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A geometric study of Wasserstein spaces: an addendum on the boundary

Jérôme Bertrand[1] and Benoît R. Kloeckner[2] *

[1] Institut de Mathématiques, Université Paul Sabatier (Toulouse) et CNRS
bertrand@math.univ-toulouse.fr
[2] Institut Fourier, Université Joseph Fourier (Grenoble) et CNRS
benoit.kloeckner@ujf-grenoble.fr

Abstract. We extend the geometric study of the Wasserstein space $\mathscr{W}_2(X)$ of a simply connected, negatively curved metric space X by investigating which pairs of boundary points can be linked by a geodesic, when X is a tree.

Let X be a *Hadamard space*, by which we mean that X is a complete globally CAT(0), locally compact metric space. Mainly, X is a space where triangles are "thin": points on the opposite side to a vertex are closer to the vertex than they would be in the Euclidean plane. This assumption can also be interpreted as X having non-positive curvature, in a setting more general than manifolds; it has a lot of consequences (the distance is convex, X is contractible, it admits a natural boundary and an associated compactification, ...) An important example of Hadamard space, on which we shall focus in this paper, is simply an infinite tree.

The set of Borel probability measures of X having finite second moment can be endowed with a natural distance defined using optimal transportation, giving birth to the Wasserstein space $\mathscr{W}_2(X)$. It is well-known that $\mathscr{W}_2(X)$ does not have non-positive curvature even when X is a tree.

This note is an addendum to [BK12], where we defined and studied the boundary of $\mathscr{W}_2(X)$. We refer to that article and references therein for the background both on Hadamard space and optimal transportation, as well as for notations. Note that a previous (long) version of [BK12] contained the present content, but has been split after remarks of a referee.

Let us quickly sum up the content of [BK12]. The boundary of X can be defined by looking at geodesic rays, and identifying rays that stay at bounded distance one to another ("asymptote" relation). We showed that there is a natural boundary $\partial\mathscr{W}_2(X)$ of the Wasserstein space that is both close to the traditional boundary of Hadamard spaces (a boundary point can be defined as an asymptote class of rays) and relevant to optimal transportation (a boundary point can be seen as a measure on the cone over ∂X, encoding the asymptotic direction and speed distribution of the mass along a ray). This boundary can

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be given a topology consistent with both points of view, and an angular metric; unsurprisingly, it carries geometric information about $\mathscr{W}_2(X)$.

Here we adress the *visibility*, or lack thereof, of $\mathscr{W}_2(X)$. A Hadamard space satisfies the visibility condition if any pair of boundary points can be linked by a geodesic (e.g. all trees have the visibility property), and the same definition makes sense for its Wasserstein space. It is easily seen that even when X has the visibility condition, $\mathscr{W}_2(X)$ does not; our result is a complete characterization of pairs of asymptotic measures that are the ends of a complete geodesic when X is a tree (Theorem 1 in Section 4).

Our motivation is twofold: first this result shows how much more constrained complete geodesics of $\mathscr{W}_2(X)$ are compared to complete rays; second the method of proof involves cyclical monotonicity in an interesting way, because we have to deal with an optimal transport problem that needs not have a finite infimum.

1 A first necessary condition: antipodality

A complete geodesic (μ_t) in $\mathscr{W}_2(X)$ defines two rays and one therefore gets two asymptotic measures, denoted by $\mu_{-\infty}$ and $\mu_{+\infty}$, also called the *ends* of the geodesic. We recall that these measures are probability measures on the cone $c\partial X$ over the geodesic boundary of X. But by Proposition 5.2 of [BK12], these measures are in fact concentrated on ∂X, viewed as a subset of $c\partial X$. In particular, $\mathscr{W}_2(X)$ is already far from satisfying the visibility condition.

Note that we shall need to consider measures μ on the set of unit complete geodesics $\mathscr{G}_1^{\mathbb{R}}(X)$ that satisfy the cyclical monotonicity, but such that $e_{t\#}\mu$ need not have finite second moment. We still call such maps dynamical transport plan and we say that $e_{\pm\infty\#}\mu$ are its ends. Such a measure μ defines a complete unit geodesic in $\mathscr{W}_2(X)$ if and only if $e_{t\#}\mu \in \mathscr{W}_2(X)$ for some, hence all $t \in \mathbb{R}$. In this section, we only consider *unit* geodesics even if it is not stated explicitly.

