_H(\rho_1, \rho_2)$ .

When considering the distance as cost function, being admissible simply means that the supports of the source and target measure have finite Hausdorff distance.

**Proposition 5.** Let  $F_0, F_1$  be entropy functions that have finite value at 0. Let  $(\rho_0, \rho_1) \in \mathcal{M}_+(M)^2$  be a pair of admissible measures. Then there exists an optimal pair  $(z_0, z_1) \in C(M)^2$  for the maximization problem in (2.5). Moreover,  $z_i$  is locally Lipschitz on  $K_i$ ,  $i = 0, 1$  and  $z_1 = \hat{z}_0$ .

Let us first prove an auxiliary technical lemma.

**Lemma 6.** Let  $(\rho_0, \rho_1)$  be an admissible pair of measures. Then, there exist  $x_1, \dots, x_k \in M$  and  $r_1, \dots, r_k > 0$  such that  $\rho_0(B(x_i, r_i)) > 0$  and for any  $y \in K_1$ , there exists  $\bar{i} \in \{1, \dots, k\}$  such that  $\sup_{x \in B(x_{\bar{i}}, r_{\bar{i}})} c(x, y) < c_H(\rho_0, \rho_1) + 1$ .

*Proof.* Since the pair  $(\rho_0, \rho_1)$  is admissible, for every  $y \in K_1$ , there exists  $B(x_y, r_y)$  and  $B(y, \delta_y)$  such that  $\sup_{x_1 \in B(x_y, r_y), y_1 \in B(y, \delta_y)} c(x_1, y_1) < c_H(\rho_0, \rho_1) + 1$  and  $\rho_1(B(x_y, r_y)) > 0$ . Since  $K_0$  is compact, there exists a finite number of points  $(x_i)_{i=1, \dots, k}$  such that the announced result is satisfied.  $\square$

*Proof of Proposition 5.* Recall that  $\mathcal{S}(z_0, z_1)$  denotes the functional in the maximization problem (2.5). Remark that  $\mathcal{S}(0, 0) = 0$ , hence the supremum in (2.5) is nonnegative. Moreover, taking the  $c$ -conjugate of  $z_0$  improves the value of  $\mathcal{S}$ , i.e.,  $\mathcal{S}(z_0, \hat{z}_0) \geq \mathcal{S}(z_0, z_1)$ . Iterating this alternate optimization enables to restrict the optimization set to pairs of potentials that satisfy  $z_1 = \hat{z}_0$  and  $z_0 = \hat{z}_1$  (indeed, the  $c$ -conjugate is an involution on its range). We prove that the set

$$(2.11) \quad \mathcal{E} = \{(z_0, z_1) \in C(M)^2 \mid (2.6) \text{ is satisfied, } \mathcal{S}(z_0, z_1) \geq 0 \text{ and } z_1 = \hat{z}_0, z_0 = \hat{z}_1\}$$

is equibounded and equi-Lipschitz, i.e., there exists a constant  $L > 0$  such that for every pair  $(z_0, z_1) \in \mathcal{E}$ ,  $z_0|_{\text{supp}(\rho_0)}$  and  $z_1|_{\text{supp}(\rho_1)}$  are locally  $L$ -Lipschitz.

Let us start by equiboundedness of  $\mathcal{E}$ . Consider  $B(x_i, r_i)$  for  $i = 1, \dots, k$  given by Lemma 6 for the measure  $\rho_0$  such that

$$\inf_{y \in \text{Supp}(\rho_1)} \min_{i=1, \dots, k} c(y, x_i) \leq c_H + 1.$$

Since  $F_0^*(x) \geq \langle x, 0 \rangle - F_0(0) = -F_0(0)$ , for every  $i \in 1, \dots, k$ , there holds

$$0 \leq \mathcal{S}(z_0, \hat{z}_0) \leq -\rho_0(B(x_i, r_i))F_0^*(-\tilde{z}) + F_0(0)\rho_0(M) + F_1(0)\rho_1(M)$$

where  $\tilde{z} = \max(\sup_{x \in B(x_i, r_i)} z_0(x), 0)$ . As a consequence, denoting  $\delta > 0$  the minimum of  $\rho_0(B(x_i, r_i))$  for  $i = 1, \dots, k$ , one has, since  $F_0^*(-\tilde{z}) \geq 0$ ,

$$(2.12) \quad -F_0(0)\rho_0(M) - F_1(0)\rho_1(M) \leq -\delta F_0^*(-\tilde{z}).$$

Moreover, since  $F_0^*(x) \geq \langle x, 1 \rangle - F_0(1) = x$ , the following lower bound

$$\tilde{z} \geq \frac{-F_0(0)\rho_0(M) - F_1(0)\rho_1(M)}{\delta}$$

holds. Set  $\kappa = (-F_0(0)\rho_0(M) - F_1(0)\rho_1(M))/\delta$ . Denote by  $\alpha \stackrel{\text{def.}}{=} \inf_{x \in M} \min_i c(x, x_i)$ , then

$$\begin{aligned} \hat{z}_0(y) &\leq \inf_x c(x, y) - z_0(x) \\ &\leq \alpha - \kappa. \end{aligned}$$

where  $x_i$  is chosen such that  $c(x_i, y) < c_H(\rho_0, \rho_1) + 1$ . Hence  $\hat{z}_0$  is bounded above. As a direct consequence,  $z_0$  is bounded below. By symmetry of the hypothesis on  $\rho_0, \rho_1$ , we obtain that there exists  $A, B$ , depending only on  $\rho_0, \rho_1, F_0^*, F_1^*$  and  $c_H(\rho_0, \rho_1)$  such that  $B \leq z_0 \leq A$  and  $B \leq \hat{z}_0 \leq A$ , for every  $(z_0, \hat{z}_0) \in \mathcal{E}$ .

We now prove that there exists a uniform constant  $L$  such that for every pair  $(z_0, z_1) \in \mathcal{E}$ ,  $z_i$  is Lipschitz continuous with constant  $L$ . Let  $(z_0, z_1) \in \mathcal{E}$ . By definition of  $\mathcal{E}$ ,  $z_0 = \hat{z}_1$ . Since  $z_1$  is bounded above by  $A$ , the infimum is attained at a point  $y(x)$  such that  $c(x, y(x)) \leq B - A$ ,

$$\hat{z}_0(x) = c(x, y(x)) - z_1(y(x))$$

and moreover, for every  $x' \in M$ ,

$$\hat{z}_0(x') \leq c(x', y(x)) - z_1(y(x)).$$

Subtracting the two previous formulas gives

$$\hat{z}_0(x') - \hat{z}_0(x) \leq c(x', y(x)) - c(x, y(x)).$$

Let  $L$  be the Lipschitz constant of  $c$  on the sublevel  $c^{-1}((-\infty, B - A])$ , then

$$|\hat{z}_0(x') - \hat{z}_0(x)| \leq Ld(x, x').$$

Therefore  $\mathcal{E}$  is not empty, equibounded and equi-Lipschitz. As a consequence, existence of an optimal pair  $(z_0, z_1)$  for (2.5) with the required properties is obtained with a standard argument based on Ascoli–Arzelà theorem for compactness and dominated convergence theorem for the convergence of the functional  $\mathcal{S}$ .  $\square$

As concerns uniqueness, an obvious sufficient condition is given by the following statement.

**Proposition 7.** *If  $F_0^*$  and  $F_1^*$  are strictly convex, the optimal pair  $(z_0, z_1)$  is unique  $\rho_0$  and  $\rho_1$  a.e.*

*Proof.* The maximization problem (2.5) is strictly convex.  $\square$

Collecting the previous results leads to existence and uniqueness of optimal Lipschitz potentials for (2.4).

**Corollary 8.** *Let  $F_0(x) = F_1(x) = x \log(x) - x + 1$  and*

$$(2.13) \quad c(x, y) = \frac{1}{2}d(x, y)^2, \text{ or } c(x, y) = -\log(\cos^2(d(x, y) \wedge \delta\pi/2))$$

*for some  $\delta > 0$ . Then, for every pair of admissible measures, there exists a unique pair of Lipschitz continuous optimal potentials for the dual formulation (2.5).*

Note that any pair of measures is admissible for the quadratic cost.

Combining Theorem 4 and Corollary 8, regularity results for the costs in (2.13) can be inferred in different ways depending on the choice of the ambient space  $M$ . When  $M = \mathbb{R}^d$ , the quadratic cost supports regularity theorems for optimal transport. For the second cost in (2.13), regularity results also hold for  $M = S^d$  the unit sphere of dimension  $d$  and for the sphere of radius  $1/2$  (see Section 2.3). In [25], such cases are named after Gaussian-Hellinger for the quadratic case, and Hellinger-Kantorovich (or Wasserstein-Fisher-Rao) for the other cost.

**2.3. Two important costs for regularity of unbalanced optimal transport.** We discuss the case of two important costs in unbalanced optimal transport. The first one is the most commonly used in practical applications, the Euclidean squared cost. The second one arises naturally from the dynamic formulation which was originally proposed to introduce this model.

**Gaussian-Hellinger distance: Euclidean space and spheres.** Regularity in these two cases is an immediate consequence of Theorem 4 and the regularity of optimal transport, for which sufficient conditions ensuring assumption (3) in Theorem 4 are well-known. We simply detail the case of the Euclidean space, for which the following statement holds true, as a consequence of [11, Theorem 3.3].

**Corollary 9.** *Let  $X, Y$  be convex sets in  $\mathbb{R}^d$  and let  $(\mu, \nu) \in \mathcal{M}_+(X) \times \mathcal{M}_+(Y)$  be a pair of measures which are absolutely continuous with respect to the Lebesgue measure, with densities  $(f, g)$  bounded away from zero and infinity. Assume the entropy functions  $F_0, F_1$  have strictly convex and differentiable Fenchel-Legendre transforms with infinite slope at 0.*

*If  $(f, g) \in C^{k, \alpha}(\bar{X}) \times C^{k, \alpha}(\bar{Y})$  for some positive integer  $k$  and  $\alpha \in (0, 1)$ , then, the pair of optimal potentials  $(z_0, z_1)$  in the dual formulation (2.5) for the quadratic cost  $\frac{1}{2}\|x - y\|^2$  belongs to  $C^{k+2, \alpha}(X) \times C^{k+2, \alpha}(Y)$  and  $\nabla z_0$  is a  $C^{k+1, \alpha}$ -diffeomorphism between  $\bar{X}$  and  $\bar{Y}$ .*

**Wasserstein-Fisher-Rao distance.** We consider the case of a  $d$ -dimensional Riemannian manifold  $M$  having constant sectional curvature, i.e.,  $M$  may be the Euclidean space, a  $d$ -sphere, or the hyperbolic space and

$$(2.14) \quad c(x, y) = -\log\left(\cos\left(d(x, y) \wedge \frac{\pi}{2}\right)^2\right).$$

Here We provide sufficient conditions to ensure assumption (3) in Theorem 4 based on the study of Ma-Trudinger-Wang tensor for the cost above on such manifolds.

