Cycle Consistent Probability Divergences
Across Different Spaces

Zhengxin Zhang\textsuperscript{a}, Youssef Mroueh\textsuperscript{b}, Ziv Goldfeld\textsuperscript{a}, and Bharath K. Sriperumbudur\textsuperscript{c}

\textsuperscript{a}Cornell University, \textsuperscript{b}IBM Research AI, \textsuperscript{c}Pennsylvania State University

November 23, 2021

Abstract

Discrepancy measures between probability distributions are at the core of statistical inference and machine learning. In many applications, distributions of interest are supported on different spaces, and yet a meaningful correspondence between data points is desired. Motivated to explicitly encode consistent bidirectional maps into the discrepancy measure, this work proposes a novel unbalanced Monge optimal transport formulation for matching, up to isometries, distributions on different spaces. Our formulation arises as a principled relaxation of the Gromov-Haussdorff distance between metric spaces, and employs two cycle-consistent maps that push forward each distribution onto the other. We study structural properties of the proposed discrepancy and, in particular, show that it captures the popular cycle-consistent generative adversarial network (GAN) framework as a special case, thereby providing the theory to explain it. Motivated by computational efficiency, we then kernelize the discrepancy and restrict the mappings to parametric function classes. The resulting kernelized version is coined the \textit{generalized maximum mean discrepancy} (GMMD). Convergence rates for empirical estimation of GMMD are studied and experiments to support our theory are provided.

1 Introduction

Discrepancy measures between probability distributions are ubiquitous in machine learning. In practice, distributions of interests are often supported on different spaces and the goal is not only to quantify discrepancy, but also to obtain a meaningful and consistent correspondence between data points. Such problems arise, e.g., in natural language processing for unsupervised matching across different languages or ontologies (Alvarez-Melis and Jaakkola, 2018; Grave et al., 2019; Alvarez-Melis et al., 2020), shape matching (Bronstein et al., 2006a; Mémoli, 2011; Xu et al., 2019), heterogenous domain adaptation (Yan et al., 2018), generative modeling (Bunne et al., 2019), and many more.

Among the most popular discrepancies between distributions on incompatible spaces is the Gromov-Wasserstein distance (GW) (Mémoli, 2011) (see Séjourné et al. (2020) for an unbalanced variant). Computationally, the GW distance amounts to a quadratic assignment problem that is NP hard (Commander, 2005). To alleviate this impasse, Peyré et al. (2016) proposed an entropic regularization to the GW problem, and derived an algorithm with cubic $O(n^3)$ complexity in the number of samples. More recently, Vayer et al. (2019) proposed slicing the GW distance, which further reduces the computational complexity to $O(n \log n)$. Despite these algorithmic advances, a common issue with GW-based discrepancies is their lack of generalization to new data points.
These approaches only quantify the distance without generating a map that captures the correspondence. This requires recomputing the distance whenever one wants to account for new data points, thereby incurring an additional cost. This shortcoming motivates us to explore computationally friendly discrepancies between distributions on different spaces that explicitly encode consistent, bidirectional measure preserving mappings that capture the correspondence. This is similar in spirit to the recent interest in learning Monge optimal transport (OT) maps (Perrot et al., 2016; Makkuva et al., 2020; Paty et al., 2020; Flamary et al., 2019).

Specifically, we propose a novel unbalanced divergence between probability measures supported on different spaces that explicitly employs two cycle-consistent maps that (approximately) push each distribution onto another. Cycle-consistency here is in the context of cycle generative adversarial networks (Zhu et al., 2017; Kim et al., 2017) (GANs), which requires that the two pushforward maps are roughly inverses one of another. Note that Mémoli and Needham (2021) recently proposed a quasi-metric called the Gromov-Monge distance that employs a single pushforward map. A key advantage of our approach is its cycle consistency that provides a mathematical framework for the popular cycle GAN and enables a principled study thereof.

The main contributions of this paper are:

- We introduce and study in Section 3 the unbalanced bidirectional Gromov-Monge (UBGM) divergence, drawing connections between UBGM and the popular cycle GAN framework.
- Motivated by computational efficiency, we kernelize UBGM in Section 4 and restrict mappings to parametric function classes, such as neural networks (NNs). We call the resulting divergence the generalized maximum mean discrepancy (GMMD). We then derive convergence rates for two-sample empirical estimation of GMMD.
- We present numerical results in Section 5 that support our theory and demonstrate the computational efficiency, and generalization capability of the proposed framework for matching across different spaces.

