Non-Aligned Distribution Distance using Metric Measure Embedding and Optimal Transport

Mokhtar Z. Alaya \textsuperscript{1} Maxime Béjar \textsuperscript{1} Gilles Gasso \textsuperscript{2} Alain Rakotomamonjy \textsuperscript{1,3}

Abstract

We propose a novel approach for comparing distributions whose supports do not necessarily lie on the same metric space. Unlike Gromov-Wasserstein (GW) distance that compares pairwise distance of elements from each distribution, we consider a method that embeds the metric measure spaces in a common Euclidean space and computes an optimal transport (OT) on the embedded distributions. This leads to what we call a sub-embedding robust Wasserstein (SERW). Under some conditions, SERW is a distance that considers an OT distance of the (low-distorted) embedded distributions using a common metric. In addition to this novel proposal that generalizes several recent OT works, our contributions stand on several theoretical analyses: \textit{i}) we characterize the embedding spaces to define SERW distance for distribution alignment; \textit{ii}) we prove that SERW mimics almost the same properties of GW distance, and we give a cost relation between GW and SERW. The paper also provides some numerical experiments illustrating how SERW behaves on matching problems in real-world.

1. Introduction

Many central tasks in machine learning often attempt to align or match real-world entities, based on computing distance of similarity (or dissimilarity) between pairs of corresponding probability distributions. Recently, optimal transport (OT) based data analysis has proven a significant usefulness to achieve such tasks, arising from designing loss functions (Frogner et al., 2015), unsupervised learning (Arjovsky et al., 2017), clustering (Ho et al., 2017), text classification (Kusner et al., 2015), domain adaptation (Courty et al., 2017), computer vision (Bonneel et al., 2011; Solomon et al., 2015), among many more applications (Kolouri et al., 2017; Peyré & Cuturi, 2019). Distances based on OT are referred to as the Monge-Kantorovich or Wasserstein distance (Monge, 1781; Kantorovich, 1942; Villani, 2009). OT tools allow for a natural geometric comparison of distributions, that takes into account the metric of the underlying space to find the most cost-efficiency way to transport mass from a set of sources to a set of targets. The success of machine learning algorithms based on Wasserstein distance is due to its nice properties (Villani, 2009) and to recent development of efficient computations using entropic regularization (Cuturi, 2013; Genevay et al., 2016; Altschuler et al., 2017; Alaya et al., 2019).

Distribution alignment using Wasserstein distance relies on the assumption that the two sets of entities in question belong to the same ground space, or at least pairwise distance between them can be computed. To overcome such limitations, one seeks to compute Gromov-Wasserstein (GW) distance (Sturm, 2006; Mémoli, 2011), which is a relaxation of Gromov-Hausdorff distance (Memoli, 2008; Bronstein et al., 2010). GW distance allows for learning an optimal transport-like plan by measuring how the distances between pairs of samples within each space are similar. The GW framework has been used for solving alignment problems in several applications, for instance shape (Mémoli, 2011), graph partitioning and matching (Xu et al., 2019a;b), vocabulary sets between different languages (Alvarez-Melis & Jaakkola, 2018), generative models (Bunne et al., 2019), matching weighted networks (Chowdhury & Mémoli, 2018), to name a few. Unfortunately, this advantage comes at the price of an expensive computation in large-scale settings, since computing GW distance is a non-convex quadratic program and NP-hard (Peyré & Cuturi, 2019). Peyré et al. (2016) propose an entropic version called entropic GW discrepancy, that leads to approximate GW distance.

Metric embedding gives an approximation algorithm for some “complex” problem in a metric space (Matoušek, 2002). Towards this end, it may be useful to establish a new representation (embedding) of data at hand in a “simpler” metric space where the distances are approximately preserved, and then solve the alignment problem there. This yields significant savings in the running time and/or space.
The improvement would particularly be impressive if an algorithm for the original problem uses space time exponential in the dimension.

**Contributions.** In the spirit of metric embedding methods for approximation, we propose a novel approach for comparing distributions whose supports do not necessarily lie on the same ground metric space. Unlike GW distance that compares pairwise distance of elements from each distribution, we consider a method that embeds the metric measure spaces into a common Euclidean space and computes a Wasserstein OT distance between the embedded distributions. Our approach generalizes the “min-max” robust OT problem recently introduced in (Paty & Cuturi, 2019), where the authors address orthogonal projections to approximate the Wasserstein distance. Furthermore, our contributions stands on several theoretical analyses. Main contributions of this work are summarized in the following three points:

- We propose a novel learning framework for distribution alignment from different spaces using a sub-embedding robust Wasserstein (SERW) distance, that mimics most of the GW distance properties.
- We characterize the embedding spaces to define SERW distance and we provide a relation between the OT costs of GW and SERW.
- We corroborate our theoretical results with numerical experiments on simulated and real datasets.

**Layout of the paper.** The remainder of the paper is organized as follows. In Section 2 we introduce the definitions of Wasserstein and GW distances, and we set up the embedding spaces. In Section 3 we investigate metric measure embedding for non-aligned distributions through an OT via SERW distance. Section 4 is dedicated to numerical experiments of matching in a simulated and real data. The proofs of the main results are postponed to the appendices in the supplementary materials.

## 2. Preliminaries

We start here by reviewing basic definitions of the materials needed to introduce the main results.

We consider two metric measure spaces (mm-space for short) (Gromov et al., 1999) $(X, d_X, \mu)$ and $(Y, d_Y, \nu)$, where $(X, d_X)$ is a compact metric space and $\mu$ is a probability measure with full support, i.e. $\mu(X) = 1$ and $\text{supp}[\mu] = X$. We recall that the support of a measure $\text{supp}[\mu]$ is the minimal closed subset $X_0 \subset X$ such that $\mu(X\setminus X_0) = 0$. Similarly, we define the mm-space $(Y, d_Y, \nu)$. Let $\mathcal{P}(X)$ be the set of probability measures in $X$ and $p \in \{1, 2\}$. We define $\mathcal{P}_p(X)$ as its subset consisting of measures with finite $p$-moment, i.e.,

$$\mathcal{P}_p(X) = \{ \eta \in \mathcal{P}(X) \text{ s.t. } M_p(\mu) < \infty \},$$

where $M_p(\mu) = \int_X \|x\|^p d\mu(x)$ with $\|x\|_X = d_X(x, 0)$. For $\mu \in \mathcal{P}(X)$ and $\nu \in \mathcal{P}(Y)$, we write $\Pi(\mu, \nu) \subset \mathcal{P}(X \times Y)$ for the collection of probability measures (couplings) on $X \times Y$ as

$$\Pi(\mu, \nu) = \{ \pi \in \mathcal{P}(X \times Y) \text{ s.t. } \forall A \subset X, B \subset Y, \pi(A \times Y) = \mu(A), \pi(X \times B) = \nu(B) \}.$$  

**Wasserstein distance.** The Monge-Kantorovich or the 2-Wasserstein distance aims at finding an optimal mass transportation plan $\pi \in \mathcal{P}(X \times Y)$ such that the marginals of $\pi$ are respectively $\mu$ and $\nu$, and these two distributions are supposed to be defined over the same ground space, i.e., $X = Y$. It reads as

$$W_2^2(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int_{X \times X} d^2(x, x') d\pi(x, x'). \quad (1)$$

The infimum in (1) is attained, and any probability $\pi$ which realizes the minimum is called an optimal transport plan.

**Gromov-Wasserstein distance.** In contrast to Wasserstein distance, GW one deals with measures that not necessarily belong to the same ground space. It learns an optimal transport-like plan which transports samples from a source metric space $X$ into a target metric space $Y$ by measuring how the distances between pairs of samples within each space are similar. Following the pioneering work of Mémoli (2011), GW distance is defined as

$$G\mathcal{W}_2^2(\mu, \nu) = \frac{1}{2} \inf_{\pi \in \Pi(\mu, \nu)} J(\mu, \nu),$$

where

$$J(\mu, \nu) = \iint_{X \times Y} \ell(d_X(x, x'), d_Y(y, y')) d\pi(x, y) d\pi(x', y')$$

with $\ell(a, b) = |a - b|^2$. Peyré et al. (2016) propose an entropic version called entropic GW discrepancy, allowing to tackle more flexible loss functions $\ell$, such as mean-square-error or Kullback-Leibler divergence.

**Metric embedding.** Metric embedding consists in characterizing a new representation of the samples based on the concept of distance preserving.