Since [26], the study of the so-called Ma-Trudinger-Wang (MTW) tensor allows to provide sufficient conditions to imply regularity of potential functions in optimal transport. In particular: MTW weak condition states that MTW tensor must be nonnegative for every pair of points and every pair of  $c$ -orthogonal vectors; MTW strong condition states that MTW weak condition holds true and the tensor vanishes only at vanishing vectors. MTW tensor for costs of the type  $c(x, y) = l(d(x, y))$  was analysed in [24] for even smooth functions  $l : \mathbb{R} \rightarrow [0, +\infty)$  having invertible derivative. In particular, authors characterize MTW weak and strong conditions on manifolds with constant sectional curvature in terms of some computable explicit functions, see [24, Theorem 5.3].

**Proposition 10.** *Let  $M$  be a Riemannian manifold with constant sectional curvature and let  $c : M \times M \rightarrow \mathbb{R} \cup \{+\infty\}$  be as in (2.14).*

*Then*

- (i) *MTW weak condition for  $c$  fails if  $M$  is either the Euclidean space, either hyperbolic space or the  $d$ -sphere of radius  $R > 1$  with the Riemannian metric induced by  $\mathbb{R}^d$ ;*



- (ii) *MTW weak condition holds for  $c$  if  $M$  is the unit  $d$ -sphere with the Riemannian metric induced by  $\mathbb{R}^d$ ;*
- (iii) *MTW strong condition holds for  $c$  if  $M$  is the  $d$ -sphere of radius  $1/2$  with the Riemannian metric induced by  $\mathbb{R}^d$ .*

*Proof.* We start by recalling the main results in [24]. Consider a cost function  $J(x, y) = l(d(x, y))$ , where  $l : \mathbb{R} \rightarrow [0, +\infty[ \rightarrow \mathbb{R}$  is a smooth, even function such that  $l''(s) > 0$ . Set  $h(s) = (l')^{-1}(s)$ . Then the  $J$ -exponential map can be computed as

$$J\text{-exp}_x(v) = \exp_x\left(\frac{h(v)}{|v|}v\right),$$

where  $\exp_x$  denotes the Riemannian exponential on  $M$ . By definition, the *MTW* tensor is

$$MTW_x(u, v, w) = -\frac{3}{2}\partial_s^2\partial_t^2|_{s=t=0}J(\exp_x(tu), J\text{-exp}_x(v+sw)),$$

where  $x \in M$ , and  $u, v, w$  are tangent vectors at  $x$ . Define  $A(s) = \frac{1}{h(s)}$ , and

$$B(s) = \begin{cases} s \coth(h(s)), & \text{if } M \text{ is the hyperbolic space,} \\ \frac{s}{h(s)}, & \text{if } M \text{ is Euclidean space,} \\ s \cot(h(s)), & \text{if } M \text{ is the unit sphere.} \end{cases}$$

By [24, Proposition 5.1], whenever  $u$  and  $w$  are  $J$ -orthogonal, the *MTW* tensor can be simplified to

$$MTW_x(u, v, w) = -\frac{3}{2}(\alpha(|v|)|u_0|^2|w_0|^2 + \beta(|v|)|u_0|^2|w_1|^2 + \gamma(|v|)|u_1|^2|w_0|^2 + \delta(|v|)|u_1|^2|w_1|^2),$$

where  $u = u_0 + u_1$ ,  $w = w_0 + w_1$ ,  $u_0, w_0 \in \text{span}\{v\}$ ,  $u_1, w_1 \in (\text{span}\{v\})^\perp$  and coefficients are given by

$$\begin{aligned} \alpha(s) &= \frac{s^2 A''(s) + 6(A(s) - B(s)) - 4s(A'(s) - B'(s))}{s^2}, \\ \beta(s) &= \frac{sA'(s) - 2(A(s) - B(s))}{s^2}, \\ \gamma(s) &= B''(s), \\ \delta(s) &= \frac{B'(s)}{s}, \end{aligned}$$

in terms of functions  $A, B$  defined above. By Theorem 5.3 in [24], *MTW* tensor satisfies *MTW* weak condition if and only if, for every  $s \in [0, |l'(D)|]$ , with  $D$  the diameter of  $M$ , four inequalities hold

$$\beta(s) \leq 0, \quad \gamma(s) \leq 0, \quad \delta(s) \leq 0, \quad \alpha(s) + \delta(s) \leq 2\sqrt{\beta(s)\gamma(s)}.$$

Moreover, *MTW* weak condition holds if and only if the four inequalities are strict.

Note that cost  $c$  in (2.14) is of the type  $l(d(x, y))$ , for  $l(s) = -\log(\cos^2(s))$ . We compute explicitly functions  $A, B$  for the hyperbolic space and for the Euclidean space. In both cases,  $\beta(0) > 0$ , whence *MTW* weak condition fails.

When  $M$  is the  $d$ -sphere of radius  $R \in (0, +\infty)$ , we can interpret the cost  $c$  in (2.14) as  $c(x, y) = l_R(d(x, y))$  where  $l_R(x, y) = -\log(\cos^2(Rs))$ . Hence we can compute *MTW* tensor by means of  $B(s) = s \cot(h_R(s))$ , with  $h_R = (l'_R)^{-1}$ . Computing explicitly,  $\beta(0) = \gamma(0) = \delta(0) = \frac{1}{3}\left(1 - \frac{1}{R^2}\right)$ . Therefore we conclude that when  $R > 1$  *MTW* weak condition fails. On the other hand, an explicit computation gives

$$\begin{aligned} \text{for } R = 1, \quad & \alpha(s) = \beta(s) = \gamma(s) = \delta(s) \equiv 0, \\ \text{for } R = \frac{1}{2}, \quad & \alpha(s) = \beta(s) = \gamma(s) = \delta(s) \equiv -1, \end{aligned}$$

Hence for  $R = 1$  *MTW* weak condition holds and *MTW* vanishes on  $c$ -orthogonal vectors, whereas for  $R = 1/2$  *MTW* strong condition holds □

Explicit computations of coefficients  $\alpha, \beta, \gamma, \delta$  on the  $d$ -sphere suggest that MTW weak condition holds if and only if the radius of the sphere satisfies  $R \in (0, 1)$ .

### 3. THE WASSERSTEIN-FISHER-RAO METRIC

In this section, we detail the case of the Wasserstein-Fisher-Rao (WFR) metric on a smooth compact Riemannian manifold  $M$ , which is the cornerstone of unbalanced optimal transport as introduced in [20, 7, 25]. Recall that the Wasserstein-Fisher-Rao corresponds to the cost function given in 2.14 and to the Kullback-Leibler divergence for the marginal penalization (i.e., both entropy functions are given by  $F(x) = x \log(x) - x + 1$ ). First we prove the equivalence of several definitions of this metric. In particular we introduce an equivalent of the Monge formulation of standard OT to this unbalanced setting. Using this formulation we prove the existence of unbalanced optimal transport maps and an unbalanced version of Brenier polar factorization Theorem on the automorphism group of the cone  $\mathcal{C}(M)$  see Theorem 18. A regularity theory for such maps is obtained in section 2 and it is linked to an unbalanced Monge-Ampère equation, see section 3.3.

**3.1. Equivalent formulations of WFR metric.** As in classical optimal transport, the Wasserstein-Fisher-Rao metric can be defined in many ways. Here we detail five of them, namely: Monge, Kantorovich, semi-couplings, dual and dynamical formulation. The Kantorovich formulation is the one introduced in Definition 2.4 and the dual formulation is given in Proposition 2. For the sake of clarity we instantiate them hereafter. Note that the starting point of the Wasserstein-Fisher-Rao metric consists in introducing the dynamical formulation given as a natural generalization of the Benamou-Brenier formulation.

**3.1.1. Dynamical formulation of WFR.** The main idea to a dynamical formulation is to consider Benamou-Brenier formula and introduce a source term in the continuity equation. This gives rise to the following optimization problem.

Consider two nonnegative Radon measures on  $M$  denoted by  $\rho_0$  and  $\rho_1$ . Denote by  $g$  the Riemannian metric on  $M$  and by  $\text{div}$  the divergence of a vector field computed with respect to the Riemannian volume. Computing the distance between  $\rho_0$  and  $\rho_1$  consists in minimizing the following functional, where  $a, b > 0$ ,

$$\inf_{\rho, v, \alpha} \frac{1}{2} \int_0^1 \left( \int_{\Omega} a^2 g_x(v(x), v(x)) + b^2 \alpha^2(x) d\rho_t(x) \right) dt$$

under the constraint of the generalized continuity equation

$$\partial_t \rho + \text{div}(\rho v) = \alpha \rho.$$

Here the control variables are  $\alpha$ , the growth rate (also called Malthusian parameter) and  $v$ , a vector field, both depending on time  $t$  and position  $x \in M$ .

**Remark 3.** For  $\alpha \equiv 0$ , the dynamic formulation above is the well-known Benamou-Brenier formulation of the optimal transport problem [3].

We now give a more rigorous definition in analytical terms.

**Definition 7** (Dynamical formulation of WFR metric). Let  $\rho_0, \rho_1 \in \mathcal{M}_+(M)$ , the WFR metric is defined by

$$\text{WFR}^2(\rho_0, \rho_1) = \inf_{\rho, \mathbf{m}, \mu} \mathcal{J}(\rho, \mathbf{m}, \mu),$$

where

$$(3.1) \quad \mathcal{J}(\rho, \mathbf{m}, \mu) = a^2 \int_0^1 \int_M \frac{g_x^{-1}(\tilde{\mathbf{m}}(t, x), \tilde{\mathbf{m}}(t, x))}{\tilde{\rho}(t, x)} d\nu(t, x) + b^2 \int_0^1 \int_M \frac{\tilde{\mu}(t, x)^2}{\tilde{\rho}(t, x)} d\nu(t, x)$$

over the set  $(\rho, \mathbf{m}, \mu)$  satisfying  $\rho \in \mathcal{M}_+([0, 1] \times M)$ ,  $\mathbf{m} \in (\Gamma_M^0([0, 1] \times M, TM))^*$  which denotes the dual of time dependent continuous vector fields on  $M$  (time dependent sections of the tangent bundle),  $\mu \in \mathcal{M}([0, 1] \times M)$  subject to the constraint

$$(3.2) \quad \int_0^1 \int_M \partial_t f d\rho + \int_0^1 \int_M (\mathbf{m}(\nabla_x f) - f \mu) d\nu = \int_M f(1, \cdot) d\rho_1 - \int_M f(0, \cdot) d\rho_0$$

satisfied for every test function  $f \in C^1([0, 1] \times M, \mathbb{R})$ . Moreover,  $\nu$  is chosen such that  $\rho, \mathfrak{m}, \mu$  are absolutely continuous with respect to  $\nu$  and  $\tilde{\rho}, \tilde{\mathfrak{m}}, \tilde{\mu}$  denote their Radon-Nikodym derivative with respect to  $\nu$ .

Note that due to the one-homogeneity of the formulas with respect to  $(\tilde{\rho}, \tilde{\mathfrak{m}}, \tilde{\mu})$ , the functional  $\mathcal{J}$  is well-defined, i.e., it does not depend on the choice of the dominating measure  $\nu$ . Moreover, the divergence is defined by duality on the space  $C^1(M)$ . Formula (3.1) in Definition 7 is called dynamic since the time variable is involved and only length-space structures can be defined in this way. It is of interest to show that the variational problem admits a so-called static formulation that does not involve the time variable.