The asymptotic formula (Theorem 4.2 of [BK12]) gives us a first necessary condition valid for any Hadamard space. Let us say that two points $\zeta, \xi \in \partial X$ are *antipodal* if they are linked by a geodesic, that two sets $A_-, A_+ \subset \partial X$ are antipodal if all pairs $(\zeta, \xi) \in A_- \times A_+$ are antipodal, and that two measures ν_-, ν_+ on ∂X are antipodal when they are concentrated on antipodal sets. Morever, let us call *uniformly antipodal* a pair of measures whose supports are antipodal.

Given a complete unit geodesic μ, the asymptotic formula readily implies that *the ends of any complete unit geodesic of $\mathscr{W}_2(X)$ must be antipodal.*

When X is a tree, every pair of boundary points is antipodal and this condition simply reads that the ends must be concentrated on disjoint sets.

2 Flows and antagonism

From now on, X is assumed to be a tree, described as a graph by a couple (V, E) where: V is the set of vertices; E is the set of edges, each endowed with one or two endpoints in V and a positive length. Since X is assumed to be complete,

the edges with only one endpoint are exactly those that have infinite length. It is assumed that vertices are incident to 1 or at least 3 edges, so that the combinatorial description of X is uniquely determined by its metric structure. Since X is locally compact, as a graph it is then locally finite. We fix a base point $x_0 \in X$ and use d to denote the distance on X.

We say that two geodesics are *antagonist* if there are two distinct points x, y such that one of the geodesics goes through x and y in this order, and the other goes through the same points in the other order.

We add to each infinite end a formal endpoint at infinity to unify notations. Each edge e has two orientations (xy) and (yx) where x, y are its endpoints. The complement in $\bar{X}$ of the interior of an edge e of endpoints x, y has two components $C_x(xy) \ni x$ and $C_y(xy) \ni y$. An oriented edge (xy) has a *future* $(xy)_+ := C_y(xy) \cap \partial X$ and a *past* $(xy)_- := C_x(xy) \cap \partial X$.

Assume ν_- and ν_+ are antipodal measures on ∂X. Define a signed measure by $\nu = \nu_+ - \nu_-$ and note that $\nu(\partial X) = 0$. The *flow* (defined by (ν_-, ν_+)) through an oriented edge (xy) is $\phi(xy) := \nu((xy)_+)$. The flow gives a natural orientation of edges: an oriented edge is *positive* if its flow is positive, *neutral* if its flow is zero, and *negative* otherwise.

Given a vertex x, let $y_1, \ldots, y_k$ be the neighbors of x such that (xy_i) is positive, and $z_1, \ldots, z_l$ be the neighbors of x such that (xz_j) is negative. Then $\sum_i \phi(xy_i) = \sum_j \phi(z_j x)$ is called the flow through x and is denoted by $\phi(x)$. If $x \neq x_0$, then there is a unique edge starting at x along which the distance to x_0 is decreasing. If this edge is a positive one, (xy_{i_0}) say, then define the *specific flow* through x as $\phi^0(x) = \sum_{i \neq i_0} \phi(xy_i)$. If this edge is a negative one, (xz_{j_0}), then let $\phi^0(x) = \sum_{j \neq j_0} \phi(z_j x)$. If this edge is neutral or if $x = x_0$, then let $\phi^0(x) = \phi(x)$. Note that $\phi(xy) = -\nu((xy)_-) = -\phi(yx)$.

Given a dynamical transport plan μ, we denote by $\mu(xy)$ the μ-measure of the set of geodesics that go through an edge (xy) in this orientation, by $\mu(x)$ the μ-measure of the set of geodesics that pass at x, and by $\mu^0(x)$ the μ-measure of those that are moreover closest to x_0 at this time.