**Definition 1** A mapping $\phi : (X, d_X) \to (Z, d_Z)$ is said an embedding with distortion $\tau$, denoted as $\tau$-embedding, if the following holds: there exists a constant $\kappa > 0$ (“scaling factor”) such that for all $x, x' \in X$,

$$\kappa d_X(x, x') \leq d_Z(\phi(x), \phi(x')) \leq \tau \kappa d_X(x, x'). \quad (3)$$

The approximation factor in metric embedding depends on a distortion parameter of the $\phi$ embedding. This distortion
we suppose hereafter \( \kappa = 1 \) in \((3)\) and denote by \( \mathcal{F}_d(X) \) and \( \mathcal{F}_d(Y) \) the set of \( \tau_\phi \)-embedding \( \phi : X \to \mathbb{R}^d \) and \( \tau_\psi \)-

embedding \( \psi : Y \to \mathbb{R}^d \), respectively. We further assume that \( \phi(0) = \psi(0) = 0 \). It is worth to note that \( \mathcal{F}_d(X) \) and \( \mathcal{F}_d(Y) \) are non empty. Indeed, suppose we are given a set of \( n \) data points \( \{x_1, x_2, \ldots, x_n\} \in X \), then Bourgain’s embedding theorem (Bourgain, 1985) guarantees the existence of an embedding \( \phi : X \to (\mathbb{R}^d, \|\cdot\|) \) with tight distortion at most \( \mathcal{O}(\log(n)) \), i.e., \( \tau_\phi = \mathcal{O}(\log(n)) \), and the target dimension \( d = \mathcal{O}(\log^2(n)) \). We stress that \( d \) is independent of the original dimensions of \( X \) and \( Y \), and depends only on the number of the given data points \( n \) and \( m \) and the accuracy-embedding parameters \( \tau_\phi \) and \( \tau_\psi \). Hence for a data points \( \{x_1, x_2, \ldots, x_n\} \in X \) and \( \{y_1, y_2, \ldots, y_m\} \in Y \)

underlying the distributions of interest, one has

\[
d = \mathcal{O}(\log^2(\max(n, m))). \tag{4}
\]

Let’s highlight all the above criteria characterizing the metric embeddings we will consider to define our novel distance and that will help us shape some of its properties.

**Assumption 1** Assume that \((X, d_X, \mu)\) and \((Y, d_Y, \nu)\) are mm-spaces with measures \( \mu \) and \( \nu \) having both finite \( p \)-moments for \( p = 1, 2 \), i.e., \( M_1(\mu) = \int_X d_X(x, 0) d\mu(x) < \infty \) and \( M_2(\mu) = \int_X d_X^2(x, 0) d\mu(x) < \infty \), (similarly for \( \nu \)). Assume also that \( X \) and \( Y \) are of cardinalities \( n \) and \( m \), the target dimension \( d \) satisfies \((4)\), and \( \mathcal{F}_d(X) = \{\phi : X \to \mathbb{R}^d, \tau_\phi \text{-embedding, } \phi(0) = 0\}, \mathcal{F}_d(Y) = \{\psi : Y \to \mathbb{R}^d, \tau_\psi \text{-embedding, } \psi(0) = 0\}, \) with distortions \( \tau_\phi \in \mathcal{D}_{\text{emb}}(X), \tau_\psi \in \mathcal{D}_{\text{emb}}(Y) \) where

\[
\mathcal{D}_{\text{emb}}(X) = [1, \mathcal{O}(\log(n))] \text{ and } \mathcal{D}_{\text{emb}}(Y) = [1, \mathcal{O}(\log(m))].
\]

**3. Metric measure embedding and OT for distribution alignment**

Let us give first the overall structure of our approach of non-aligned distributions, which generalizes a recent works (Alvarez-Melis & Jaakkola, 2018; Paty & Cuturi, 2019). Paty & Cuturi (2019) prove an equivalence of Wasserstein distance through linear projection embeddings. In this work, we aim at proposing a novel distance between two measures defined on different mm-spaces. As this distance will be defined as the optimal objective of some optimization problem, in the first part of this section, we provide technical details and conditions ensuring its existence. The second part of the section presents formally our novel distances and its properties including its cost relation with GW distance.

In a nutshell, our distribution alignment distance between \( \mu \) and \( \nu \) is obtained as a Wasserstein distance between pushfowards (see Definition 2) of \( \mu \) and \( \nu \) w.r.t. some appropriate couple \((\phi, \psi)\)-embeddings belonging to \( \mathcal{F}_d(X) \times \mathcal{F}_d(Y) \).

Towards this end, we need to exhibit some topological properties of the embeddings spaces, allowing at first the existence of the constructed OT approximate distances.

**3.1. Topological properties of the embedding spaces**

We may consider the function \( \Gamma_X : \mathcal{F}_d(X) \times \mathcal{F}_d(X) \to \mathbb{R}_+ \) such that \( \Gamma_X(\phi, \phi') = \sup_{x \in X} \|\phi(x) - \phi'(x)\| \), for each pair of embeddings \( \phi, \phi' \in \mathcal{F}_d(X) \). This function defines a proper metric on the space of embeddings \( \mathcal{F}_d(X) \) and it is referred to as the supremum metric on \( \mathcal{F}_d(X) \). Indeed, \( \Gamma_X \) satisfies all the conditions that define a general metric. We define analogously the metric \( \Gamma_Y \) on \( \mathcal{F}_d(Y) \). With the aforementioned preparations, the embeddings spaces satisfy the following topological property.

**Proposition 1** \((\mathcal{F}_d(X), \Gamma_X) \) and \((\mathcal{F}_d(Y), \Gamma_Y) \) are both compact metric spaces.

Endowing the embedding spaces with the supremum metrics is fruitful, since we get benefits from some existing topological results, based on this functional space metric, to prove the statement in Proposition 1. To let it more readable, the proof of Proposition 1 is divided into 5 steps summarized as follows: first step is for metric property of \( \mathcal{F}_d(X) \); second one shows completeness of \( \mathcal{F}_d(X) \); third establishes the totally boundedness of \( \mathcal{F}_d(X) \), namely that one can recover this space using balls centred on a finite number of embedding points; the last is a conclusion using Arzela-Ascoli’s Theorem for characterizing compactness of subsets of functional continuous space, see Appendix A.1 for all these details and their proofs.

Let us now give a definition of pushforward measures.

**Definition 2** (Pushforward measure). Let \((S, \mathcal{S})\) and \((T, \mathcal{T})\) be two measurable spaces, \( f : S \to T \) be a mapping, and \( \eta \) be a measure on \( S \). The pushforward of \( \eta \) by \( f \), written \( f_\# \eta \), is the measure on \( T \) defined by \( f_\# \eta(A) = \eta(f^{-1}(A)) \) for \( A \in \mathcal{T} \). If \( \eta \) is a measure and \( f \) is a measurable function,
then $f\#\eta$ is a measure.

### 3.2. Sub-Embedding OT

Let assume that Assumption 1 holds. Following Paty & Cuturi (2019), we define an embedding robust version of Wasserstein distance between pushforwards $\phi\#\mu, \psi\#\nu \in \mathcal{P}_p(\mathbb{R}^d)$ and $\psi\#\nu \in \mathcal{P}_p(\mathbb{R}^d)$ for some appropriate couple $(\phi, \psi)$-embeddings belonging to $\mathcal{F}_d(X) \times \mathcal{F}_d(Y)$. We then consider the worst possible OT cost over all possible low-distortion embeddings.

**Definition 3** The $d$-dimensional embedding robust 2-Wasserstein distance (ERW) between $\mu$ and $\nu$ reads as

$$E_d^2(\mu, \nu) := \sup_{\phi \in \mathcal{F}_d(X), \psi \in \mathcal{F}_d(Y)} \mathcal{W}_2^2\left(\frac{1}{\sqrt{2}}\phi\#\mu, \frac{1}{\sqrt{2}}\psi\#\nu\right).$$

Note that $E_d^2(\mu, \nu)$ is finite since the considered embeddings are Lipschitz and both of the distributions $\mu$ and $\nu$ have finite 2-moment due to Assumption 1. Next, using results of pushforward measures, for instance see Lemmas 4 and 5 in the supplementary materials, we explicit ERW in Lemma 1, whereas Lemmas 2 and 3 establish the existence of embeddings that achieve the supremaums defining both ERW and SERW.

**Lemma 1** One has

$$E_d^2(\mu, \nu) = \sup_{\phi \in \mathcal{F}_d(X), \psi \in \mathcal{F}_d(Y)} \frac{1}{2} \inf_{\pi \in \Pi(\mu, \nu)} J_{\phi, \psi}(\mu, \nu),$$

where $J_{\phi, \psi}(\mu, \nu) = \int_{X \times Y} \|\phi(x) - \psi(y)\|^2 \, d\pi(x, y)$.

By the compactness property of the embedding spaces (see Proposition 1), the set of optimums defining $E_d^2(\mu, \nu)$ is not empty.

**Lemma 2** There exists a couple $(\phi^*, \psi^*)$-embeddings in $\mathcal{F}_d(X) \times \mathcal{F}_d(Y)$ such that

$$E_d^2(\mu, \nu) = \mathcal{W}_2^2\left(\frac{1}{\sqrt{2}}\phi^*\#\mu, \frac{1}{\sqrt{2}}\psi^*\#\nu\right).$$

Clearly, the quantity $E_d^2(\mu, \nu)$ is difficult to compute, since an OT is a linear programming problem that requires generally super cubic arithmetic operations. Based on this observation, we focus on the corresponding “min-max” problem to define the $d$-dimensional sub-embedding robust $2$-Wasserstein distance (SERW). For the sake, we make the next definition.