3.1.2. *Semi-couplings formulation of WFR.* The semi-couplings formulation already appears in [8] and in another form in [25] where the equivalence with the dynamical formulation was proved in both papers only in the Euclidean case. We now extend these results to a Riemannian setting.

**Theorem 11** (Semi-couplings formulation of WFR metric). *Given  $\rho_0, \rho_1 \in \mathcal{M}_+(M)$ , we set*

$$\Gamma(\rho_0, \rho_1) \stackrel{\text{def.}}{=} \left\{ (\gamma_0, \gamma_1) \in (\mathcal{M}_+(M^2))^2 : p_*^1 \gamma_0 = \rho_0, p_*^2 \gamma_1 = \rho_1 \right\},$$

where  $p^1$  and  $p^2$  denote the projection on the first and second factors of the product  $M^2$ . The variational problem associated with the Wasserstein-Fisher-Rao distance satisfies

$$(3.3) \quad \text{WFR}^2(\rho_0, \rho_1) = \min_{(\gamma_0, \gamma_1) \in \Gamma(\rho_0, \rho_1)} \int_{M^2} d_{\mathcal{C}(M)}^2 \left( \left( x, \frac{d\gamma_0}{d\gamma} \right), \left( y, \frac{d\gamma_1}{d\gamma} \right) \right) d\gamma(x, y),$$

where  $d_{\mathcal{C}(M)}^2$  is the square of the cone distance given by

$$g(x, r)(dx, dr) = a^2 r^2 dx^2 + 4b^2 dr^2,$$

and  $\gamma$  is any measure that dominates  $\gamma_0, \gamma_1$ .

**Remark 4.** *The fact that  $S(\gamma_1, \gamma_2) \stackrel{\text{def.}}{=} \int_{M^2} d_{\mathcal{C}(M)}^2 \left( \left( x, \frac{d\gamma_1}{d\gamma} \right), \left( y, \frac{d\gamma_2}{d\gamma} \right) \right) d\gamma(x, y)$  is well-defined follows from the application of [30, Theorem 5]. It does not depend on the choice of the measure  $\gamma$  since the function  $d^2$  is one-homogeneous w.r.t. the mass variables. As a consequence of Rockafellar's theorem [30, Theorem 5],  $\mathcal{S}$  is convex and lower-semicontinuous on the space of Radon measures as the Legendre-Fenchel transform of a convex functional on the space of continuous functions.*

Our proof of Theorem 11 is an adaptation to the Riemannian case of the one in [8, Theorem 4.3], to which we refer the reader for technical details. Under minor adaptations, the same argument, based on a simple regularization argument which is intrinsic on Riemannian manifolds, applies to the standard Wasserstein  $L^2$  metric on Riemannian manifolds, see for instance the comments in [37, Remark 8.3]. A different demonstration of the standard Wasserstein case is given in [1] which uses the Nash isometric embedding theorem.

*Proof of Theorem 11.* The fact that the minimum for  $S$  is attained follows by application of the direct method of calculus of variations. The set  $\Gamma$  is weakly closed and the functional is weakly continuous and  $S$  is lower semicontinuous. In the following, we denote by  $\mathcal{S}^2(\rho_1, \rho_2)$  the minimization of the r.h.s. of (3.3).

Since  $d$  is a distance on the cone, one can prove that  $\mathcal{S}$  is a distance on the space of nonnegative Radon measures which is continuous w.r.t. the weak-\* topology, as done in [8, Theorems 2,3].

On the set of measures that are finite sum of Dirac masses, the minimization problem (3.3) can be reduced to a linear optimization problem in finite dimension. Indeed, the optimal semi-couplings can be proved to have support on the product of the support of  $\rho_1$  and  $\rho_2$ . Denoting  $\rho_1 = \sum_i a_i \delta_{x_i}$  and  $\rho_2 = \sum_j b_j \delta_{y_j}$  for  $x_i, y_j$  a finite number of points in  $M$ , optimal semi-couplings can be written

as  $\gamma^k = \sum_{i,j} m_{i,j}^k \delta_{x_i, x_j}$  for  $k = 1, 2$ . Then, one has

$$\begin{aligned} \mathcal{S}^2(\rho_1, \rho_2) &= \sum_{i,j} d^2((x_i, m_{i,j}^1), (y_j, m_{i,j}^2)) \\ &\geq \sum_{i,j} \text{WFR}^2(m_{i,j}^1 \delta_{x_i}, m_{i,j}^2 \delta_{y_j}) \geq \text{WFR}^2(\rho_1, \rho_2), \end{aligned}$$

where the first inequality comes from the fact that the distance on the cone (with mass coordinates) for a geodesic  $(x(t), m(t))$  is given by the evaluation of WFR on the path  $m(t)\delta_{x(t)}$ . The second inequality is given by subadditivity of  $\text{WFR}^2$ . By density of this set of measures and weak-\* continuity of WFR and  $\mathcal{S}$ , one has  $\mathcal{S} \geq \text{WFR}$ .

The reverse inequality follows using the convexity of  $\text{WFR}^2$ . By subadditivity of  $\text{WFR}^2$ , one has, for any positive Radon measure  $\rho_3$

$$(3.4) \quad \text{WFR}^2(\rho_1 + \rho_3, \rho_2 + \rho_3) \leq \text{WFR}^2(\rho_1, \rho_2).$$

Using the triangular inequality and the fact that the WFR metric is bounded above (up to a multiplicative constant) by the Hellinger distance, we also have, for  $\varepsilon_1 > 0$

$$(3.5) \quad \text{WFR}(\rho_0, \rho_1) \leq \text{WFR}(\rho_0 + \varepsilon_1 \text{vol}, \rho_1 + \varepsilon_1 \text{vol}) + 2 \text{cst} \sqrt{\varepsilon_1}.$$

Let us be more precise on the previous inequality: Consider now a path  $\rho, \mathbf{m}, \mu$  which is a solution to the continuity equation (3.2), then so is the path  $\rho + \varepsilon_1 \text{vol}, \mathbf{m}, \mu$  satisfying the boundary conditions  $\rho(0) = \rho_0, \rho(1) = \rho_1$ . Note that  $\varepsilon_1 \text{vol}$  is constant in time and space. In addition, it is obvious that

$$\mathcal{J}(\rho + \varepsilon_1 \text{vol}, \mathbf{m}, \mu) \leq \mathcal{J}(\rho, \mathbf{m}, \mu).$$

To prove the final result, it suffices to prove that  $\mathcal{S}(\rho_0 + \varepsilon_1 \text{vol}, \rho_1 + \varepsilon_1 \text{vol}) \leq \mathcal{J}(\rho + \varepsilon \text{vol}, \mathbf{m}, \mu) + \varepsilon_0$  for any  $\varepsilon_0 > 0$ . This will be done via a smoothing argument which is standard in the Euclidean case using convolution but has never been adapted, to the best of our knowledge, to work on Riemannian manifolds (see [37, Remarks 8.3]).

Our goal is to prove that there exists a path of smooth quantities  $(\rho_\varepsilon, \mathbf{m}_\varepsilon, \mu_\varepsilon)$  for which  $\mathcal{J}(\rho_\varepsilon, \mathbf{m}_\varepsilon, \mu_\varepsilon)$  is close to  $\mathcal{J}(\rho, \mathbf{m}, \mu)$  and  $\rho_\varepsilon$  is strictly positive and the time endpoints of the path are close in the weak-\* topology. The conclusion can then be obtained by integrating the flow defined by the vector field  $(\mathbf{m}_\varepsilon/\rho_\varepsilon, \mu_\varepsilon/\rho_\varepsilon)$ . It gives that  $\mathcal{S}(\rho_\varepsilon(0), \rho_\varepsilon(1)) \leq \mathcal{J}(\rho_\varepsilon, \mathbf{m}_\varepsilon, \mu_\varepsilon)$  and the conclusion is similar to the Euclidean case [8, Theorem 5].

By compactness of  $M$ , it is sufficient to locally smooth the path on  $M$  by iteration of this smoothing. Therefore, we will work on a chart  $U$  around a point  $x_0 \in M$ . By Moser's lemma, it is possible to choose the chart such that the volume form is the Lebesgue measure.

**Averaging over perturbations of identity:** We construct perturbations (of compact support) of the identity which will be local translations around  $x_0$  and which will play the role of the translations in the standard convolution formula. We consider a ball  $B(x_0, r_0)$  and a function  $u$  whose support is contained in  $B(x_0, r_0)$  and is constant equal to 1 on  $B(x_0, r_1)$  for  $0 < r_1 < r_0$ . For a given vector  $v \in \mathbb{R}^d$ , we consider the map  $\Phi_v(x) = x + u(x)v$  which is a smooth diffeomorphism. We extend  $\Phi$  to the whole manifold  $M$  by defining it as identity outside of  $U$ .

Let  $k : \mathbb{R}^{d+1} \rightarrow \mathbb{R}_+$  be a smooth symmetric function whose support is contained in the unit ball and such that  $\int k(y) dy = 1$  and define for  $\varepsilon > 0$ ,  $k_\varepsilon(x) = k(x/\varepsilon)/\varepsilon^{d+1}$  whose support is thus contained in the ball of radius  $\varepsilon$ . We define the mollifier  $k_\varepsilon \star$  acting on  $f \in C([0, 1] \times U, \mathbb{R})$  by

$$(3.6) \quad (k_\varepsilon \star f)(s, x) = \int_{\mathbb{R}} \int_U k_\varepsilon(s, v) f(t + s, \Phi_v^{-1}(x)) dv ds,$$

which is well defined for  $\varepsilon$  small enough, extending the function outside the time interval  $[0, 1]$  as a constant. Moreover, for  $\varepsilon$  sufficiently small, it coincides with the usual convolution on a neighborhood of  $x_0$ . By duality, it is well defined on Radon measures and extends trivially to vector

valued measures as follows:

$$(3.7) \quad (\mathbf{k}_\varepsilon \star \rho)(s, x) = \int_{\mathbb{R}} \int_U k_\varepsilon(s, v) (\Phi_v)_*(\rho(t+s)) \, dv \, ds,$$

$$(3.8) \quad (\mathbf{k}_\varepsilon \star m)(s, x) = \int_{\mathbb{R}} \int_U k_\varepsilon(s, v) \text{Ad}_{\Phi_v^{-1}}^*(m(t+s)) \, dv \, ds.$$

We consider the path  $(\Phi_v)_*(\rho)$  which satisfies the continuity equation for the triple of measures  $\left( (\Phi_v)_*(\rho), \text{Ad}_{\Phi_v^{-1}}^*(m), (\Phi_v)_*(\mu) \right)$  and average over  $v$  to consider

$$(3.9) \quad (\rho_\varepsilon, \mathbf{m}_\varepsilon, \mu_\varepsilon) = (\mathbf{k}_\varepsilon \star \rho, \mathbf{k}_\varepsilon \star m, \mathbf{k}_\varepsilon \star \mu).$$

As a convex combination, this path satisfies the continuity equation and the boundary conditions are close in the weak-\* topology when  $\varepsilon$  tends to 0. An important remark is that, for  $\varepsilon$  small enough,  $\mathbf{k}_\varepsilon \star \text{Ad}_{\Phi_v^{-1}}^*(m)$  reduces to the standard convolution on  $m$  in a small neighborhood of  $x_0$  since  $D\Phi_v = \text{Id}$  in a neighborhood of  $x_0$  since  $u \equiv 1$  on  $B(x_0, r_1)$ .