Lemma 1. *If μ is any dynamical transport plan with ends $\nu_\pm$, then:*

1. *for all edge (xy) we have $\mu(xy) \geqslant \max(\phi(xy), 0)$,*
2. *for all vertex x we have $\mu(x) \geqslant \phi(x)$.*

and each of these inequality is an equality for all (xy), respectively all x, if and only if μ contains no pair of antagonist geodesics in its support. In this case, we moreover have $\mu^0(x) = \phi^0(x)$ for all x.

Proof. We prove the first point, the other ones are similar. Denote by $\mu(C_y(xy))$ the measure of the set of geodesic that lie entirely in $C_y(xy)$. We have

$$\mu(xy) + \mu(C_y(xy)) = \nu_+((xy)_+) = \phi(xy) + \nu_-((xy)_+)$$

and

$$\nu_-((xy)_+) = \mu(C_y(xy)) + \mu(yx).$$

It follows that $\phi(xy) = \mu(xy) - \mu(yx)$ so that $\mu(xy) \geqslant \phi(xy)$. Moreover the case of equality $\mu(xy) = \max(\phi(xy), 0)$ implies that $\mu(yx) = 0$ whenever $\mu(xy) > 0$, and we get the conclusion.

Lemma 2. *A dynamical transport plan μ is d^2-cyclically monotone if and only if $\mu \otimes \mu$-almost no pairs of geodesics are antagonist.*

Proof. Assume that the support of μ contains two antagonist geodesics γ, β and let x, y be points such that $\gamma_t = x, \gamma_u = y$ where $u > t$ and $\beta_v = y, \beta_w = x$ where $w > v$. Let $r = \min(t, v)$ and $s = \max(u, w)$. Then

$$d(\gamma_r, \beta_s)^2 + d(\gamma_s, \beta_r)^2 < d(\gamma_r, \gamma_s)^2 + d(\beta_r, \beta_s)^2)$$

so that the transport plan $(e_r, e_s)_\# \mu$ between μ_r and μ_s would not be cyclically monotone (see Figure 1).

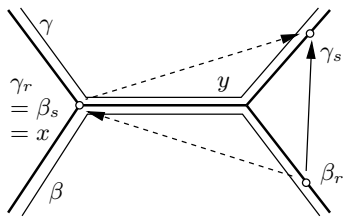

Fig. 1. The transport plan corresponding to the solid arrow is cheaper than the one corresponding to the dashed arrows.

Assume now that $\mu \otimes \mu$-almost no pairs of geodesics are antagonist. Let $\tau : X \to \mathbb{R}$ be a function that is continuous, increasing isometric on each positive edge and constant on neutral edges. Such a function can be defined locally around any point, and we can design it globally since X has no cycle. By Lemma 1, we see that τ is isometric when restricted to any geodesic in the support of μ (such a geodesic must go through positive edges only). Given times $r < s$, the only $|\cdot|^2$-cyclically monotone transport plan in $\mathbb{R}$ from $\tau_\# \mu_r$ to $\tau_\# \mu_s$ is known to be the increasing rearrangement by convexity of the cost. Here $\tau_\# \mu_s$ is the $r - s$ translate of $\tau_\# \mu_r$, so that this transport plan has cost $(r - s)^2$. But τ is 1-Lipschitz, so that any transport plan from μ_r to μ_s has cost at least $(r - s)^2$. This proves the cyclical monotonicity of μ.

Note that here for example, μ_r and μ_s need not have finite second moment; however μ induces a transport plan with finite cost between them, and that peculiarity has therefore no incidence on the proof.

3 Gromov product

Before we state the main result, let us turn to a second point of view.

Given $\xi_- \neq \xi_+$ in ∂X, we denote by $(\xi_-, \xi_+) \subset X$ the locus of a geodesic whose ends are ξ_- and ξ_+. Then we write $D_0(\xi_-, \xi_+)$ the distance between the

base point x_0 and the geodesic (ξ_-, ξ_+). Since X is a tree, this quantity is equal to what is usually called the *Gromov product* $(\xi_- \cdot \xi_+)_{x_0}$, see e.g. [BH99]; however the present definition is adapted to our needs. Set $D_0(\xi, \xi) = \infty$ and denote by $\gamma(\xi_-, \xi_+)$ the parametrized unit complete geodesic whose ends are $\xi_\pm$ at $\pm\infty$, and such that its time 0 realizes D_0: $d(x_0, \gamma(\xi_-, \xi_+)_0) = D_0(\xi_-, \xi_+)$.