**Definition 4** The $d$-dimensional sub-embedding robust $2$-Wasserstein distance between $\mu$ and $\nu$ is defined as

$$S_d^2(\mu, \nu) := \frac{1}{2} \inf_{\pi \in \Pi(\mu, \nu)} \sup_{\phi \in \mathcal{F}_d(X), \psi \in \mathcal{F}_d(Y)} J_{\phi, \psi}(\mu, \nu). \tag{5}$$

Thanks to the minimax inequality we have that $E_d^2(\mu, \nu) \leq S_d^2(\mu, \nu)$. We emphasize that ERW and SERW quantities play a crucial role in our approach to match distributions in the common space $\mathbb{R}^d$ regarding pushforwards of the measures $\mu$ and $\nu$ realized by a couple of optimum embeddings.

Optimal solutions for $S_d^2(\mu, \nu)$ exist, namely:

**Lemma 3** There exist a couple $(\phi^*, \psi^*)$-embeddings in $\mathcal{F}_d(X) \times \mathcal{F}_d(Y)$ such that

$$S_d^2(\mu, \nu) = \frac{1}{2} \inf_{\pi \in \Pi(\mu, \nu)} J_{\phi^*, \psi^*}(\mu, \nu).$$

The proofs of Lemmas 2 and 3 rely on the continuity under integral sign Theorem (Schilling), and the compactness property of both the embeddings spaces and the couplings transport plan $\Pi(\mu, \nu)$, see Appendices A.4 and A.3 for more details.

![Illustration of the preserving measure mappings between the mm-spaces](image)

Figure 1. Illustration of the preserving measure mappings between the mm-spaces $(X, d_X, \mu)$ and $(Y, d_Y, \nu)$ given in (6). $\psi^*$ maps from the Y space to $\mathbb{R}^d$ while $\phi^*$ maps from X to $\mathbb{R}^d$. Our distance $S_d^2(\mu, \nu)$ vanishes if and only if $\mu$ and $\nu$ are mapped through the embedding $\phi^*-1, \psi^*-1$.

### 3.3. Cost relation between GW and SERW

Recall that we are interested in distribution alignment for measures coming from different mm-spaces. One hence expects that SERW mimics some metric properties of GW distance. To proceed in this direction, we first prove that SERW defines a proper metric on the set of all weakly isomorphism classes of mm-spaces. In our setting the terminology of weakly isomorphism means that there exists a pushforward mapping between mm-spaces. If such a pushforward is 1-embedding the class is called strongly isomorphism.

**Proposition 2** Let Assumption 1 holds and assume $X \subseteq \mathbb{R}^D$ and $Y \subseteq \mathbb{R}^{D'}$ with $D \neq D'$. Then, $S_d^2(\mu, \nu) = 0$ hap-
pens if and only if the couple \((\phi^*,\psi^*)\)-embedding optima of \(S^2_d(\mu,\nu)\) verifies
\[
\mu = (\phi^{-1} \circ \psi^*) \# \nu \quad \text{and} \quad \nu = (\psi^{-1} \circ \phi^*) \# \mu,
\]
where \(\circ\) stands for the composition operator between functions.

Figure 1 illustrates the mappings between the embedding spaces and how they are assumed to interact in order to satisfy condition in Prop. 2.

In (Mémoli, 2011) (Theorem 5, property (a)), it is shown that GW distance, \(GW^2_d(\mu,\nu) = 0\) if and only if \((X, d_X, \mu)\) and \((Y, d_Y, \nu)\) are strongly isomorphic. This means that there exists a Borel measurable bijection \(\varphi : X \to Y\) (with Borel measurable inverse \(\varphi^{-1}\)) such that \(\varphi\) is 1-embedding and \(\varphi \# \mu = \nu\). The statement in Prop. 2 seems to be a “weak” version of the aforementioned result, because neither \(\phi^{-1} \circ \psi^*\) nor \(\psi^{-1} \circ \phi^*\) are isometric embeddings. However, we succeed to find a measure-preserving mapping relating \(\mu\) and \(\nu\) to each other via the given pushforwards in (6).

With these elements, we can now prove that both ERW and SERW are further distances.

**Proposition 3** Assume that statement of Prop. 2 holds. Then, ERW and SERW define a proper distance between weakly isomorphism mm-spaces.

The additional assumption on the mm-spaces being subsets of \(\mathbb{R}^D\) and \(\mathbb{R}^{D'}\) allows us to use the Cramér and Wold Theorem (Cramér & Wold, 1936) to compare two probabilities measures. The fundamental theorem of Cramér and Wold states that a Borel probability measure on Euclidean space is determined by the values it assigns to all half-spaces, see Appendix A.6 for the details.

We end up this section by proving a cost relation metric between GW and the SERW distances. The obtained upper and lower bounds depend on approximation constants that are linked to the distortions of the embeddings.

**Proposition 4** Let Assumption 1 holds. Then, one has
\[
\frac{1}{2} GW^2_d(\mu, \nu) \leq S^2_d(\mu, \nu) + \alpha M_{\mu,\nu},
\]
where \(\alpha = 2 \inf_{\tau_0 \in D_{\text{out}}(X), \tau_0 \in D_{\text{out}}(Y)} (\tau_0 \tau_0 - 1)\) and \(M_{\mu,\nu} = 2(M_1(\mu) + M_1(\nu))\).

**Proposition 5** Let Assumption 1 holds. Define \(\beta = 2 \sup_{\tau_0 \in D_{\text{out}}(X), \tau_0 \in D_{\text{out}}(Y)} (\tau_0^2 + \tau_0^2)\). Then, one has
\[
S^2_d(\mu, \nu) \leq \beta GW^2_d(\mu, \nu) + 4 \beta M_{\mu,\nu},
\]
where \(M_{\mu,\nu} = \sqrt{M_2(\mu) + M_1(\mu)} + \sqrt{M_2(\nu) + M_1(\nu)}\).

Proofs of Propositions 4 and 5 are presented in Appendices A.8 and A.7. We use upper and lower bounds of GW distance as provided in (Memoli, 2008). The cost relation between SERW and GW distances obtained in (4) and (5) are up to the constants \(\alpha, \beta\) which are depending on the distortion parameters of the embeddings, and up to an additive constant through the \(p\)-moments \(M_p\) of the measures \(\mu\) and \(\nu\). In the following discussion we highlight some particular cases leading to closed form of the upper and lower bounds for the cost relation between GW and SERW distances.

Discussion. From the computational point of view, computing SERW distance seems a daunting task, since one would have to optimize over the product of two huge embedding spaces \(D_d(X) \times D_d(Y)\). For this reason, we suggest to tailor our experiments using known embeddings in advance. Hence the cost relation guarantees given in Propositions 3 and 4 are dependent on the distortions of the fixed embeddings, i.e., the constants \(\alpha, \beta\) become:\(\alpha = \tau_0^2 \tau_0 - 1\) and \(\beta = \tau_0^2 + \tau_0^2\). In a particular case of isometric embeddings, our procedure gives the following cost relation
\[
\frac{1}{2} GW^2_d(\mu, \nu) \leq S^2_d(\mu, \nu) \leq 2 GW^2_d(\mu, \nu) + 8 M_{\mu,\nu}.
\]

Roughly speaking, our SERW procedure with respect to a fixed embeddings can be viewed as an embedding-dependent distribution alignment. More precisely, the alignment quality is strongly dependent on the given embeddings; the more low distorted embeddings, the more accurate alignment. On the other hand, the additive constants \(M_{\mu,\nu}\) and \(M_{\mu,\nu}\) can be upper bounded in a setting of data preprocessing, for instance in the case of a normalization preprocessing we have \(M_{\mu,\nu} \leq 4\) and \(M_{\mu,\nu} \leq 6\).

3.4. Practical implementation

Based on the above presented theory, we have several options for computing the distance between non-aligned measures and they all come with some guarantees compared to a Gromov-Wasserstein distance.

In practice, for fixed embedding setting, one may proceed in various possible ways. If original spaces are subspace of \(\mathbb{R}^d\), any distance preserving embedding can be a good option for having an embedding with low distortion. Typically, methods like multidimensional scaling (MDS), Isomap or Local linear embedding (LLE) can be good candidates (Kruskal & Wish, 1978; Balasubramanian & Schwartz, 2002; Roweis & Saul, 2000). One of the key advantage of SERW is that it considers non-linear embedding before measure alignments. Hence, it has the ability of leveraging over the large zoo of recent embedding methods that act on different data structures like text (Mikolov et al., 2013; Grave et al., 2018), graphs (Grover & Leskovec, 2016; Narayanan et al., 2017).
or even histogram (Courty et al., 2018). While most of these methods have not been designed for minimizing their distortions, one potential future work is to reshape those methods so as to integrate a distance preserving loss in their objective function.

4. Numerical experiments

In this section, we provide some illustrative examples that show how SERW distance behaves on numerical problems. We apply it on some toy problems as well as on some problems usually addressed using Gromov-Wasserstein distance.

4.1. Toy example

In this example, we extracted randomly \( n = m = 1000 \) samples from MNIST, USPS and fashion MNIST databases, denoted by \( X, Y \) and \( Z \). We compare GW distances between three possible matchings with the assorted SERW distances computed for two classical manifold learning approaches Isomap and Locally Linear Embedding. We preprocess the data in order to fix the parameter \( \tilde{\beta}_d \) and \( \tilde{\beta}_d \) as discussed previously. We then vary the dimension of the embedded data from \( \log(n)^2 \) up to the smallest dimension of the original samples.