**Use of convexity of  $\mathcal{J}$ :** For notation convenience, we denote by  $f$  the integrand of  $\mathcal{J}$  and we make the abuse of notation to use  $\rho, m, \mu$  instead of their corresponding densities w.r.t.  $\nu$  a dominating measure.

Under the change of variables  $y = \Phi_v^{-1}(x)$  (we use one homogeneity hereafter) leads to

$$(3.10) \quad \mathcal{J}(\rho_\varepsilon, \mathbf{m}_\varepsilon, \mu_\varepsilon) = \int_{[0,1] \times M} f(x, (\rho_\varepsilon, \mathbf{m}_\varepsilon, \mu_\varepsilon)) \, d\nu(x) \leq \int_{\mathbb{R}} \int_U \int_{[0,1] \times M} k_\varepsilon(s, v) f(\Phi_v(y), (\rho(t+s), D\Phi_v(t, y)m(t+s), \mu(t+s))) \, d\nu(t, y) \, dt \, ds \, dv.$$

Moreover, since the metric  $g$  on  $M$  is smooth and in particular uniformly continuous on  $M$  and since  $\|D\Phi_v - \text{Id}\| \leq \text{cst}\|v\|$  for a constant that only depends on  $u$ , we thus have, for any  $\varepsilon_2 > 0$ , the existence of  $\delta > 0$  such that if  $\|v\| \leq \delta$  then,

$$(3.11) \quad |g(x)(w, w) - g(\Phi_v(x))(D\Phi_v(x)w, D\Phi_v(x)w)| \leq \varepsilon_2 g(x)(w, w),$$

for every  $w \in T_x M$ . Therefore, a direct estimation leads to

$$(3.12) \quad \left| \int_{\mathbb{R} \times M} k_\varepsilon(s, v) f(\Phi_v(x), (\rho(t+s), m(t+s), \mu(t+s))) \, d\nu(t, x) - \int_{[0,1] \times M} f(x, (\rho(t), m(t), \mu(t))) \, d\nu(t, x) \right| \leq \varepsilon_2 \mathcal{J}(\rho, m, \mu),$$

and as a consequence the desired result,

$$(3.13) \quad \mathcal{J}(\rho_\varepsilon, \mathbf{m}_\varepsilon, \mu_\varepsilon) \leq \mathcal{J}(\rho, m, \mu) + \varepsilon_2 \mathcal{J}(\rho, m, \mu).$$

Since this averaging reduces to standard convolution in the coordinate chart  $U$  in a small neighborhood of  $x_0$ , it implies that  $(\rho_\varepsilon, \mathbf{m}_\varepsilon, \mu_\varepsilon)$  is smooth in a neighborhood of  $x_0$  and  $\rho_\varepsilon \geq \varepsilon_1 \text{vol}$ . By compactness of  $M$ , iterating a finite number of times this argument gives the desired path.  $\square$

Next, we prove the equivalence of these two formulations with a particular UOT problem introduced in Section 2.

**3.1.3. Kantorovich and dual formulation of WFR.** As in [8] the application of Fenchel-Rockafellar duality Theorem gives the dual formulation of WFR. This is summarized in the following proposition.

**Proposition 12** (Dual formulation of WFR). *On  $(M, g)$ , it holds*

$$(3.14) \quad \text{WFR}^2(\rho_0, \rho_1) = \sup_{(\phi, \psi) \in \mathcal{C}(M)^2} \int_M \phi(x) \, d\rho_0(x) + \int_M \psi(y) \, d\rho_1(y)$$

subject to  $\forall(x, y) \in M^2$ ,

$$(3.15) \quad \begin{cases} \phi(x) \leq 1, & \psi(y) \leq 1, \\ (1 - \phi(x))(1 - \psi(y)) \geq \cos^2(d(x, y) \wedge (\pi/2)). \end{cases}$$

A reformulation of this linear optimization problem is

$$(3.16) \quad \text{WFR}^2(\rho_0, \rho_1) = \sup_{(z_0, z_1) \in C(M)^2} \int_M 1 - e^{-z_0(x)} d\rho_0(x) + \int_M 1 - e^{-z_1(y)} d\rho_1(y)$$

subject to  $\forall(x, y) \in M^2$ ,

$$(3.17) \quad z_0(x) + z_1(y) \leq -\log(\cos^2(d(x, y) \wedge (\pi/2))).$$

Interestingly this last formulation is exactly the dual formulation of UOT defined in Proposition 2 with the cost  $c(x, y) = -\log(\cos^2(d(x, y) \wedge (\pi/2)))$  and dual entropy functions  $F_0^*(x) = F_1^*(x) = F^*(x) = e^x - 1$ . As noticed in Remark 1 the associated entropy function is therefore  $F(x) = x \log(x) - x + 1$  leading to the Kullback-Leibler divergence, which reads

$$(3.18) \quad \text{KL}(\mu, \nu) = \int \frac{d\mu}{d\nu} \log\left(\frac{d\mu}{d\nu}\right) d\nu + |\nu| - |\mu|.$$

Existence of Lipschitz solutions to the dual problem has been proved under admissibility condition on the measures in Section 2.2. Without these assumptions, existence of potentials can be proved in a less regular space of functions in [25, Section 6.2].

**Proposition 13** (Kantorovich formulation of WFR). *With the same notations as above it holds*

$$(3.19) \quad \text{WFR}^2(\rho_0, \rho_1) = \inf_{\gamma \in \mathcal{M}_+(M^2)} \text{KL}(p_*^1 \gamma, \rho_0) + \text{KL}(p_*^2 \gamma, \rho_1) - \int_{M^2} \log(\cos^2(d(x, y) \wedge (\pi/2))) d\gamma(x, y).$$

**3.2. A Monge formulation for WFR.** OT supports an interesting geometric framework. Indeed, the pushforward action of the diffeomorphisms group on the space of densities is a (formal) Riemannian submersion to the space of densities endowed with the Wasserstein metric, see [19, 13] for more details. This structure also exists in the case of UOT, as already explained in [18]. We briefly recall it hereafter.

**3.2.1. The formal Riemannian submersion and Monge formulation of WFR.** Recall that a Riemannian submersion is a submersion  $\pi$  between two Riemannian manifolds  $M$  and  $N$ , such that  $d\pi$  is an isometry between the orthogonal of its kernel and its range. An important property of Riemannian submersion is that every geodesic on  $N$  can be lifted (called horizontal lift) to a unique geodesic on  $M$  (having the same length), up to the choice of a basepoint in  $M$ . In the following, the roles of  $M$  and  $N$  are taken by  $\text{Diff}(M)$ , the group of diffeomorphisms of  $M$  and  $\text{Dens}_p(M)$  the space of probability densities on  $M$ . We choose the reference volume form  $\rho_0$  on  $M$  and define

$$\begin{aligned} \pi_0 : \text{Diff}(M) &\rightarrow \text{Dens}_p(M) \\ \pi(\varphi) &= \varphi_* \rho_0 \end{aligned}$$

which is a (formal) Riemannian submersion of the metric  $L^2(M, \rho_0)$  on  $\text{Diff}(M)$  to the Wasserstein  $W_2$  metric on  $\text{Dens}_p(M)$ . Using the horizontal lift property of geodesics mentioned above, the Benamou and Brenier dynamic formulation [3] can be rewritten on the group  $\text{Diff}(M)$  as the Monge problem,

$$(3.20) \quad W_2(\rho_0, \rho_1)^2 = \inf_{\varphi \in \text{Diff}(M)} \left\{ \int_{\Omega} d_M^2(\varphi(x), x) \rho_0(x) d\text{vol}(x) : \varphi_* \rho_0 = \rho_1 \right\}.$$

In the unbalanced case, the group  $\text{Diff}(M)$  is replaced with the semidirect product of groups between  $\text{Diff}(M)$  and the space of positive functions on  $M$  which is a group under pointwise multiplication. It is not a direct product but a semidirect one, where the composition law is defined such

that the map  $\pi$  given by

$$\begin{aligned}\pi_1 &: (\text{Diff}(M) \times C(M, \mathbb{R}_{>0})) \times \text{Dens}(M) \mapsto \text{Dens}(M) \\ \pi_1 &((\varphi, \lambda), \rho) \stackrel{\text{def.}}{=} \varphi_*(\lambda\rho)\end{aligned}$$

is a left-action of the group  $\text{Diff}(M) \times C(M, \mathbb{R}_{>0})$  on the space of densities. Similarly to the optimal transport case, this action is actually a Riemannian submersion between  $L^2(M, M \times \mathbb{R}_{>0})$  and  $\text{Dens}(M)$  endowed with the WFR metric. Note that the  $L^2$  metric is defined by a density (the initial density) on  $M$  and a metric on  $M \times \mathbb{R}_{>0}$  (see [15] for more details) and this Riemannian metric is completely specified by the unbalanced optimal transport model, namely

$$(3.21) \quad g_{(x,m)}(dx, dm) = a^2 m dx^2 + b^2 \frac{dm^2}{m}.$$

Up to the change of variable  $m = r^2$ , we find that the metric can be rewritten as

$$(3.22) \quad g_{(x,r)}(dx, dr) = a^2 r^2 dx^2 + 4b^2 dr^2,$$

which is called a cone metric<sup>1</sup>. Since it is a classical formulation of this metric, we adopt this change of variable in the rest of the paper. In particular, the action is changed into

$$\begin{aligned}\pi &: (\text{Diff}(M) \times C(M, \mathbb{R}_{>0})) \times \text{Dens}(M) \mapsto \text{Dens}(M) \\ \pi &((\varphi, \lambda), \rho) \stackrel{\text{def.}}{=} \varphi_*(\lambda^2 \rho),\end{aligned}$$

and the metric on  $M \times \mathbb{R}_{>0}$  is the cone metric (3.22). We now adopt the notation  $\mathcal{C}(M)$  for the  $M \times \mathbb{R}_{>0}$  equipped with the cone metric. In fact, as done in [18] we can identify this semidirect product of groups with the automorphism group of the cone  $\mathcal{C}(M)$  (since it has a multiplicative group structure in the  $\mathbb{R}_{>0}$  component). Thus, to shorten the notations, we use  $\text{Aut}(\mathcal{C}(M))$  instead of  $\text{Diff}(M) \times C(M, \mathbb{R}_{>0})$ . We now state the (formal) Riemannian submersion result obtained in [18].

**Proposition 14.** *Let  $\rho_0 \in \text{Dens}(M)$  be a positive density and  $\pi$  be the map*

$$\begin{aligned}\pi &: \text{Aut}(\mathcal{C}(M)) \mapsto \text{Dens}(M) \\ \pi(\varphi, \lambda) &= \varphi_*(\lambda^2 \rho_0).\end{aligned}$$

*Then,  $\pi$  is a Riemannian submersion between  $\text{Aut}(\mathcal{C}(M))$  endowed with the metric  $L^2(M, \rho_0, \mathcal{C}(M))$  and  $\text{Dens}(M)$  with the WFR metric.*

For details about the proof, we refer the reader to [18]. This proposition can be used to deduce a static or Monge formulation of the variational problem.