For any $\varepsilon > 0$, $e^{-\varepsilon D_0}$ metrizes the cone topology on ∂X so that $D_0(\xi_n, \zeta) \to \infty$ if and only if $\xi_n \to \zeta$. Moreover by compactness if $D_0(\xi_n, \zeta_n) \to \infty$ then there are increasing indices (n_k) such that ξ_{n_k} and ζ_{n_k} converge to a common point. D_0 is continuous, and locally constant outside the diagonal; the map

$$\begin{aligned} F : \partial X \times \partial X &\to \mathscr{G}_1^{\mathbb{R}}(X) \\ (\xi_-, \xi_+) &\mapsto \gamma(\xi_-, \xi_+) \end{aligned}$$

is easily seen to be continuous. when $\mathscr{G}_1^{\mathbb{R}}(X)$ is endowed with the topology of uniform convergence on compact subsets.

Since F is a right inverse to $(e_{-\infty}, e_{+\infty})$, a transport plan $\Pi \in \Gamma(\nu_-, \nu_+)$ can always be written $(e_{-\infty}, e_{+\infty})_\# \mu$ by taking $\mu = F_\# \Pi$. We shall denote also by D_0 the map $\gamma \mapsto d(x_0, \gamma)$ where γ is any parametrized or unparametrized complete geodesic.

Lemma 3. *A transport plan $\Pi_0 \in \Gamma(\nu_-, \nu_+)$ such that*

$$\int -D_0^2 \, \Pi_0 > -\infty$$

is $-D_0^2$-cyclically monotone if and only if $F_\# \Pi_0$ contains no pair of antagonist geodesics in its support. In this case, Π_0 is a solution to the optimal transport problem

$$\inf_{\Pi \in \Gamma(\nu^-, \nu^+)} \int -D_0^2(\xi, \zeta) \, \Pi(d\xi, d\zeta). \tag{1}$$

Proof. Consider $\Pi_0 \in \Gamma(\nu_-, \nu_+)$ and let $\mu = F_\# \Pi_0$.

Assume first that there are antagonist geodesics γ, β in the support of μ. Then permuting $\gamma_{+\infty}$ and $\beta_{+\infty}$ contradicts the $-D_0^2$-cyclical monotonicity.

To prove the other implication, assume that $\operatorname{supp} \mu$ contains no pair of antagonist geodesics but that Π_0 does not achieve the infimum in (1). This happens notably when Π_0 is not cyclically monotone.

Then there is some $\Pi_1 \in \Gamma(\nu_-, \nu_+)$ such that $\int -D_0^2 \, \Pi_0 > \int -D_0^2 \, \Pi_1$. If $F_\# \Pi_1$ has couples of antagonist geodesics in its support, then we can still improve Π_1. Choosing any numbering $e_2, e_3, \ldots$ of the non-oriented edges of X, we inductively construct transport plans $\Pi_2, \Pi_3, \ldots$ in $\Gamma(\nu_-, \nu_+)$ such that $F_\# \Pi_k$ has no antagonist geodesics through the edges $e_2, \ldots, e_k$ in its support, and $(-D_0^2)_\# \Pi_k([x, +\infty)) \leq (-D_0^2)_\# \Pi_{k-1}([x, +\infty))$ for all x (proceed as follows: for all (ζ, ξ) going through e_k in the negative direction, replace ξ by some ξ' in the future of e_k and corresponding to a $(\zeta', \xi') \in \operatorname{supp} \Pi_{k-1}$, and replace (ζ', ξ') by (ζ', ξ); there are many choices to do but they can be made in a arbitrary manner). Then we get $\int -D_0^2 \, \Pi_{k-1} \geqslant \int -D_0^2 \, \Pi_k$ where some, or even all of this integrals can be negative infinite.