In Figure 2 we report plots of the distortion rate, the additive constant \( \beta \tilde{M}_{\mu, \nu} \) in the upper bound in Proposition 5, and the distance ratio of SERW for the three data sets \( X, Y \) and \( Z \). As can be seen the rates decrease as the embedding dimension increase. Note that to determine the distortion coefficient for each given embedding dimension, we just compute the quotient of the pairwise distances both in the origin and the embedded spaces. Thus, this high magnitudes of the upper bounds are due to a “simple” estimation of the distortion rate. One may investigate a good estimation to lead to a more closed upper bound. For this toy set, we investigate a useful property in our approach called proximity preservation is the property stating that: \( GW_2(\mu, \nu) \leq GW_2(\mu, \eta) \Rightarrow S_d(\mu, \nu) \leq S_d(\mu, \eta) \). In order to confirm this property, we compute the ratio between \( S_d(X, Y) / S_d(Y, Z) \) and \( S_d(X, Z) / S_d(Y, Z) \) for various embeddings and compare the resulting order with \( GW_2(X, Y) / GW_2(Y, Z) \) and \( GW_2(X, Z) / GW_2(Y, Z) \). As seen in Figure 2, while the ratios vary their order is preserved when changing the embedding dimensions and types.

4.2. Meshes comparison

Gromov-Wasserstein distance is frequently used in computer graphics for computing correspondence between meshes. Those distances are then exploited for organizing shape collection, for instance for shape retrieval or search. One of the useful key property of Gromov-Wasserstein distance for those applications is that it is isometry-invariant. In order to show that our proposed approach approximately satisfies this property, we reproduce an experiment already considered by Solomon et al. (2016) and Vayer et al. (2019).

We have at our disposal a time-series of 45 meshes of a galloping horses. When comparing all meshes with the first one, the goal is to show that the distance presents a cyclic nature related to galop cycle. Each mesh if composed of 8400 samples and in our case, we have embedded them into a 2-dimensional space using an multi-dimensional scaling algorithm. This provides us a low-distorsion embedding as pairwise distances are approximately preserved through MDS.

Figure 3 shows the (max-normalized) distances between meshes we obtain with SERW and with asliced Gromov-Wasserstein distance. In both cases, due to the random aspect of both algorithms, distances are averaged over 10
we have images labeled by some nouns modified by some (Isola et al., 2015). In the dataset discussed in this paper, the embeddings of dimension $256 \times 4096$ have been computed for coupling labels and images in the two extracted from the first dense layer of a VGG-16. These embeddings are issued by a model trained on the first 1 billion bytes of En- dembedded into $\mathbb{R}^{4096}$ and extracted all the classes associated with those adjectives, ruffled, weathered, engraved considered only three of them adjectives describing state of the object or scenes. In our experiment, we want to show that our approach provides coupling between labels and images similar to those obtained by a Gromov-Wasserstein approach. As for proof of concept, from the 115 available adjectives, we have conceived only three of them ruffled, weathered, engraved and extracted all the classes associated with those adjectives. In total, we obtain 109 different classes of objects and about 525 images in total (as each class contains at most 5 objects).

The embeddings of dimension 100 for the labels have been obtained using Fasttext (Grave et al., 2018). Specifically, the composed name (adjective + noun) of each label is embedded into $\mathbb{R}^{100}$ using a word vector representation issued by a model trained on the first 1 billion bytes of English Wikipedia according to (Mikolov et al., 2018). The 256 $\times$ 256 images have been embedded into a vector of dimension 4096 using a pre-trained VGG-16 model (Simonyan & Zisserman, 2015). These embeddings are extracted from the first dense layer of a VGG-16.

The Gromov-Wasserstein distance of those embeddings has been computed for coupling labels and images in the two different embedding spaces. For our SERW approach, we have further reduce the dimension of the image embeddings using MDS with 100 dimensions. When computing the distance matrix, objects have been organized by class of adjectives for an easy visual inspection.

Figure 4 presents an example of coupling matrix obtained using Gromov-Wasserstein and our SERW approach. Since in both cases, the Wasserstein distance is not approximated by the Sinkhorn algorithm, the obtained matching is not smooth. Our results show that both Gromov-Wasserstein and our SERW distances are able to retrieve the 3 classes of adjectives and matches appropriate images with the relevant labels. Interestingly, it seems that our approach is able to provide a better matching as the lower-right structure is more consistent than in the Gromov-Wasserstein case.

Figure 5 illustrates the best matched images by GW and SERW (according to the transportation map) to the texts En- graved Copper and Engraved Metal. We can remark that in both cases GW and SERW do not suggest the same images. However, the retrieved images are meaningful according to the text queries. We shall notice that the embeddings used by SERW do not distort the discriminative information, leading to interesting matched images as shown by the last row of Figure 5.

4.3. Text-Image Alignment

In order to show that our proposed approach also provides relevant coupling when considering out-of-the-shelves embeddings, we present here results on aligning text and images distributions. The problem we address is related to identifying different states of objects, scene and materials (Isola et al., 2015). In the dataset discussed in this paper, we have images labeled by some nouns modified by some adjectives describing state of the object or scenes. In our experiment, we want to show that our approach provides coupling between labels and images similar to those obtained by a Gromov-Wasserstein approach. As for proof of concept, from the 115 available adjectives, we have considered only three of them ruffled, weathered, engraved and extracted all the classes associated with those adjectives. In total, we obtain 109 different classes of objects and about 525 images in total (as each class contains at most 5 objects).

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5. Conclusion

In this paper we introduced the SERW distance for distribution alignment lying in different mm-spaces. It is based on metric measure embedding of the original mm-spaces into a common Euclidean space and computes an optimal transport on the (low-distorted) embedded distributions. We prove that SERW defines a proper distance behaving like GW distancen and we further show a cost relation between SERW and GW. The numerical experiments are tailored regarding fixed embeddings, since the exact computation of SERW needs an optimization algorithm over the product of two very large embedding spaces. Nevertheless, SERW can be viewed as an embedding-dependent alignment for distributions coming from different mm-spaces. Thus its quality is strongly dependent on the given embeddings. A line of future work to SERW procedure includes a nonlinear embedding learning using deep neural network tools, that can after be incorporated on the optimal transport computation.

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Figure 5. Best matched images obtained through GW transportation plan, and our SERW distance. The first block of images correspond to the class Engraved Copper and the second one to Engraved Metal. Within each block, the top row shows the results of GW and the bottom row illustrates the matching proposed by SERW.

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A. Proofs

In the proofs, we frequently use the two following lemmas. Lemma 4 writes an integration result using push-forward measures; it relates integrals with respect to a measure \( \eta \) and its push-forward under a measurable map \( f : X \to Y \). Lemma 5 proves that the admissible set of couplings between the embedded measures are exactly the embedded of the admissible couplings between the original measures.

**Lemma 4** Let \( f : S \to T \) be a measurable mapping, let \( \eta \) be a measurable measure on \( S \), and let \( g \) be a measurable function on \( T \). Then \( \int_T g f_# \eta = \int_S (g \circ f) d\eta \).

**Lemma 5** (Paty & Cuturi, 2019) For all \( \phi \in \mathcal{F}_d(X), \psi \in \mathcal{F}_d(Y) \), and \( \mu, \nu \in \mathcal{P}(X, \nu) \), one has \( \Pi(\phi_# \mu, \psi_# \nu) = \left\{ \left( \phi \otimes \psi \right) \# \pi \text{ s.t. } \pi \in \Pi(\mu, \nu) \right\} \), where \( \phi \otimes \psi : X \times Y \to X \times Y \) such that \( (\phi \otimes \psi)(x, y) = (\phi(x), \psi(y)) \) for all \( x, y \in X \times Y \).

A.1. Proof of Proposition 1

Since the arguments of the proof are similar for the two spaces, we only focus on proving the topological property of \( \mathcal{F}_d(X) \). Let us refresh the memories by some results in topology: we denote \( \mathcal{C}(X, \mathbb{R}^d) \) the set of all continuous mappings of \( X \) into \( (\mathbb{R}^d, \| \cdot \|) \) and recall the notions of totally boundedness in order to characterize the compactness of \( (\mathcal{F}_d(X), \Gamma_X) \). The material here is taken from (Kubrusly, 2011) and (O’Searcoid, 2006).

**Definition 5** i) (Totally bounded) Let \( A \) be a subset of a metric space \((S, d_S)\). A subset \( A_\varepsilon \) of \( A \) is an \( \varepsilon \)-net for \( A \) if for every point \( s \) of \( A \) there exists a point \( t \) in \( A_\varepsilon \) such that \( d(t, s) < \varepsilon \). A subset \( A \) of \( S \) is totally bounded (precompact) in \((S, d_S)\) if for every real number \( \varepsilon > 0 \) there exists a finite \( \epsilon \)-net for \( A \).

ii) (Pointwise totally bounded) A subset \( S \) of \( \mathcal{C}(S, d_S), (T, d_T) \) is pointwise totally bounded if for each \( s \) in \( S \) the set \( S(s) = \{ f(s) \in T : f \in S \} \) is totally bounded in \( T \).

iii) (Equicontinuous) A subset \( \mathcal{F}(S, T) \) is equicontinuous at a point \( s_0 \) in \( S \) if for each \( \varepsilon > 0 \) there exists a \( \delta > 0 \) such that \( d_T(f(s), f(s_0)) < \varepsilon \) whenever \( d_S(s, s_0) < \delta \) for every \( f \in S \).