**Definition 8.** Let  $(\rho_0, \rho_1) \in \mathcal{M}_+(M^2)$ . The Monge formulation of WFR is given by

$$(3.23) \quad \begin{aligned}\text{M-WFR}^2(\rho_0, \rho_1) &= \inf_{(\varphi, \lambda)} \left\{ \int_M d_{\mathcal{C}(M)}^2((\varphi(x), \lambda(x)), (x, 1)) d\rho_0(x) : \varphi_*(\lambda^2 \rho_0) = \rho_1 \right\} \\ &= \inf_{(\varphi, \lambda)} \left\{ d_{\text{Aut}(\mathcal{C}(M))}^2((\varphi, \lambda), (\text{Id}, 1)) : \varphi_*(\lambda^2 \rho_0) = \rho_1 \right\}\end{aligned}$$

where the infimum is taken over  $(\varphi, \lambda) \in \text{Diff}(M) \times C(M, \mathbb{R}_{>0})$  and  $(\text{Id}, 1)$  denotes the identity in  $\text{Aut}(\mathcal{C}(M))$ .

A consequence of the semi-couplings formulation is the relaxation inequality  $\text{M-WFR}^2(\rho_0, \rho_1) \geq \text{WFR}^2(\rho_0, \rho_1)$ . The converse inequality does not hold in general since in the case of unbalanced transport not only the particles can split but also they can reach the apex of the cone. However under our admissibility condition on  $(\rho_0, \rho_1)$  we prove that  $\text{M-WFR}^2(\rho_0, \rho_1) = \text{WFR}^2(\rho_0, \rho_1)$  in Proposition 17.

---

<sup>1</sup>It is interesting to check that other Riemannian metrics on the cone can be chosen provided they are two-homogeneous in the radial variable. Some of the results of this article carry over such cases.

**3.3. Monge solution and polar factorization on the automorphism group.** The geometric structure used to show Brenier's polar factorization theorem [5] in standard optimal transport relies on the Riemannian submersion and solution of Monge problem. Thanks to results given in Section 3.2.1 and after finding a solution to the Monge problem M-WFR we generalise in this section polar factorization to the unbalanced framework.

3.3.1. *Monge solution of WFR.* To show the existence of a solution to Monge problem (3.23) we start by solving  $\text{WFR}(\rho_0, \rho_1)$ , in the dual form (3.16), (3.17) and we provide geometric properties of such solution (see Proposition 16). To prove Proposition 16 there are two different arguments: one is based on results in Section 2 and the existence of Lipschitz potentials; the other one mimics the standard case of optimal transport with minor adaptations due to the cost. This latter approach leads to a pair of approximately differentiable potentials. For completeness we give both proofs.

**Lemma 15** (sub-differentiability). *Let  $y \in M$ , the function  $g$  defined on  $M$  by  $g(x) = \cos^2(d(x, y))$  is sub-differentiable.*

*Proof.* The function  $d^2(\cdot, y)$  is super-differentiable see [27, Proposition 6] for instance. Therefore  $d_{\pi/2}^2(\cdot, y) = (d(x, y) \wedge (\pi/2))$  is also super-differentiable and the function  $g$  is sub-differentiable as the combination of a decreasing  $C^1$  function and the super-differentiable function  $d_{\pi/2}^2(\cdot, y)$ , see [27, Lemma 5].  $\square$

**Proposition 16** (Brenier's weak solution of WFR-Monge-Ampère). *Let  $(\rho_0, \rho_1) \in \mathcal{M}_+(M^2)$  and let  $(z_0, z_1)$  be the generalized optimal potentials for  $\text{WFR}^2(\rho_0, \rho_1)$ . Suppose that  $(\rho_0, \rho_1)$  is admissible and  $\rho_0 \ll \text{vol}$ , then  $z_0$  is  $\rho_0$  a.e. unique and approximate differentiable on  $\text{Supp}(\rho_0)$ . The optimal plan  $\gamma$  in the formulation (13) is unique, with marginals  $\gamma_0 = e^{-z_0}\rho_0$ ,  $\gamma_1 = e^{-z_1}\rho_1$  and concentrated on the graph of*

$$(3.24) \quad x \mapsto \varphi(x) = \exp_x^M \left( -\arctan \left( \frac{\|\tilde{\nabla} z_0(\bar{x})\|}{2} \right) \frac{\tilde{\nabla} z_0(\bar{x})}{\|\tilde{\nabla} z_0(\bar{x})\|} \right) = \text{c-exp}(-\nabla z_0(x)),$$

that is  $\varphi_*\gamma_0 = \gamma_1$  and  $\gamma = (\text{Id} \times \varphi)_*\gamma_0$ . Finally

$$(3.25) \quad \text{WFR}^2(\rho_0, \rho_1) = \int_M 1 - e^{-z_0(x)} d\rho_0(x) + \int_M 1 - e^{-z_1(y)} d\rho_1(y).$$

Note that  $(z_0, z_1)$  may not be continuous as needed in (3.16) but (3.25) still holds true. The approximate differentiable proof of this proposition (being more technical) is given in Appendix A, we prefer to discuss the corresponding formulation of the Monge-Ampère equation hereafter and a simple sketch of proof following the results in Section 2.

*Direct proof.* Corollary 8 gives a pair of Lipschitz potentials  $(z_0, z_1)$  solution of  $\text{WFR}^2(\rho_0, \rho_1)$ . Lemma 3 proves that this pair is also solution of a classical Optimal Transport problem between  $\gamma_0 = e^{-z_0}\rho_0$ ,  $\gamma_1 = e^{-z_1}\rho_1$  for the cost  $c(x, y) = -\log(\cos^2(d(x, y) \wedge (\pi/2)))$ . The hypothesis on  $\rho_0$  and Classical optimal transport theory arguments gives the existence of a map  $\varphi(x) = \text{c-exp}(-\nabla z_0(x))$  solution of this OT problem. In particular  $\varphi_*\gamma_0 = \gamma_1$ .  $\square$

**Remark 5.** *Note that the map  $\varphi(x) = \text{c-exp}(-\nabla z_0(x))$  is a solution to a standard OT problem from  $\gamma_0 = e^{-z_0}\rho_0$  to  $\gamma_1 = e^{-z_1}\rho_1$  for the cost  $c(x, y) = -\log(\cos^2(d(x, y) \wedge (\pi/2)))$ . Therefore, OT regularity theory applies to  $z_0$  with fixed marginals  $\gamma_0, \gamma_1$ . In particular, higher regularity of  $z_0$  increases regularity of  $\gamma_0$  and  $\gamma_1$  and, in turn, a bootstrap argument improves regularity of  $z_0$  (see also the strategy in the proof of Theorem 4).*

As a consequence of the underlying classical OT structure, the potential found in Proposition 16, denoted by  $z$ , is a solution of a Monge-Ampère equation with a right-hand side that also depends on the potential. We recall how to derive the equation supposing that  $z$  is  $C^2$ . Remember that



$c(x, y) = -\log(\cos^2(d_{\pi/2}(x, y)))$  and  $\varphi(x) = \exp_x^M \left( -\arctan \left( \frac{1}{2} \|\nabla z(x)\| \right) \frac{\nabla z(x)}{\|\nabla z(x)\|} \right)$ , therefore

$$2\sqrt{2} \tan(d_{\pi/2}(x, \varphi(x))) \frac{\sqrt{2}}{2d_{\pi/2}(x, \varphi(x))} \nabla \left( \frac{1}{2} d_{\pi/2}^2(x, \varphi(x)) \right) = (\nabla_x c)(x, \varphi(x))$$

and the sub-differentiable equality (A.4) reads

$$(3.26) \quad \nabla z(x) - (\nabla_x c)(x, \varphi(x)) = 0.$$

Observe that by definition of  $c\text{-exp}_x(v) = [(-\nabla_x c)(x, \cdot)]^{-1}(v)$  (3.26) is exactly

$$\varphi(x) = c\text{-exp}(-\nabla z(x)).$$

Differentiating (3.26) and taking the determinant yields

$$(3.27) \quad \det [-\nabla^2 z(x) + (\nabla_{xx}^2 c)(x, \varphi(x))] = |\det [(\nabla_{x,y} c)(x, \varphi(x))]| |\det(\nabla \varphi)|.$$

Notice that the  $c$ -convexity property of  $z$  implies that  $-\nabla^2 z + (\nabla_{xx}^2 c)(x, \varphi(x))$  is a nonnegative symmetric matrix. To obtain the equation on  $z$ , observe that  $\varphi_* \left( (1 + \frac{1}{4} \|\nabla z\|^2) e^{-2z} \rho_0 \right) = \rho_1$  (see the proof of Proposition 17 below for details) or equivalently

$$|\det(\nabla \varphi)| = e^{-2z} \left( 1 + \frac{1}{4} \|\nabla z\|^2 \right) \frac{f}{g \circ \varphi},$$

for smooth  $z$  and smooth positive measures  $\rho_0$  and  $\rho_1$  with densities  $f$  and  $g$  with respect to the volume measure  $\text{vol}$ . Together with (3.27), we obtain the WFR-Monge-Ampère equation defined by (3.28)

$$\det [-\nabla^2 z(x) + (\nabla_{xx}^2 c)(x, \varphi(x))] = |\det [(\nabla_{x,y} c)(x, \varphi(x))]| e^{-2z(x)} \left( 1 + \frac{1}{4} \|\nabla z(x)\|^2 \right) \frac{f(x)}{g \circ \varphi(x)},$$

where  $\varphi$  is given by (3.29) and satisfies the second boundary value problem:  $\varphi$  maps the support of  $\rho_0$  to the support of  $\rho_1$ .

**Remark 6.** Another possibility is to write directly the Monge-Ampère equation satisfied by  $\varphi$  as on optimal map pushing  $\gamma_0$  to  $\gamma_1$  that is

$$\det [-\nabla^2 z(x) + (\nabla_{xx}^2 c)(x, \varphi(x))] = |\det [(\nabla_{x,y} c)(x, \varphi(x))]| \frac{e^{-z_0(x)} \rho_0(x)}{e^{-z_1(\varphi(x))} \rho_1 \circ \varphi(x)}.$$

Using  $z_0(x) + z_1(\varphi(x)) = c(x, \varphi(x))$  and  $1 + \frac{1}{4} \|\nabla z_0(x)\|^2 = e^{c(x, \varphi(x))}$  one recovers the WFR-Monge-Ampère equation (3.28).

**Remark 7.** Following Brenier [5, Section 1.4] Proposition 16 can be taken as a definition of weak solutions for the WFR-Monge-Ampère equation (3.28) with second boundary value problem. The question of regularity of such a solution of a WFR-Monge-Ampère equation is a consequence of the results proved in Section 2. In particular as we saw it depends on the regularity of classical OT and therefore on the study of the Ma-Trudinger-Wang tensor associated to  $c$  see [10], [36, Section 12].

Thanks to Proposition 16 we are now able to prove the existence, under some assumptions on the initial density, of a solution to the Monge problem M-WFR.