We shall use a weak convergence, but $-D_0^2$ is not bounded; we therefore introduce the functions $f_T = -\min(D_0^2, T)$ for $T \in \mathbb{N}$. For all T, the transport plans Π_k also satisfy

$$\int f_T \, \Pi_{k-1} \geqslant \int f_T \, \Pi_k$$

Since ∂X is compact, so is $\Gamma(\nu_-, \nu_+)$ and we can extract a subsequence of (Π_k) that weakly converges to some $\tilde{\Pi}$, and $\tilde{\mu} := F_\# \tilde{\Pi}$ has no pair of antagonist geodesics in its support.

The monotone convergence theorem implies that for T large enough, we have $\int f_T \, \Pi_1 < \int -D_0^2 \, \Pi_0$, and by weak convergence we get $\int f_T \, \tilde{\Pi} \leqslant \int f_T \, \Pi_1$. Since $-D_0^2 \leqslant f_T$, we get

$$\int -D_0^2 \, \tilde{\Pi} < \int -D_0^2 \, \Pi.$$

But then by Lemma 1 we get that $\tilde{\mu}^0(x) = \mu^0(x)$ for all $x \in V$, and since $\int -D_0^2 \, \Pi_0 = \sum_x -d^2(x_0, x)\mu^0(x)$ it follows that $\int -D_0^2 \, \Pi_0$ and $\int -D_0^2 \, \tilde{\Pi}$ must be equal, a contradiction.

Note that the lemma stays true if $-D_0^2$ is replaced with any decreasing function of D_0, but that we shall need precisely $-D_0^2$ later.

Remark 1. In this proof we cannot use Theorem 4.1 of [Vil09] since we do not have the suitable lower bounds on the cost.

4 Characterization of ends

We can now state and prove our result.

Theorem 1. *Assume that X is a tree and let ν_-, ν_+ be two antipodal measures on ∂X. The following are equivalent:*

1. *there is a complete geodesic in $\mathscr{W}_2(X)$ with $\nu_\pm$ as ends;*
2. *the optimal transport problem* (1) *is finite:*

$$\inf_{\Pi \in \Gamma(\nu^-, \nu^+)} \int -D_0^2(\xi, \zeta) \, \Pi(d\xi, d\zeta) > -\infty;$$

3. *the specific flow defined by $\nu_\pm$ satisfies*

$$\sum_{x \in V} \phi^0(x) d(x, x_0)^2 < +\infty.$$

When these conditions are satisfied, then the optimal transport problem (1) *has a minimizer Π_0 and $\Gamma_\# \Pi_0$ define a geodesic of $\mathscr{W}_2(X)$ with the prescribed ends.*

Moreover, the above conditions are satisfied as soon as $\nu_\pm$ are uniformly antipodal.

Proof. First assume that there is a complete geodesic in $\mathscr{W}_2(X)$ with $\nu_\pm$ as ends and denote by μ one of its displacement interpolations; by Lemma 2, the support of μ does not contain any pair of antagonist geodesics. From Lemma 1 it follows that

$$\sum_{x\in V} \phi^0(x) d(x,x_0)^2 \leqslant \int_X d(x,x_0)^2 \mu_0(dx) < \infty$$

since by hypothesis $\mu_0 \in \mathscr{W}_2(X)$. We have also

$$\int -D_0^2(\xi,\zeta)\, \Pi_0(d\xi, d\zeta) \geqslant -\int_X d(x,x_0)^2 \mu_0(dx) > -\infty$$

so that Lemma 3 implies that $\Pi_0 := (e_{-\infty}, e_{+\infty})_\# \mu$ is a solution to problem 1.

Now consider the case when $\nu_\pm$ are uniformly antipodal. Since the supports of ν^- and ν^+ are disjoint, the map D_0, when restricted to $\operatorname{supp}\nu^- \times \operatorname{supp}\nu^+$, is bounded. Therefore, since it is a continuous map, the optimal mass transport problem is well-posed and admits minimisers.