**Proposition 6** If \( S \) is a metric space, then \( S \) is compact if and only if \( S \) is complete and totally bounded.

Let \( \mathcal{C}((S, d_S), (T, d_T)) \) consisting of all continuous bounded mappings of \( S \) into \( (T, d_T) \), endowed with the supremum metric \( d_\infty(f, g) = \sup_{x \in S} d_T(f(x), g(x)) \). Proving the totally boundedness of some topological spaces may need more technical tricks. Fortunately, in our case we use Arzelà–Ascoli Theorem that gives compactness criteria for subspaces of \( \mathcal{C}((S, d_S), (T, d_T)) \) in terms of pointwise totally bounded and equicontinuous, namely they are a necessary and sufficient condition to guarantee that the totally boundedness of a subset \( S \) in \( \mathcal{C}(S, T), d_\infty \).

**Theorem 1** (Arzelà–Ascoli Theorem) If \( S \) is compact, then a subset of the metric space \( \mathcal{C}((S, d_S), (T, d_T)) \) is totally bounded if and only if it is pointwise totally bounded and equicontinuous.

The proof is divided on 5 Steps:

- **Step 1.** \( \mathcal{F}_d(X), \Gamma_X \) is a metric space. It is clear that for all \( \phi, \phi' \in \mathcal{F}_d(X), \Gamma_X(\phi, \phi') \geq 0 \) (nongenativeness) and \( \Gamma_X(\phi, \phi') = 0 \) if and only if \( \phi = \phi' \). To verify the triangle inequality, we proceed as follows. Take and arbitrary \( x, x' \in X \) and note that, if \( \phi, \phi' \), and \( \phi'' \) are embeddings in \( \mathcal{F}_d(X) \) then by triangle inequality in the Euclidean space \( \mathbb{R}^d \):

\[
\|\phi(x) - \phi'(x)\| \leq \|\phi(x) - \phi''(x)\| + \|\phi''(x) - \phi'(x)\| \leq \Gamma_X(\phi, \phi'') + \Gamma_X(\phi'', \phi'),
\]

hence \( \Gamma_X(\phi, \phi') \leq \Gamma_X(\phi, \phi'') + \Gamma_X(\phi'', \phi'), \) and therefore \( \mathcal{F}_d(X), \Gamma_X \) is a metric space.

- **Step 2.** \( \mathcal{F}_d(X) \subset \mathcal{C}(X, \mathbb{R}^d) \). First recall that for each \( \phi \in \mathcal{F}_d(X) \) is a \( \tau_\phi \)-embedding then it is Lipshitzian mapping. It is readily verified that every Lipshitzian mapping is uniformly continuous, that is for each real number \( \varepsilon > 0 \) there exists a real number \( \delta > 0 \) such that \( d(x, x') < \delta \) implies \( \|\phi(x) - \phi(x')\| < \varepsilon \) for all \( x, x' \in X \). So it is sufficient to take \( \delta = \frac{\varepsilon}{\tau_\phi} \).

- **Step 3.** \( \mathcal{F}_d(X), \Gamma_X \) is complete. The proof of this step is classic in the topology literature of the continuous space endowed with the supremum metric. For the sake of completeness, we adapt it in our case. Let \( \{\phi_k\}_{k \leq 1} \) be a Cauchy sequence in \( \mathcal{F}_d(X), \Gamma_X \). Thus \( \{\phi_k(x)\}_{k \leq 1} \) is a Cauchy sequence in \( (\mathbb{R}^d, \| \cdot \|) \) for every \( x \in X \). This can be as follows: \( \|\phi_k(x) - \phi_k(x')\| \leq \sup_{x \in X} \|\phi_k(x) - \phi_k(x')\| = \Gamma_X(\phi, \phi') \) for each pair of integers \( k, k' \) and every \( x, x' \in X \), and hence \( \{\phi_k(x)\}_{k \leq 1} \) converges in \( \mathbb{R}^d \) for every \( x \in X \) (since \( \mathbb{R}^d \) is complete). Let \( \phi(x) = \lim_{k \to \infty} \phi_k(x) \) for each \( x \in X \) (i.e.,
\( \phi_k(x) \to \phi(x) \) in \( \mathbb{R}^d \), which defines a mapping of \( \phi \) of \( X \) into \( \mathbb{R}^d \). We shall show that \( \phi \in \mathcal{F}_d(X) \) and that \( \{ \phi_k \} \) converges to \( \phi \) in \( \mathcal{F}_d(X) \), thus proving that \( \mathcal{F}_d(X) \) is complete. Note that for any integer \( n \) and every pair of points \( x, x' \in \mathcal{F}_d(X) \), we have \( \| \phi(x) - \phi(x') \| \leq \| \phi(x) - \phi_k(x) \| + \| \phi_k(x) - \phi_k(x') \| + \| \phi_k(x') - \phi(x') \| \) by the triangle inequality. Now take an arbitrary real number \( \varepsilon > 0 \). Since \( \{ \phi_k(x) \}_k \) is a Cauchy sequence in \( \mathcal{F}_d(X) \), it follows that there exists a positive integer \( k_0 \in \mathbb{N} \) such that \( \Gamma(\phi_k, \phi_{k_0}) < \varepsilon \), and hence \( \| \phi_k(x) - \phi_{k_0}(x) \| < \varepsilon \) for all \( x \in \mathbb{R}^d \), whenever \( k, k' \geq k_0 \). Moreover, since \( \phi_k(x) \to \phi(x) \) in \( \mathbb{R}^d \) for every \( x \in \mathbb{R}^d \), and the Euclidean distance is a continuous function from the metric space \( \mathbb{R}^d \) to the metric space \( \mathbb{R}^d \), it also follows that \( \| \phi(x) - \phi_k(x) \| = \lim_{k \to \infty} \| \phi_k(x) - \phi(x) \| \) for each positive integer \( k \) and every \( x \in \mathbb{R}^d \). Thus \( \| \phi(x) - \phi_k(x) \| \leq \varepsilon \) for all \( x \in \mathbb{R}^d \) whenever \( k \geq k_0 \). Furthermore, since each \( \phi_k \) lies in \( \mathcal{F}_d(X) \), it follows that there exists a real number \( \gamma(k_0) \) such that \( \sup_{x \in \mathbb{R}^d} \| \phi(x) - \phi(x') \| \leq 2 \varepsilon + \gamma(k_0) \) for all \( x, x' \in \mathbb{R}^d \) so that \( \phi \in \mathcal{F}_d(X) \).\( \Gamma_X \phi, \phi' \subseteq \mathbb{R}^d \) and every pair of points \( x, x' \in \mathbb{R}^d \) satisfies \( \| \phi(x) - \phi(x') \| \leq 2 \varepsilon + \gamma(k_0) \) for all \( x \in \mathbb{R}^d \) whenever \( k \geq k_0 \), so that \( \phi_k \) converges to \( \phi \) in \( \mathcal{F}_d(X) \).

- **Step 4.** \( \mathcal{F}_d(X) \) is pointwise totally bounded and equicontinuous. From (iii) in Definition 5 and the details in **Step 3**, \( \mathcal{F}_d(X) \) is readily equicontinuous. Next we shall prove that the subset \( \{ \hat{x} \} = \{ \phi(x) \in \mathbb{R}^d : \phi \in \mathcal{F}_d(X) \} \) is totally bounded in \( \mathbb{R}^d \). To proceed we use another result characterizing totally boundedness that reads as:

\[
(S, d_S) \text{ is totally bounded metric space if and only if every sequence in } S \text{ has a Cauchy subsequence.}
\]

Since for any \( \phi \in \mathcal{F}_d(X) \) is Lipschitzian then it is uniformly continuous as explained above. Furthermore uniformly continuous functions have some very nice conserving properties. They map totally bounded sets onto totally bounded sets and Cauchy sequences onto Cauchy sequences.

Now suppose that Suppose \( \{ y_l \}_{l \geq 1} \) is any sequence in \( \{ \hat{x} \} \subset \phi(X) \). For each \( l \in \mathbb{N} \), the subset \( X \cap \phi^{-1}(\{ y_l \}) \subset X \) is non empty for each \( l \in \mathbb{N} \) (Axiom of Countable Choice see [O’Searcoid, 2006]). Then \( \phi(x_l) = y_l \) for each \( l \in \mathbb{N} \). By the Cauchy criterion for complete boundedness of \( X \), the sequence \( \{ x_l \} \) has a Cauchy subsequence \( \{ x_{l_i} \} \). Then, by what we have just proved, \( \phi(x_{l_i}) \to \gamma \) as \( i \to \infty \) is a Cauchy subsequence of \( \{ y_l \} \). Since \( \{ y_l \} \) is an arbitrary sequence in \( \{ \hat{x} \} \), \( \{ \hat{x} \} \) satisfies the Cauchy criterion for total boundedness and so is totally bounded.