**Proposition 17** (Solution to the Monge problem M-WFR and equivalence to WFR). *Let  $\rho_0, \rho_1$  be admissible and such that  $\rho_0$  has density w.r.t. the volume measure on  $M$ . Then, there exists a  $\rho_0$  a.e. unique  $c$ -convex function on  $M$ ,  $z$ , approximately differentiable  $\rho_0$ -a.e., such that the associated unbalanced transport couple  $(\varphi, \lambda)$  defined by*

$$(3.29) \quad \varphi(x) = \exp_x^M \left( -\arctan \left( \frac{1}{2} \|\tilde{\nabla} z(x)\| \right) \frac{\tilde{\nabla} z(x)}{\|\tilde{\nabla} z(x)\|} \right)$$

and

$$(3.30) \quad \lambda(x) = e^{-z(x)} \sqrt{1 + \frac{1}{4} \|\tilde{\nabla} z(x)\|^2}$$

is a solution of the Monge problem (3.23) and satisfies

$$(3.31) \quad \pi[(\varphi, \lambda), \rho_0] = \varphi_* (\lambda^2 \rho_0) = \varphi_* \left( \left(1 + \frac{1}{4} \|\tilde{\nabla} z\|^2\right) e^{-2z} \rho_0 \right) = \rho_1.$$

Moreover,  $(\varphi, \lambda)$  is the unique  $\rho_0$  a.e. unbalanced transport couple associated to a  $c$ -convex potential, also unique, such that  $\pi[(\varphi, \lambda), \rho_0] = \rho_1$ . The potential  $z$  is characterized by

$$(3.32) \quad \text{M-WFR}^2(\rho_0, \rho_1) = \text{WFR}^2(\rho_0, \rho_1) = \int_M 1 - e^{-z(x)} d\rho_0(x) + \int_M 1 - e^{-z^c(y)} d\rho_1(y),$$

*Proof. Existence:* Let  $(z_0, z_1)$  be the optimal potentials for  $\text{WFR}^2(\rho_0, \rho_1)$ . From Proposition 16, we know that  $x \mapsto \varphi(x) = \exp_x^M \left( -\arctan \left( \frac{\|\tilde{\nabla} z_0(x)\|}{2} \right) \frac{\tilde{\nabla} z_0(x)}{\|\tilde{\nabla} z_0(x)\|} \right)$  is well defined  $\rho_0$  a.e. and  $\varphi_*(\gamma_0) = \gamma_1$  where  $\gamma_i = \sigma_i \rho_i = e^{-z_i} \rho_i$ ,  $i = 0, 1$ . Therefore

$$\begin{aligned} \rho_1 &= \sigma_1^{-1} \gamma_1 = \sigma_1^{-1} \varphi_*(\gamma_0) = \sigma_1^{-1} \varphi_*(\sigma_0 \rho_0) \\ &= \varphi_* (e^{-z_0} \sigma_1^{-1} \circ \varphi \rho_0) = \varphi_* (e^{-z_0} e^{z_1 \circ \varphi} \rho_0) = \varphi_* \left( e^{-z_0} e^{c(\cdot, \varphi(\cdot))} e^{-z_0} \rho_0 \right) \\ &= \varphi_* \left( e^{-2z_0} \left(1 + \frac{1}{4} \|\tilde{\nabla} z_0\|^2\right) \rho_0 \right) = \varphi_* \left( \left( e^{-z_0} \sqrt{1 + \frac{1}{4} \|\tilde{\nabla} z_0\|^2} \right)^2 \rho_0 \right) \\ &= \pi \left[ \left( \varphi, e^{-z_0} \sqrt{1 + \frac{1}{4} \|\tilde{\nabla} z_0\|^2} \right), \rho_0 \right]. \end{aligned}$$

We used that  $\rho_0$  a.e.  $z_0(x) + z_1(\varphi(x)) = c(x, \varphi(x))$ ,  $1 + \tan^2(x) = 1/\cos^2(x)$  and thus  $1 + \frac{1}{4} \|\tilde{\nabla} z_0(x)\|^2 = e^{c(x, \varphi(x))}$ . Equation (3.25) is exactly (3.32).

To prove uniqueness, consider  $z$  to be a  $c$ -convex function, such that  $(\varphi, \lambda)$  are well defined through (3.29) and (3.31) and  $\pi[(\varphi, \lambda), \rho_0] = \rho_1$ . Then, we claim that  $\gamma = [\text{Id} \times \varphi]_*(e^{-z} \rho_0)$  is an optimal plan for  $\text{WFR}^2(\rho_0, \rho_1)$  in (13). Indeed, let us check that  $\gamma$  satisfies the optimality conditions of [25, Theorem 6.3(b)].

- $\gamma$  is concentrated on the set of equality for a pair  $(z, z^c)$  of  $c$ -convex functions. By definition of  $\varphi$ , it holds  $\rho_0$  a.e. and therefore  $\gamma_0 = e^{-z} \rho_0$  a.e.

$$(3.33) \quad z(x) + z^c(\varphi(x)) = c(x, \varphi(x)).$$

Thus,  $(z, z^c)$  satisfies for all  $(x, y) \in M \times M$ ,  $z(x) + z^c(y) \leq c(x, y)$  with equality  $\gamma$  a.e.

- The marginals are absolutely continuous with respect to  $\rho_0$  and  $\rho_1$ . It holds true for  $\gamma_0 = e^{-z} \rho_0$ . Note then that  $\rho_0$  a.e.

$$\lambda^2(x) = e^{-2z(x)} \left(1 + \frac{1}{4} \|\tilde{\nabla} z(x)\|^2\right) = e^{-z(x)} e^{z^c(\varphi(x))}.$$

It yields

$$\rho_1 = \varphi_*(\lambda^2 \rho_0) = \varphi_*(e^{z^c(\varphi(x))} e^{-z(x)} \rho_0) = e^{z^c} \varphi_*(\gamma_0) = e^{z^c} \gamma_1,$$

thus  $\gamma_1 = e^{-z^c} \rho_1$  and  $\gamma$  is optimal for  $\text{WFR}^2(\rho_0, \rho_1)$ .

In particular it implies  $\text{M-WFR}^2(\rho_0, \rho_1) = \text{WFR}^2(\rho_0, \rho_1)$ . The computation (A.5) yields (3.32) and uniqueness of the generalized optimal potentials for  $\text{WFR}^2(\rho_0, \rho_1)$  in Proposition (16) implies uniqueness of  $(z, \varphi, \lambda)$ .  $\square$

**3.3.2. Polar factorization.** We are left with proving a polar factorization theorem for the automorphism group of the cone  $\text{Aut}(\mathcal{C}(M))$ .

**Definition 9.** We define the *generalized automorphism semigroup* of  $\mathcal{C}(M)$  as the set of measurable maps  $(\varphi, \lambda)$  from  $M$  to  $\mathcal{C}(M)$

$$(3.34) \quad \overline{\text{Aut}}(\mathcal{C}(M)) = \{(\varphi, \lambda) \in \text{Mes}(M, M) \times \text{Mes}(M, \mathbb{R}_{>0y})\},$$

endowed with the semigroup law

$$(\varphi_1, \lambda_1) \cdot (\varphi_2, \lambda_2) = (\varphi_1 \circ \varphi_2, (\lambda_1 \circ \varphi_2)\lambda_2).$$

We also consider the stabilizer of the volume measure in the automorphisms of  $\mathcal{C}(M)$ . It is defined by

$$(3.35) \quad \overline{\text{Aut}}_{\text{vol}}(\mathcal{C}(M)) = \{(s, \lambda) \in \overline{\text{Aut}}(\mathcal{C}(M)) : \pi((s, \lambda), \text{vol}) = \text{vol}\}.$$

By abuse of notation, any  $(s, \lambda) \in \overline{\text{Aut}}_{\text{vol}}(\mathcal{C}(M))$  will be denoted  $(s, \sqrt{\text{Jac}(s)})$  meaning that for every continuous function  $f \in C(M, \mathbb{R})$

$$(3.36) \quad \int_M f(s(x)) \sqrt{\text{Jac}(s)}^2 \, d \text{vol}(x) = \int_M f(x) \, d \text{vol}(x).$$

**Theorem 18** (Polar factorization). *Let  $(\phi, \lambda) \in \overline{\text{Aut}}(\mathcal{C}(M))$  be an element of the generalized automorphism group of the half-densities bundle such that  $\rho_1 = \pi_0[(\phi, \lambda), \text{vol}]$  is an absolute continuous admissible measure. Then, there exists a unique minimizer, characterized by a  $c$ -convex function  $z_0$ , to the Monge formulation (3.23) between  $\text{vol}$  and  $\rho_1$  and there exists a unique measure preserving generalized automorphism  $(s, \sqrt{\text{Jac}(s)}) \in \overline{\text{Aut}}_{\text{vol}}(\mathcal{C}(M))$  such that  $\text{vol}$  a.e.*

$$(3.37) \quad (\phi, \lambda) = \exp^{\mathcal{C}(M)} \left( -\frac{1}{2} \tilde{\nabla} p_{z_0}, -p_{z_0} \right) \circ (s, \sqrt{\text{Jac}(s)})$$

or equivalently

$$(3.38) \quad (\phi, \lambda) = \left( \varphi, e^{-z_0} \sqrt{1 + \|\tilde{\nabla} z_0\|^2} \right) \cdot (s, \sqrt{\text{Jac}(s)}),$$

where  $p_{z_0} = e^{z_0} - 1$  and

$$(3.39) \quad \varphi(x) = \exp_x^M \left( -\arctan \left( \frac{1}{2} \|\tilde{\nabla} z_0(x)\| \right) \frac{\tilde{\nabla} z_0(x)}{\|\tilde{\nabla} z_0(x)\|} \right).$$

Moreover  $(s, \sqrt{\text{Jac}(s)})$  is the unique  $L^2(M, \mathcal{C}(M))$  projection of  $(\phi, \lambda)$  onto  $\overline{\text{Aut}}_{\text{vol}}(\mathcal{C}(M))$ .

*Proof of Theorem 18.* We denote  $\rho_0 = \text{vol}$  and  $\rho_1 = \pi_0[(\phi, \lambda), \rho_0]$ . Let  $(z_0, z_1)$  be a solution of  $\text{WFR}^2(\rho_0, \rho_1)$  and  $\gamma$  be an optimal unbalanced transport plan. By symmetry,  $(z_1, z_0)$  is a solution of  $\text{WFR}^2(\rho_1, \rho_0)$  and  $\gamma^t$  is an optimal unbalanced transport plan. Let finally  $(\varphi_0, \lambda_0)$  and  $(\varphi_1, \lambda_1)$  be the two transport couples given by application of Proposition 16 to  $(\rho_0, \rho_1)$  and  $(\rho_1, \rho_0)$ . We divide the proof into four small steps. We also denote  $\text{dom}(f)$  the domain of definition of the function  $f$ .

**Step 1:  $\varphi_0$  and  $\varphi_1$  are inverse maps.** On  $U = \varphi_0^{-1}(\text{dom} \tilde{\nabla} z_1) \cap \text{dom} \tilde{\nabla} z_0$  which has full  $\gamma_0$  and therefore  $\rho_0$  measure (we use here the admissible condition to say that  $\gamma_0$  and  $\rho_0$  have the same support), we have

$$z_0(x) + z_1(\varphi_0(x)) = c(x, \varphi_0(x))$$

and thus  $\varphi_1(\varphi_0(x)) = x$ . Similarly, it holds  $\varphi_0(\varphi_1(y)) = y$  on  $V = \varphi_1^{-1}(\text{dom} \tilde{\nabla} z_0) \cap \text{dom}(\tilde{\nabla} z_1)$  which has full  $\rho_1$  measure.