More generally when the infimum in problem (1) is finite, by using the regularity of Borel probability measures on ∂X we can approximate ν^- and ν^+ by probability measures whose supports are disjoint sets. Then, the previous paragraph gives us a sequence of plans which are $-D_0^2$-cyclically monotone. Since D_0 is a continuous map, Prokhorov's theorem allows us to extract a converging subsequence whose limit Π_0 is $-D_0^2$-cyclically monotone. By the finiteness assumption,

$$\int -D_0^2(\xi,\zeta)\, \Pi_0(d\xi, d\zeta) > -\infty$$

and Π_0 is a $-D_0^2$-optimal transport plan.

As soon as a minimizer Π_0 to (1) exists,by Lemma 3 $\mu := \Gamma_\# \Pi_0$ is a dynamical transport plan that has no antagonist pair of geodesics in its support. By Lemma 2 μ is cyclically monotone. By its definition

$$\int_X d(x,x_0)^2 \mu_0(dx) = \int D_0^2(\xi,\zeta)\, \Pi_0(d\xi, d\zeta) < +\infty$$

so that μ defines a geodesic of $\mathscr{W}_2(X)$. It has the prescribed ends since $\Pi_0 \in \Gamma(\nu_-, \nu_+)$.

We have only left to consider the case when $\sum_{x\in V} \phi^0(x) d(x,x_0)^2 < \infty$. For this, let us construct a suitable complete geodesic by hand. Let τ be the time function such that $\tau(x_0) = 0$, as in the proof of Lemma 2. The levels of the time function are finite unions of isolated points and of subtrees of X all of whose edges are neutral. Indeed, consider a point a: if it lies inside a neutral edge, then all the edge has time $\tau(a)$. Otherwise, let (xy) be the orientation of this edge that is positive: points on $[x,a)$ have time lesser than $\tau(a)$, while points on $(a,y]$ have time greater than $\tau(a)$. If a is a vertex, then similarly one sees that nearby a, only the points lying on an incident neutral edge can have time equal to $\tau(a)$. Let $\dot{\tau}^{-1}(t)$ be the union of the isolated points of the level $\tau^{-1}(t)$ and of the points that lie (in X) on the boundary of the neutral subtrees of the same level.

In other words, $\dot{\tau}^{-1}(t)$ is the level t of the map induced by τ on the subforest of X where all neutral edges have been removed.

Define now

$$\tilde{\mu}_t = \sum_{a \in \dot{\tau}^{-1}(t)} \phi(a)\, \delta_a$$

where $\phi(a) = \phi(xy)$ if a lies inside a positive edge (xy). Note that $\tilde{\mu}_t$ is a probability measure thanks to the antipodality of ν_- and ν_+: without it, it would have mass less than 1. It is a good first candidate to be the geodesic we are looking for, except the second moment of μ_t need not be finite! To remedy this problem, proceed as follows. First, there is a displacement interpolation $\tilde{\mu}$ of $(\tilde{\mu}_t)$, which is a probability measure on $\mathscr{G}_1^{\mathbb{R}}(X)$. Now, construct a random geodesic γ as follows : draw $\tilde{\gamma}$ with law $\tilde{\mu}$, and let γ be the geodesic that has the same geometric locus and the same orientation as $\tilde{\gamma}$, and such that γ is nearest to x_0 at time 0. The condition $\sum_{x \in V} \phi^0(x) d(x, x_0)^2 < \infty$ ensures that the law of γ_0 has finite second moment and (μ_t) is the desired geodesic.

The example shown in Figure 2 shows that antipodality is not sufficient for $\nu_\pm$ to be the ends of a geodesic.

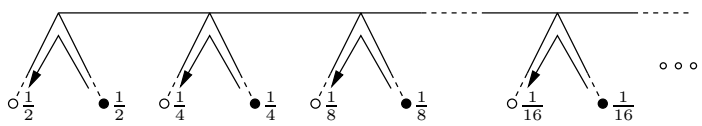

Fig. 2. The measures ν_- (black dots) and ν_+ (white dots) are antipodal. However, the only possible geodesics having these measures as ends, depicted by simple arrows, are not in $\mathscr{W}_2(X)$ if the horizontal edges are long enough.

As a last remark, let us stress that the condition 2 in Theorem 1 is clearly necessary when X is a general Hadamard space, but it might not be a sufficient condition in general.

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