- **Step 5.** \( \mathcal{F}_d(X) \) is compact. Using Arzela-Ascoli Thereom and **Step 2** we conclude that \( \mathcal{F}_d(X) \) is totally bounded. Together with **Step 3** \( \mathcal{F}_d(X) \) is compact.

### A.2. Proof of Lemma 1

Notice that for \( \mu \in \mathcal{P}(X), \nu \in \mathcal{P}(Y) \), and \( (\phi, \psi) \in \mathcal{F}_d(X) \times \mathcal{F}_d(Y) \), one has \( W_2^2 \left( \frac{1}{\sqrt{2}} \phi \# \mu, \frac{1}{\sqrt{2}} \psi \# \nu \right) < \infty \). It can be seen easily using the fact that \( \int_X \| x \|^2 d(\frac{1}{\sqrt{2}} \phi \# \mu) = \frac{1}{2} \int_X \| \phi(x) \|^2 d\mu(x) \leq \frac{1}{2} M_2(\mu) \), where \( M_2(\mu) = \int_X \| x \|^2 d\mu(x) < \infty \). Now, thanks to Lemmas 4 and 5, we have

\[
\begin{align*}
\mathcal{E}^2_d(\mu, \nu) &= \sup_{\phi \in \mathcal{F}_d(X), \psi \in \mathcal{F}_d(Y)} \inf_{\gamma \in \Pi(\phi, \psi \# \mu)} \int_{X \times X} \| u - v \|^2 d\gamma(u, v) \\
&= \sup_{\phi \in \mathcal{F}_d(X), \psi \in \mathcal{F}_d(Y)} \inf_{\gamma \in \Pi(\mu, \nu)} \int_{X \times X} \| u - v \|^2 d\left( \frac{1}{\sqrt{2}} \phi \otimes \frac{1}{\sqrt{2}} \psi \right) \# \gamma(u, v) \\
&= \sup_{\phi \in \mathcal{F}_d(X), \psi \in \mathcal{F}_d(Y)} \inf_{\gamma \in \Pi(\mu, \nu)} \frac{1}{2} \int_{X \times Y} \| \phi(x) - \psi(y) \|^2 d\gamma(x, y) \\
&= \sup_{\phi \in \mathcal{F}_d(X), \psi \in \mathcal{F}_d(Y)} \frac{1}{2} \inf_{\gamma \in \Pi(\mu, \nu)} J_{\phi, \psi}(\mu, \nu).
\end{align*}
\]

### A.3. Proof of Lemma 2

In one hand, for any fixed \( \pi \in \Pi(\mu, \nu) \) the application \( h_{\pi} : (\phi, \psi) \to \int_{X \times Y} \| \phi(x) - \psi(y) \|^2 d\pi(x, y) \) is continuous. To show that, we use the continuity under integral sign Theorem. Indeed,

- for \( \pi \)-almost \( (x, y) \), the mapping \( (\phi, \psi) \to \| \phi(x) - \psi(y) \|^2 \) is continuous. To show that fix \( \varepsilon > 0 \), and \( \phi, \psi, \phi_0, \psi_0 \in \mathcal{F}_d(X) \times \mathcal{F}_d(Y) \). We endow the product sace \( \mathcal{F}_d(X) \times \mathcal{F}_d(Y) \) by the metric \( \Gamma_{X \times Y} \) defined as
follows: $\Gamma_{X,Y}((\phi, \psi), (\phi', \psi')) = \Gamma_X(\phi, \phi') + \Gamma_Y(\psi, \psi')$. We have

$$
\|\phi(x) - \psi(y)\|^2 - \|\phi_0(x) - \psi_0(y)\|^2 \leq \|\phi(x) - \phi_0(x)\| + \|\psi(y) - \psi_0(y)\|^2
\leq 2\|\phi(x) - \phi_0(x)\|^2 + \|\psi(y) - \psi_0(y)\|^2
\leq 2\Gamma_X^2(\phi, \phi_0) + \Gamma_Y^2(\psi, \psi_0)
\leq 2\Gamma_{X,Y}^2((\phi, \psi), (\phi_0, \psi_0)).
$$

Letting $\delta_\varepsilon = \sqrt{\varepsilon/2}$, then if $\Gamma_{X,Y}((\phi, \psi), (\phi_0, \psi_0)) < \delta_\varepsilon$, one has $\|\phi(x) - \psi(y)\|^2 - \|\phi_0(x) - \psi_0(y)\|^2 < \varepsilon$. This yields that $\lim_{(\phi, \psi) \to (\phi_0, \psi_0)} \|\phi(x) - \psi(y)\|^2 = \|\phi_0(x) - \psi_0(y)\|^2$.

- for a fixed $(\phi, \psi)$ and $(x, y)$, we have $\|\phi(x) - \psi(y)\|^2 \leq \|\phi(x)\|^2 + \|\psi(y)\|^2 \leq g(x, y) := \tau_\phi^2\|x\|^2 + \tau_\psi^2\|y\|^2$ with $\int_{X \times Y} g(x, y) d\pi(x, y) = \tau_\phi^2 \int_X \|x\|^2 d\mu(x) + \tau_\psi^2 \int_Y \|y\|^2 d\nu(x) < \infty$.

Therefore, the family $(h_\pi)_{\pi \in \Pi(\mu, \nu)}$ is continuous then it is upper semicontinuous. We know that the pointwise infimum of a family of upper semicontinuous functions is upper semicontinuous (see Lemma 2.41 in (Aliprantis & Border, 2006)). This entails $\inf_{\pi \in \Pi(\mu, \nu)} h_\pi$ is upper semicontinuous. Since the product of two compact sets is a compact set (Tychonoff Theorem), then $F_d(X) \times F_d(Y)$ is compact, hence $\sup_{\phi \in F_d(X), \psi \in F_d(Y)} \inf_{\pi \in \Pi(\mu, \nu)} h_\pi(\phi, \psi)$ attains a maximum value (see Theorem 2.44 in (Aliprantis & Border, 2006)).

**A.4. Proof of Lemma 3**

As we proved in Lemma 2 that for any fixed $\pi \in \Pi(\mu, \nu)$, $h_\pi(\phi, \psi) = \int_{X \times Y} ||\phi(x) - \psi(y)||^2 d\pi(x, y)$ is continuous, then it is lower semicontinuous. The pointwise supremum of a family of lower semicontinuous functions is lower semicontinuous (Lemma 2.41 in (Aliprantis & Border, 2006)), and hence $\pi \mapsto \sup_{\phi \in F_d(X), \psi \in F_d(Y)} \int_{X \times Y} ||\phi(x) - \psi(y)||^2 d\pi(x, y)$ is lower semicontinuous. Furthermore $\Pi(\mu, \nu)$ is compact set with respect to the topology of narrow convergence (Villani, 2003), then $\inf_{\pi \in \Pi(\mu, \nu)} \sup_{\phi \in F_d(X), \psi \in F_d(Y)} \int_{X \times Y} ||\phi(x) - \psi(y)||^2 d\pi(x, y)$ exists (see Theorem 2.44 in (Aliprantis & Border, 2006)).

**A.5. Proof of Proposition 2**

- \"\rightarrow\" Suppose that $S_d(\mu, \nu) = 0$ then $E_d(\mu, \nu) = 0$, that gives the Wasserstein distance $W_2(\frac{\sqrt{\mu}}{\sqrt{\nu}}, \frac{\sqrt{\nu}}{\sqrt{\mu}}) = 0$ and hence $\phi_# \mu = \psi_# \nu$ for any $\phi, \psi \in F_d(X) \times F_d(Y)$. Then for any $C \subseteq \mathbb{R}^d$ Borel, we have $\mu(\phi^{-1}(C)) = \nu(\psi^{-1}(C))$. Recall that $X \subseteq \mathbb{R}^D$ and $Y \subseteq \mathbb{R}^{D'}$, then through the proof lines we regard to $\mu$ and $\nu$ as probability measures on $\mathbb{R}^D$ and $\mathbb{R}^{D'}$, allowing us to use a the following key result of (Cramér & Wold, 1936).

**Theorem 2** (Cramér & Wold, 1936) Let $\gamma, \beta$ be Borel probability measures on $\mathbb{R}^D$ and agree at every open half-space of $X$. Then $\gamma = \beta$. In other words if for $\omega \in S^D = \{x \in \mathbb{R}^D : \|x\| = 1\}$ and $\alpha \in \mathbb{R}$ we write $H_{\omega, \alpha} = \{x \in \mathbb{R}^D : \langle \omega, x \rangle < \alpha\}$ and if $\gamma(H_{\omega, \alpha}) = \beta(H_{\omega, \alpha})$, for all $\omega \in S^D$ and $\alpha \in \mathbb{R}$ then one has $\gamma = \beta$.

The fundamental Cramér-Wold theorem states that a Borel probability measure $\mu$ on $\mathbb{R}^D$ is uniquely determined by the values it gives to halfspaces $H_{\omega, \alpha} = \{x \in \mathbb{R}^D : \langle \omega, x \rangle < \alpha\}$ for $\omega \in S^D$ and $\alpha \in \mathbb{R}$. Equivalently, $\gamma$ is uniquely determined by its one-dimensional projections $(\Delta_\omega)_{\#} \mu$, where $\Delta_\omega$ is the projection $x \in \mathbb{R}^D \mapsto \langle x, \omega \rangle \in \mathbb{R}$ for $\omega \in S^D$. 