**Step 2:  $(\varphi_0, \lambda_0)$  and  $(\varphi_1, \lambda_1)$  are inverse in  $\overline{\text{Aut}}$ .** From Step 1,  $\rho_1$  a.e. it holds  $\varphi_0(\varphi_1(y)) = y$ . Thus,  $\rho_1$  a.e.

$$(\varphi_0, \lambda_0) \cdot (\varphi_1, \lambda_1) = (\varphi_0 \circ \varphi_1, \lambda_0 \circ \varphi_1 \lambda_1) = (\text{Id}, (\lambda_0 \circ \varphi_1)\lambda_1).$$

Moreover by (3.31) of Proposition 17 applied twice

$$\pi[(\varphi_0, \lambda_0) \cdot (\varphi_1, \lambda_1), \rho_1] = \pi[(\varphi_0, \lambda_0), \pi[(\varphi_1, \lambda_1), \rho_1]] = \pi[(\varphi_0, \lambda_0), \rho_0] = \rho_1.$$

It implies that

$$\pi[(\text{Id}, (\lambda_0 \circ \varphi_1)\lambda_1), \rho_1] = \pi[(\varphi_0, \lambda_0) \cdot (\varphi_1, \lambda_1), \rho_1] = \rho_1.$$

In other words, we have  $\rho_1$  a.e.  $(\lambda_0 \circ \varphi_1)\lambda_1 = 1$  and  $\rho_1$  a.e.

$$(\varphi_0, \lambda_0) \cdot (\varphi_1, \lambda_1) = (\text{Id}, 1).$$

**Step 3: polar factorization.** Let  $(s, \lambda_s) = (\varphi_1, \lambda_1) \cdot (\phi, \lambda) = (\varphi_1 \circ \phi, \lambda_1 \circ \phi \lambda)$ . By construction, one has

$$\pi[(s, \lambda_s), \rho_0] = \pi[(\varphi_1, \lambda_1) \cdot (\phi, \lambda), \rho_0] = \pi[(\varphi_1, \lambda_1), \pi[(\phi, \lambda), \rho_0]] = \pi[(\varphi_1, \lambda_1), \rho_1] = \rho_0.$$

Therefore,  $(s, \lambda_s)$  belongs to  $\overline{\text{Aut}}_{\text{vol}}$  and  $\lambda_s = \sqrt{\text{Jac}(s)}$  holds in the weak sense (3.36). Thus

$$(\phi, \lambda) = (\text{Id}, 1) \cdot (\phi, \lambda) = (\varphi_0, \lambda_0) \cdot (\varphi_1, \lambda_1) \cdot (\phi, \lambda) = (\varphi_0, \lambda_0) \cdot (s, \sqrt{\text{Jac}(s)}).$$

It proves the polar factorization.

**Step 4: Uniqueness.** The pair of c-convex potentials  $(z_0, z_1)$  is optimal for  $\text{WFR}(\rho_0, [(\varphi_0, \lambda_0), \rho_0]) = \text{WFR}(\rho_0, \rho_1)$  and therefore by Proposition 17,  $z_i$  are unique  $\rho_i$  a.e.. We deduce that the projection  $(s, \sqrt{\text{Jac}(s)}) = (\varphi_1, \lambda_1) \cdot (\phi, \lambda)$  is also unique  $\rho_0$  a.e.. Indeed the positivity of  $\lambda$  implies that  $\text{Supp}(\lambda^2 \rho_0) = \text{Supp}(\rho_0)$ , thus  $\phi$  maps  $\text{Supp}(\rho_0)$  onto  $\text{Supp}(\rho_1)$  and the uniqueness of  $\varphi_1$  and  $\lambda_1, \rho_1$  a.e., implies the uniqueness of  $s$  and  $\sqrt{\text{Jac}(s)}, \rho_0$  a.e.. To prove that  $(s, \sqrt{\text{Jac}(s)})$  is the  $L^2(M, \mathcal{C}(M))$  projection of  $(\phi, \lambda)$  onto  $\overline{\text{Aut}}_{\text{vol}}(\mathcal{C}(M))$ , we observe

$$\begin{aligned} \inf_{(\sigma, \sqrt{\text{Jac}(\sigma)}) \in \overline{\text{Aut}}_{\text{vol}}(\mathcal{C}(M))} \int_M d_{\mathcal{C}(M)}^2 \left( (\phi, \lambda), (\sigma, \sqrt{\text{Jac}(\sigma)}) \right) \rho_0 &\geq \text{WFR}^2(\rho_0, \rho_1) \\ &= \int_M d_{\mathcal{C}(M)}^2 \left( (\varphi_0, \lambda_0), (\text{Id}, 1) \right) \rho_0 \\ &= \int_M d_{\mathcal{C}(M)}^2 \left( (\varphi_0, \lambda_0) \cdot (s, \sqrt{\text{Jac}(s)}), (s, \sqrt{\text{Jac}(s)}) \right) \rho_0 \\ &= \int_M d_{\mathcal{C}(M)}^2 \left( (\phi, \lambda), (s, \sqrt{\text{Jac}(s)}) \right) \rho_0, \end{aligned}$$

which gives the result.  $\square$

As in OT, Theorem 18 could be extended, for example, to any admissible  $\rho_1$  without the absolute continuity assumption. In such a case, one loses uniqueness of the measure preserving generalized automorphism  $(s, \sqrt{\text{Jac}(s)})$ . An other extension is to project on the subset of  $\overline{\text{Aut}}(\mathcal{C}(M))$ :

$$\overline{\text{Aut}}_{\rho_0, \mu_0}(\mathcal{C}(M)) = \{(s, \lambda) \in \overline{\text{Aut}}(\mathcal{C}(M)) \mid \pi((s, \lambda), \rho_0) = \mu_0\},$$

in the spirit of [37, Theorem 3.15]. The proof is similar to the one given above. Last, linearization of this polar factorization leads to an Helmholtz decomposition for velocity vector fields. We leave it for future works.

#### 4. FUTURE DIRECTIONS

We have shown, not unsurprisingly, that regularity for unbalanced optimal transport can be reduced to the one of optimal transport through linearization of the dual problem. Regularity, being a structural result in itself, is interesting outside analysis. For instance, regularity of optimal transport maps is the key to be able to mitigate the curse of dimensionality of statistical optimal transport as done in [34] and to obtain minimax rate of convergence for the statistical estimation of optimal potentials [28]. Our results should allow similar gains in the statistical estimation of unbalanced optimal transport. We focus on Wasserstein-Fisher-Rao metric since it is the natural length space associated with the problem. This particular case leads us to examine the MTW condition of the induced cost. Interestingly, it seems that when the MTW condition on the cone is satisfied, the same holds true for the MTW condition for the induced cost on the base manifold. We conjecture that this implication is true, possibly for other costs than the geodesic distance on the base space. This is an open direction for future works. Another open application of polar factorization can lead to new numerical scheme for the Camassa-Holm equation as done for incompressible Euler in [16].

## REFERENCES

- [1] L. Ambrosio and N. Gigli. *A user's guide to optimal transport*. Lecture Notes in Mathematics. Springer Berlin Heidelberg, 2013.
- [2] Martin Bauer, Emmanuel Hartman, and Eric Klassen. The square root normal field distance and unbalanced optimal transport, 2021.
- [3] J-D. Benamou and Y. Brenier. A computational fluid mechanics solution to the Monge-Kantorovich mass transfer problem. *Numerische Mathematik*, 84(3):375–393, 2000.
- [4] Kristian Bredies, Marcello Carioni, and Silvio Fanzon. A superposition principle for the inhomogeneous continuity equation with hellinger-kantorovich-regular coefficients, 2020.
- [5] Yann Brenier. Polar factorization and monotone rearrangement of vector-valued functions. *Comm. Pure Appl. Math.*, 44(4):375–417, 1991.
- [6] L. Caffarelli. The regularity of mappings with a convex potential. *J. Amer. Math. Soc.*, 5:99–104, 1992.
- [7] L. Chizat, B. Schmitzer, G. Peyré, and F.-X. Vialard. An Interpolating Distance between Optimal Transport and Fisher-Rao. *Found. Comp. Math.*, 2016.
- [8] Lenaïc Chizat, Gabriel Peyre, Bernhard Schmitzer, and François-Xavier Vialard. Unbalanced optimal transport: dynamic and Kantorovich formulations. *J. Funct. Anal.*, 274(11):3090–3123, 2018.
- [9] Lenaïc Chizat, Gabriel Peyré, Bernhard Schmitzer, and François-Xavier Vialard. Scaling algorithms for unbalanced transport problems. *Mathematics of Computation*, 2018.
- [10] G. De Philippis and A. Figalli. The Monge-Ampère equation and its link to optimal transportation. *Bull. Amer. Math. Soc.*, 51:527–580, 2014.
- [11] Guido De Philippis and Alessio Figalli. The Monge-Ampère equation and its link to optimal transportation. *Bulletin of the American Mathematical Society*, 51(4):527–580, 2014.
- [12] Guido De Philippis and Alessio Figalli. The Monge-Ampère equation and its link to optimal transportation. *Bull. Amer. Math. Soc. (N.S.)*, 51(4):527–580, 2014.
- [13] Philippe Delanoë. Differential geometric heuristics for riemannian optimal mass transportation. In Boris Kruglikov, Valentin Lychagin, and Eldar Straume, editors, *Differential Equations - Geometry, Symmetries and Integrability*, volume 5 of *Abel Symposia*, pages 49–73. Springer Berlin Heidelberg, 2009.
- [14] Jean Feydy, Benjamin CHARLIER, François-Xavier Vialard, and Gabriel Peyré. Optimal transport for diffeomorphic registration. In *MICCAI 2017*, Quebec, Canada, September 2017.
- [15] D. S. Freed and D. Groisser. The basic geometry of the manifold of riemannian metrics and of its quotient by the diffeomorphism group. *Michigan Math. J.*, 36(3):323–344, 1989.
- [16] Thomas Gallouët and Quentin Mérigot. A lagrangian scheme for the incompressible euler equation using optimal transport, 2016.
- [17] Thomas Gallouët, Andrea Natale, and François-Xavier Vialard. Generalized compressible fluid flows and solutions of the camassa-holm variational model. *ARMA*, June 2019. working paper or preprint.
- [18] Thomas Gallouët and François-Xavier Vialard. The camassa-holm equation as an incompressible euler equation: A geometric point of view. *Journal of Differential Equations*, 264(7):4199 – 4234, 2018.
- [19] B. Khesin and R. Wendt. *The geometry of infinite-dimensional groups*, volume 51. Springer Science & Business Media, 2008.
- [20] S. Kondratyev, L. Monsaingeon, and D. Vorotnikov. A new optimal transport distance on the space of finite Radon measures. *Adv. Differential Equations*, 21(11):1117–1164, 2016.
- [21] Stanislav Kondratyev and Dmitry Vorotnikov. Convex sobolev inequalities related to unbalanced optimal transport, 2019.
- [22] Stanislav Kondratyev and Dmitry Vorotnikov. Spherical hellinger-kantorovich gradient flows, 2019.
- [23] Vaïos Laschos and Alexander Mielke. Geometric properties of cones with applications on the hellinger-kantorovich space, and a new distance on the space of probability measures, 2018.
- [24] Paul W. Y. Lee and Jiayong Li. New examples satisfying Ma-Trudinger-Wang conditions. *SIAM J. Math. Anal.*, 44(1):61–73, 2012.
- [25] M. Liero, A. Mielke, and G. Savaré. Optimal Entropy-Transport problems and a new Hellinger-Kantorovich distance between positive measures. *Inventiones Math.*, August 2018.
- [26] Xi-Nan Ma, Neil S. Trudinger, and Xu-Jia Wang. Regularity of potential functions of the optimal transportation problem. *Arch. Ration. Mech. Anal.*, 177(2):151–183, 2005.
- [27] R.J. McCann. Polar factorization of maps on riemannian manifolds. *Geometric & Functional Analysis GAFA*, 11(3):589–608, 2001.
- [28] Boris Muzellec, Adrien Vacher, Francis Bach, François-Xavier Vialard, and Alessandro Rudi. Near-optimal estimation of smooth transport maps with kernel sums-of-squares, 2021.
- [29] Nicolás De Ponti and Andrea Mondino. Entropy-transport distances between unbalanced metric measure spaces, 2020.
- [30] R.T. Rockafellar. Integrals which are convex functionals. II. *Pacific Journal of Mathematics*, 39(2):439–469, 1971.
- [31] Zhengyang Shen, Jean Feydy, Peirong Liu, Ariel Hernán Curiale, Ruben San Jose Estepar, Raul San Jose Estepar, and Marc Niethammer. Accurate point cloud registration with robust optimal transport, 2021.

- [32] Thibault Sjourn, Jean Feydy, Franois-Xavier Vialard, Alain Trouv, and Gabriel Peyr. Sinkhorn divergences for unbalanced optimal transport. 2019.
- [33] Thibault Sjourn, Franois-Xavier Vialard, and Gabriel Peyr. The unbalanced gromov wasserstein distance: Conic formulation and relaxation, Sep 2020.
- [34] Adrien Vacher, Boris Muzellec, Alessandro Rudi, Francis Bach, and Francois-Xavier Vialard. A dimension free computational upper-bound for smooth optimal transport estimation, Jan 2021.
- [35] Franois-Xavier Vialard and Andrea Natale. Embedding camassa-holm equations in incompressible euler. *Journal of Geometric Mechanics*, page arXiv:1804.11080, Apr 2018.
- [36] C. Villani. *Optimal transport: old and new*, volume 338. Springer Science & Business Media, 2008.
- [37] Cdric Villani. *Topics in optimal transportation*, volume 58 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, 2003.
- [38] Zihao Wang, Datong Zhou, Ming Yang, Yong Zhang, Chenglong Rao, and Hao Wu. Robust document distance with wasserstein-fisher-rao metric. In Sinno Jialin Pan and Masashi Sugiyama, editors, *Proceedings of The 12th Asian Conference on Machine Learning*, volume 129 of *Proceedings of Machine Learning Research*, pages 721–736. PMLR, 18–20 Nov 2020.

## APPENDIX A. PROOFS

*Proof of Proposition 16 (Approximate differentiability).* The proof is an adaptation of [25, Theorem 6.7] using arguments in [27, 36]. In particular we use the notation of [25]. Let  $(z_0, z_1)$  be a generalized optimal potential pair for  $\text{WF}^2(\rho_0, \rho_1)$  and  $\gamma$  an optimal coupling [25, Theorem 6.3]. We define the associated densities  $\sigma_i = e^{-z_i}$ ,  $i = 0, 1$ . Since  $\rho_0$  and  $\rho_1$  are admissible [25, Theorem 6.3,b] implies  $\text{Supp}(p_*^1(\gamma) = \gamma_0) = \text{Supp}(\rho_0)$  and  $\text{Supp}(p_*^2(\gamma) = \gamma_1) = \text{Supp}(\rho_1)$ . Therefore, there exist Borel sets  $A_i \subset \text{Supp}(\rho_i)$  with  $\rho_i(M \setminus A_i) = 0$  such that

$$(A.1) \quad \sigma_0(x)\sigma_1(y) \geq \cos^2(d_{\pi/2}(x, y)) \quad \text{in } A_0 \times A_1,$$

$$(A.2) \quad \sigma_0(x)\sigma_1(y) = \cos^2(d_{\pi/2}(x, y)) \quad \gamma - \text{a. e. in } A_0 \times A_1.$$

To construct the set of approximate differentiability let

$$A_{1,n} = \{y \in M; \sigma_1(y) \geq 1/n\}$$

and consider, the function

$$s_{0,n} = \sup_{y \in A_{1,n}} \frac{\cos^2(d_{\pi/2}(x, y))}{\sigma_1(y)}.$$

By construction,  $s_{0,n}$  is bounded, Lipschitz and thus differentiable vol a.e. Still by definition, we have  $\sigma_0 \geq s_{0,n}$  and thus the sets  $A_{0,n} = \{x \in M; \sigma_0(x) = s_{0,n}(x)\}$  are increasing. Since (A.2) is valid  $\gamma$  a.e. the set  $\bigcap_{n=1}^{\infty} (X \setminus A_{0,n})$  is  $\rho_0$  negligible. Let

$$A'_{0,n} = \left\{ x \in A_{0,n}; \lim_{r \rightarrow 0} \frac{\text{vol}(B(x, r) \cap A_{0,n})}{\text{vol}(B(x, r))} = 1 \text{ and } s_{0,n} \text{ is differentiable at } x \right\}$$

be the set of points of  $A_{0,n}$  with vol density 1. Remark that  $\bigcap_{n=1}^{\infty} (X \setminus A'_{0,n})$  is also  $\rho_0$  negligible. Let  $(\bar{x}, \bar{y}) \in A'_{0,n} \times A_{1,n}$  be such that

$$s_{0,n}(\bar{x})\sigma_1(\bar{y}) = \cos^2(d_{\pi/2}(\bar{x}, \bar{y})) = \sigma_0(\bar{x})\sigma_1(\bar{y}).$$

Using (A.1), it holds, for all  $x \in A_1$

$$\sigma_1(y) \geq \cos^2(d_{\pi/2}(x, \bar{y}))/s_{0,n}(x).$$

In particular,  $\cos^2(d_{\pi/2}(x, \bar{y}))/s_{0,n}(x)$  achieves its maximum at  $\bar{x}$ , implying  $0 \in \nabla_{\bar{x}}^+ (\cos^2(d_{\pi/2}(\cdot, \bar{y}))/s_{0,n}(\cdot))$ . Since  $s_{0,n}$  is differentiable at  $\bar{x}$ , it yields that  $d^2(\cdot, y)$  is super-differentiable. By Lemma 15, it is also sub-differentiable and thus differentiable at  $\bar{x}$ . It holds

$$(A.3) \quad 0 = \nabla \cos^2 \left( \sqrt{2} \sqrt{\frac{1}{2} d_{\pi/2}^2(\bar{x}, \bar{y})} \right) / s_{0,n}(\bar{x}) - \cos^2(d_{\pi/2}(\bar{x}, \bar{y})) \nabla s_{0,n}(\bar{x}) / s_{0,n}^2(\bar{x})$$

$$(A.4) \quad = -2\sqrt{2} \tan(d_{\pi/2}(\bar{x}, \bar{y})) \frac{\sqrt{2}}{2d_{\pi/2}(\bar{x}, \bar{y})} \nabla \left( \frac{1}{2} d_{\pi/2}^2(\bar{x}, \bar{y}) \right) - \nabla \ln s_{0,n}(\bar{x}).$$

Let  $-\nabla\left(\frac{1}{2}d_{\pi/2}^2(\bar{x}, \bar{y})\right) = v_{\bar{x}\rightarrow\bar{y}} \in T_{\bar{x}}M$  be the unique vector such that  $\bar{y} = \exp_{\bar{x}}^M(v_{\bar{x}\rightarrow\bar{y}})$ , the last equality reads

$$\tilde{\nabla}z_0(\bar{x}) = -\tilde{\nabla}\ln\sigma_0(\bar{x}) = -\nabla\ln s_{0,n}(\bar{x}) = -2\tan(\|v_{\bar{x}\rightarrow\bar{y}}\|)\frac{v_{\bar{x}\rightarrow\bar{y}}}{\|v_{\bar{x}\rightarrow\bar{y}}\|}.$$

Therefore,  $\bar{y}$  is unique  $\rho_1$  a.e. and given by

$$\bar{y} = \exp_{\bar{x}}^M(v_{\bar{x}\rightarrow\bar{y}}) = \exp_{\bar{x}}^M\left(-\arctan\left(\frac{\|\tilde{\nabla}z_0(\bar{x})\|}{2}\right)\frac{\tilde{\nabla}z_0(\bar{x})}{\|\tilde{\nabla}z_0(\bar{x})\|}\right) = \varphi(\bar{x}).$$

It implies that  $\gamma$  is concentrated on the graph of  $\varphi$  in particular  $\gamma = (Id, \varphi)_* \gamma_0$  and  $\varphi_* \gamma_0 = \gamma_1$ . The strict convexity of KL implies that the marginals  $\gamma_0$  and  $\gamma_1$  are unique [25, Theorem 6.7] thus

$$z_0 = -\log(\sigma_0) = -\log\left(\frac{d\gamma_0}{d\rho_0}\right)$$

is unique  $\rho_0$  a.e. and  $\gamma$  is also unique. Note that we used the admissible condition to say that  $\sigma_0$  is  $\rho_0$  a.e. positive. In order to prove (3.25), we start from (13) and a direct computation yields

(A.5)

$$\begin{aligned} \text{WFR}^2(\rho_0, \rho_1) &= \text{KL}(\gamma_0, \rho_0) + \text{KL}(\gamma_1, \rho_1) + \int_{M^2} c(x, y) d\gamma(x, y) \\ &= \int_M \log(e^{-z_0}) e^{-z_0} d\rho_0 + \int_M (1 - e^{-z_0}) d\rho_0 + \int_M \log(e^{-z_1}) e^{-z_1} d\rho_1 + \int_M (1 - e^{-z_1}) d\rho_1 \\ &\quad + \int_{M^2} c(x, \varphi(x)) d\gamma(x) \\ &= \int_M (1 - e^{-z_0}) d\rho_0 + \int_M (1 - e^{-z_1}) d\rho_1 + \int_M [c(x, \varphi(x)) - z_0(x) - z_1(\varphi(x))] d\gamma_0(x) \\ &= \int_M (1 - e^{-z_0}) d\rho_0 + \int_M (1 - e^{-z_1}) d\rho_1. \end{aligned}$$

□

INRIA, PROJECT TEAM MOKAPLAN, UNIVERSITÉ PARIS-DAUPHINE, PSL RESEARCH UNIVERSITY, UMR CNRS 7534-CEREMADE.

*Email address:* [thomas.gallouet@inria.fr](mailto:thomas.gallouet@inria.fr)

DIPARTIMENTO DI MATEMATICA, UNIVERSITÀ DEGLI STUDI DI ROMA “TOR VERGATA”, ROME ITALY

*Email address:* [ghezzi@mat.uniroma2.it](mailto:ghezzi@mat.uniroma2.it)

UNIVERSITÉ GUSTAVE EIFFEL, LIGM, CNRS, INRIA, PROJECT TEAM MOKAPLAN

*Email address:* [fxvialard@normalesup.org](mailto:fxvialard@normalesup.org)