Straightforwardly, we have
\[
\phi^{-1}_w(\psi_\#(H_{\omega,\alpha})) = \psi_\#(\phi^{-1}((H_{\alpha,\omega}))) = \psi_\#(\nu(u \in X : \phi^{-1}(u) \in H_{\omega,\alpha})) = \psi_\#(\nu(u \in X : \{w, \phi^{-1}(u) < \alpha\})) = \phi_\#(\mu(u \in X : \{w, \phi^{-1}(u) < \alpha\})(by hypothesis)) = \mu(\phi^{-1}((u \in X : \{w, \phi^{-1}(u) < \alpha\}))) = \mu(\{x \in X : \phi(x) \in \{x \in X : \{w, \phi^{-1}(u) < \alpha\}\}) = \mu(\{x \in X : \{w, \phi^{-1}(\phi(x)) < \alpha\}) = \mu(\{x \in X : \{w, \phi^{-1}(\phi(x)) < \alpha\}))(since \phi is one-to-one) = \mu(H_{\omega,\alpha}).
\]

Analogously, we prove that \(\psi^{-1}_w(\phi_\#(\mu(H_{\omega,\alpha}))) = \nu(H_{\omega,\alpha}). \) Therefore, for all \(A \subseteq X \) and \(B \subseteq Y \) Borels, we have \(\mu(A) = \phi^{-1}_w(\psi_\#(\nu)(A)) \) and \(\nu(B) = \psi^{-1}_w(\phi_\#(\mu))(B).\)

- \(\ast \Leftrightarrow \) Thanks to Lemma 3 in the core of the paper, there exists a couple \((\phi^*, \psi^*)\)-embeddings optimum for \(S^2_2(\mu, \nu)\). We assume now that \(\nu = (\psi^{-1}_w \circ \phi^*)_\# \mu\), then
\[
S^2_2(\mu, \nu) = \frac{1}{2} \inf_{\pi \in \Pi(\mu, \phi^*_w(\# \mu))} \int_{X \times Y} \|\phi^*(x) - \psi^*(y)\|^2 d\pi(x, y)
= \frac{1}{2} \inf_{\pi \in \Pi(\mu, \phi^*_w(\# \mu))} \int_{X \times Y} \|\phi^*(x) - \psi^*(y)\|^2 d(I \otimes (\psi^*)^{-1})_\# \pi(x, y)
= \frac{1}{2} \inf_{\pi \in \Pi(\mu, \phi^*_w(\# \mu))} \int_{X \times Y} \|\phi^*(x) - \psi^*(y)\|^2 d(I \otimes \phi^*)_\# ((I \otimes (\psi^*)^{-1})_\# \pi(x, y)).
\]

On the other hand, it is clear that \((I \otimes \phi^*)_\# ((I \otimes (\psi^*)^{-1})_\# \pi)(\cdot) = \mu(\phi^* \circ (\psi^*)^{-1})(\pi(\cdot). Using the fact that \(\phi^*\) is \(\tau_{\phi^*}\)-embedding then we get
\[
S^2_2(\mu, \nu) = \frac{1}{2} \inf_{\pi \in \Pi(\mu, \phi^*_w(\# \mu))} \int_{X \times Y} \|\phi^*(x) - \psi^*(y)\|^2 d(\phi^* \circ (\psi^*)^{-1})_\# \pi(x, y))
= \frac{1}{2} \inf_{\pi \in \Pi(\mu, \phi^*_w(\# \mu))} \int_{X \times Y} \|\phi^*(x) - \phi^*(x')\|^2 d\pi(x, x')
\leq \frac{\tau_{\phi^*}^2}{2} \inf_{\pi \in \Pi(\mu, \phi^*_w(\# \mu))} \int_{X \times X} d^2_{\phi^*}(x, x') d\pi(x, x')
\leq \frac{\tau_{\phi^*}^2}{2} W^2_2(\mu, \mu)
= 0.
\]

A.6. Proof of Proposition 3

Symmetry is clear for both objects. In order to prove the triangle inequality, we use a classic lemma known as “gluing lemma” that allows to produce a sort of composition of two transport plans, as if they are maps.

**Lemma 6** (Villani, 2003) *Let \(X, Y, Z\) be three Polish spaces and let \(\gamma^1 \in \mathcal{P}(X \times Y), \gamma^2 \in \mathcal{P}(Y \times Z), \) be such that \(\Delta^Y_\# \gamma^1 = \Delta^Y_\# \gamma^2\) where \(\Delta^Y_\#\) is the natural projection from \(X \times Y\) (or \(Y \times Z\)) onto \(Y.\) Then there exists a measure \(\gamma \in \mathcal{P}(X \times Y \times Z)\) such that \(\Delta^X_\# \gamma = \gamma^1\) and \(\Delta^Y_\# \gamma = \gamma^2.\)"

Let \(\eta \in \mathcal{P}_2(Z)\) and \(\pi^1 \in \Pi(\mu, \nu)\) and \(\pi^2 \in \Pi(\nu, \eta).\) By the gluing lemma we know that there exists \(\gamma \in \mathcal{P}_2(X \times Y \times Z)\) such that \(\Delta^X_\# \gamma = \pi^1\) and \(\Delta^Y_\# \gamma = \pi^2.\) Since \(\Delta^X_\# \gamma = \mu\) and \(\Delta^Y_\# \gamma = \eta,\) we have \(\pi = \Delta^Z_\# \gamma \in \Pi(\mu, \eta).\) On the
other hand
\[
\int_{X \times Z} \|\phi(x) - \zeta(z)\|^2 d\pi(x, z) = \int_{X \times Y \times Z} \|\phi(x) - \zeta(z)\|^2 d\gamma(x, y, z)
\]
\[
\leq 2 \int_{X \times Y \times Z} (\|\phi(x) - \psi(y)\|^2 + \|\psi(y) - \zeta(z)\|^2) d\gamma(x, y, z)
\]
\[
= 2 \int_{X \times Y} \|\phi(x) - \psi(y)\|^2 d\pi_1(x, y) + 2 \int_{X \times Z} \|\psi(y) - \zeta(z)\|^2 d\pi_2(y, z).
\]
Hence, we end up with the desired result, \( S^2_d(\mu, \eta) \leq S^2_d(\mu, \nu) + S^2_d(\nu, \eta). \)

**A.7. Proof of Proposition 4**

As the embedding \( \phi \) is Lipschitzian then it is continuous. Since \( X \) is compact hence \( \phi(X) \) is also compact. Consequently \( \text{supp}[\phi_{\#}\mu] \subset \phi(X) \) is compact (closed subset of a compact). The same observation is fulfilled by \( \text{supp}[\psi_{\#}\nu] \subset \psi(Y) \). Letting \( Z = \{\text{supp}[\phi_{\#}\mu] \cup \text{supp}[\psi_{\#}\nu]\} \subset \mathbb{R}^d \). Hence, \((Z, \| \cdot \|)\) is compact metric space and \( \phi_{\#}\mu \) and \( \psi_{\#}\nu \) are Borel probability measures on \( Z \). Thanks to Theorem 5 (property (c)) in (Mémoli, 2011), we have that

\[
W_2^2\left(\frac{1}{\sqrt{2}} \phi_{\#}\mu, \frac{1}{\sqrt{2}} \psi_{\#}\nu\right) \geq GW_2^2\left(\frac{1}{\sqrt{2}} \phi_{\#}\mu, \frac{1}{\sqrt{2}} \psi_{\#}\nu\right), \text{ for any } \phi \in F_d(X), \psi \in F_d(Y).
\]

So
\[
S^2_d(\mu, \nu) \geq \sup_{\phi \in F_d(X), \psi \in F_d(Y)} GW_2^2\left(\frac{1}{\sqrt{2}} \phi_{\#}\mu, \frac{1}{\sqrt{2}} \psi_{\#}\nu\right).
\]

Together with the minimax inequality we arrive at

\[
S^2_d(\mu, \nu) \geq \sup_{\phi \in F_d(X), \psi \in F_d(Y)} \frac{1}{2} GW_2^2\left(\frac{1}{\sqrt{2}} \phi_{\#}\mu, \frac{1}{\sqrt{2}} \psi_{\#}\nu\right)
\]
\[
\geq \sup_{\phi \in F_d(X), \psi \in F_d(Y)} \frac{1}{4} \inf_{\pi \in \Pi(\mu, \nu)} \int_{Z \times Z} (\|u - u'\|_2 - \|v - v'\|_2)^2 d\gamma(u, v)d\gamma(u', v')
\]
\[
\geq \sup_{\phi \in F_d(X), \psi \in F_d(Y)} \frac{1}{4} \inf_{\pi \in \Pi(\mu, \nu)} \int_{X \times Y} (\|\phi(x) - \phi(x')\|_2 - \|\psi(y) - \psi(y')\|_2)^2 d\pi(x, y)d\pi(x', y')
\]
\[
\geq \sup_{\phi \in F_d(X), \psi \in F_d(Y)} \frac{1}{4} \inf_{\pi \in \Pi(\mu, \nu)} \int_{X \times Y} (d^2_X(x, x') + d^2_Y(y, y') - 2\tau_{\phi, \psi} d_X(x, x')d_Y(y, y'))d\pi(x, y)d\pi(x', y')
\]
\[
\geq \frac{1}{2} GW_2^2(\mu, \nu) + \frac{1}{2} \sup_{\phi \in F_d(X), \psi \in F_d(Y)} \left(1 - \tau_{\phi, \psi}\right) \inf_{\pi \in \Pi(\mu, \nu)} \int_{X \times Y} d_X(x, x')d_Y(y, y')d\pi(x, y)d\pi(x', y').
\]

Using the fact that \( -\sup -x = \inf x \), we get
\[
GW_2^2(\mu, \nu) \leq 2S^2_d(\mu, \nu) + \inf_{\phi \in F_d(X), \psi \in F_d(Y)} (\tau_{\phi, \psi} - 1)I(\mu, \nu),
\]
where \( I_1(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \int_{X \times Y} d_X(x, x')d_Y(y, y')d\pi(x, y)d\pi(x', y') \). Using Bourgain’s embedding theorem (Bourgain, 1985), \( \tau_{\phi} \in [1, O(\log n)] \) and \( \tau_{\psi} \in [1, O(\log m)] \), then
\[
GW_2^2(\mu, \nu) \leq 2S^2_d(\mu, \nu) + \inf_{\tau_{\phi} \in D_{emb}(X), \tau_{\psi} \in D_{emb}(Y)} (\tau_{\phi, \psi} - 1)I_1(\mu, \nu).
\]
In another hand, we have

\[ \mathcal{I}_1(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \int_{X \times Y} d_X(x, x')d_Y(y, y')d\pi(x, y)d\pi(x', y') \]

\[ \leq \int_{X \times Y} d_X(x, x')d\mu(x)d\nu(y)d\mu(x')d\nu(y') \]

\[ \leq \int_{X \times X} d_X(x, x')d\mu(x)\int_{Y \times Y} d_Y(y, y')d\nu(y)d\nu(y') \]

\[ \leq 4 \left( \int_X d_X(x, 0)d\mu(x) + \int_Y d_Y(y, 0)d\nu(y) \right) \]

\[ \leq 4 \left( \int_X \|x\|_Xd\mu(x) + \int_Y |y|d\nu(y) \right) \]

\[ \leq 4(M_1(\mu) + M_1(\nu)), \]

\[ M_1(\mu) = \int_X \|x\|_Xd\mu(x) < \infty. \]

Hence,

\[ \frac{1}{2} \mathcal{GW}_2^2(\mu, \nu) \leq S_2^2(\mu, \nu) + 2 \inf_{\tau_0 \in D_{\text{amb}}(X), \tau_\psi \in D_{\text{amb}}(Y)} (\tau_0 \tau_\psi - 1)(M_1(\mu) + M_1(\nu)). \]

**A.8. Proof of Proposition 5**

The proof of this proposition is based on a lower bound for the Gromov-Wasserstein distance (Proposition 6.1 in (Mémoli, 2011)):

\[ \mathcal{GW}_2^2(\mu, \nu) \geq \text{FLB}_2^2(\mu, \nu) := \frac{1}{2} \inf_{\pi \in \Pi(\mu, \nu)} \int_{X \times Y} |s_{X,2}(x) - s_{Y,2}(y)|^2d\pi(x, y), \]

where \( s_{X,2} : X \to \mathbb{R}_+, s_{X,2}(x') = \left( \int_X d_X^2(x, x')d\mu(x') \right)^{1/2} \) defines an eccentricity function. Note that FLB_2^2 leads to a mass transportation problem for the cost \( c(x, y) := |s_{X,2}(x) - s_{Y,2}(y)|^2 \).

Now, for any \( x, y \in X \times Y \), and \( \phi, \psi \in \mathcal{F}_d(X) \times \mathcal{F}_d(Y) \) we have (by triangle inequality)

\[ \|\phi(x) - \psi(y)\|_2^2 \]

\[ = \int_{X \times Y} \|\phi(x) - \psi(y)\|_2^2d\mu(x')d\nu(y') \]

\[ \leq 4 \int_X \|\phi(x) - \phi(x')\|_2^2d\mu(x') + 4 \int_Y \|\psi(y) - \psi(y')\|_2^2d\nu(y') + 2 \int_{X \times Y} \|\phi(x') - \psi(y')\|_2^2d\mu(x')d\nu(y') \]

\[ \leq 4\tau_\phi^2 + 4\tau_\psi^2 \left( \int_X d_X^2(x, x')d\mu(x') + \int_Y d_Y^2(y, y')d\nu(y') \right) \]

\[ + 8\tau_\phi^2 + 8\tau_\psi^2 \int_X d_X^2(x, x')d\mu(x') \]

\[ \leq 4(\tau_\phi^2 + \tau_\psi^2)|s_{X,2}(x) - s_{Y,2}(y)|^2 + 8(\tau_\phi^2 + \tau_\psi^2)\sqrt{\mathcal{I}_{2,x,y}(\mu, \nu)} \]

\[ + 2 \int_{X \times Y} \|\phi(x') - \psi(y')\|_2^2d\mu(x')d\nu(y'), \]

where

\[ \mathcal{I}_{2,x,y}(\mu, \nu) := \left( \int_X d_X^2(x, x')d\mu(x') \right) \left( \int_Y d_Y^2(y, y')d\nu(y') \right). \]

We observe that

\[ \mathcal{I}_{2,x,y}(\mu, \nu) \leq 4(M_2(\mu) + d_X^2(x, 0))(M_2(\nu) + d_Y^2(y, 0)). \]
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Moreover,

\[ \int_{X \times Y} \| \phi(x') - \psi(y') \|^2 d\mu(x')d\nu(y') \leq 2(\tau_{\phi}^2 + \tau_{\psi}^2)(M_2(\mu) + M_2(\nu)). \]

Therefore, for any \( \pi \in \Pi(\mu, \nu) \)

\[ \int_{X \times Y} \| \phi(x) - \psi(y) \|^2 d\pi(x, y) \leq 2(\tau_{\phi}^2 + \tau_{\psi}^2) \int_{X, Y} |s_{X, 2}(x) - s_{Y, 2}(y)|^2 d\pi(x, y) + 8(\tau_{\phi}^2 + \tau_{\psi}^2) \int_{X \times Y} \sqrt{4(M_2(\mu) + d_X^2(x, 0))(M_2(\nu) + d_Y^2(y, 0))d\pi(x, y)} 
+ 2(\tau_{\phi}^2 + \tau_{\psi}^2)(M_2(\mu) + M_2(\nu)) \leq 4(\tau_{\phi}^2 + \tau_{\psi}^2) \int_{X \times Y} |s_{X, 2}(x) - s_{Y, 2}(y)|^2 d\pi(x, y) + 16(\tau_{\phi}^2 + \tau_{\psi}^2) \int_X \sqrt{M_2(\mu) + d_X^2(x, 0)}d\mu(x) \int_Y \sqrt{M_2(\nu) + d_Y^2(y, 0)}d\nu(y) 
+ 2(\tau_{\phi}^2 + \tau_{\psi}^2)(M_2(\mu) + M_2(\nu)). \]

Note that

\[ \int_X \sqrt{M_2(\mu) + d_X^2(x, 0)}d\mu(x) \leq \sqrt{M_2(\mu)} + \int_X d_X(x, 0)d\mu(x) \leq \sqrt{M_2(\mu)} + \sqrt{M_1(\mu)}, \]

and

\[ \int_Y \sqrt{M_2(\nu) + d_Y^2(y, 0)}d\nu(y) \leq \sqrt{M_2(\nu)} + \int_Y d_Y(y, 0)d\nu(y) \leq \sqrt{M_2(\nu)} + \sqrt{M_1(\nu)}. \]

So

\[ \int_{X \times Y} \| \phi(x) - \psi(y) \|^2 d\pi(x, y) \leq 4(\tau_{\phi}^2 + \tau_{\psi}^2) \int_{X, Y} |s_{X, 2}(x) - s_{Y, 2}(y)|^2 d\pi(x, y) + 16(\tau_{\phi}^2 + \tau_{\psi}^2)(\sqrt{M_2(\mu)} + \sqrt{M_1(\mu)})(\sqrt{M_2(\nu)} + \sqrt{M_1(\nu)}) 
+ 2(\tau_{\phi}^2 + \tau_{\psi}^2)(M_2(\mu) + M_2(\nu)). \]

Finally,

\[ \mathcal{S}_d^2(\mu, \nu) \leq 2 \sup_{\tau_{\phi} \in \mathcal{D}_{\text{emb}}(X), \tau_{\psi} \in \mathcal{D}_{\text{emb}}(Y)} (\tau_{\phi}^2 + \tau_{\psi}^2)(GW_d^2(\mu, \nu) + \overline{M}_{\mu, \nu}), \]

where

\[ \overline{M}_{\mu, \nu} = 8(\sqrt{M_2(\mu)} + \sqrt{M_1(\mu)})(\sqrt{M_2(\nu)} + \sqrt{M_1(\nu)}) + (M_2(\mu) + M_2(\nu)). \]

This finishes the proof.