2 Background and Preliminaries

2.1 Notations

Let \((X, d_X)\) be a compact metric space. The diameter of a set \(A \subseteq X\) is \(\text{diam}(A) := \sup_{x,x' \in A} d_X(x, x')\). We use \(B(x, r)\) to denote the open ball of radius \(r > 0\) centered at \(x \in X\). For \(\epsilon > 0\), a set \(\mathcal{X}_\epsilon\) is called an \(\epsilon\)-cover of \(X\) if for any \(x \in X\), \(\inf_{x' \in \mathcal{X}_\epsilon} d_X(x, x') < \epsilon\). The \(\epsilon\)-covering number of \(X\) is \(N(X, d_X, \epsilon) := \inf\{|\mathcal{X}_\epsilon| : \mathcal{X}_\epsilon \text{ is an } \epsilon\text{-cover of } X\}\). When \(X\) is a subset of \(\mathbb{R}^d\), we always use the metric induce by the Euclidean norm, denoted as \(\| \cdot \|\). For a metric space \((X, d_X)\), the diameter of \(X\) is defined as \(\sup_{x,x' \in X} d_X(x, x')\).

For \(1 \leq p \leq \infty\), the \(L^p\) space over \(X\) is denoted by \(L^p(X)\) with \(\| \cdot \|_p\) designating the norm. The Lipschitz constant of a function \(f : X \to \mathcal{Y}\) is \(\|f\|_{\text{Lip}} = \sup_{x,x' \in X} \frac{d_Y(f(x), f(x'))}{d_X(x, x')}\), with \(\text{Lip}_L(X, \mathcal{Y}) = \{f : \|f\|_{\text{Lip}} \leq L\}\) denoting the Lipschitz ball of radius \(L > 0\). A mapping \(f : X \to \mathcal{Y}\) between metric spaces is called an isometry if \(d_X(x, x') = d_Y(f(x), f(x'))\), for all \(x, x' \in X\), i.e., \(f\) preserves the metric structure. For a class of mappings from \(X\) to \(\mathcal{Y}\), define the sup-metric on \(\mathcal{F}\) as \(d_{\mathcal{F}}(f_1, f_2) := \sup_{x \in X} d_Y(f_1(x), f_2(x))\).

The probability space on which all random variables are defined is denoted by \((\Omega, \mathcal{A}, \mathbb{P})\) (assumed to be sufficiently rich), with \(\mathbb{E}\) designating the corresponding expectation. The class of Borel probability measures over \(X\) is denoted by \(\mathcal{P}(X)\). For \(n \in \mathbb{N}\), \(\mathcal{P}^\otimes n\) denotes the \(n\)-fold product measure of \(\mathcal{P}\). Given a measurable \(f : X \to \mathcal{Y}\) and \(P \in \mathcal{P}(X)\), the pushforward of \(P\)
through $f$ is $f_\sharp P(B) := P(f^{-1}(B))$, for any Borel set $B$. Clearly $f_\sharp P \in \mathcal{P}(\mathcal{Y})$. A sequence of probability measures $P_n \in \mathcal{P}(\mathcal{X})$ converges to a probability measure $P$, denoted as $P_n \xrightarrow{w} P$, if for any bounded continuous function $\phi(x)$ on $\mathcal{X}$, $\lim_n \int \phi(x) \, dP_n(x) = \int \phi(x) \, dP(x)$ \textbf{We also write $a \lesssim b$ when $a \leq C_x b$, where $C_x$ is a constant depending only on $x$, and write $a \lesssim b$ if the omitted constant is universal. Also denote $n \wedge m = \min\{n, m\}$.

2.2 Gromov-Hausdorff Distance

To motivate our proposed discrepancy measure, we start by recalling the Gromov-Hausdorff distance between metric spaces, which is defined as

$$d_{GH}(\mathcal{X}, \mathcal{Y}) := \inf_{Z, \phi_X, \phi_Y} d_H^Z(\phi_X(\mathcal{X}), \phi_Y(\mathcal{Y})), \quad (1)$$

where the infimum is on an ambient metric space $(Z, d_Z)$ and isometric embeddings $\phi_X : \mathcal{X} \to Z$ and $\phi_Y : \mathcal{Y} \to Z$, with $d_H^Z$ as the Hausdorff distance on $Z$.

Evidently, the formulation above is not computable. Nevertheless, $d_{GH}$ has several equivalent forms (Mémoli, 2011) that, with appropriate relaxations, can be computed efficiently. Two such forms are as follows.

**Correspondence set reformulation.** Following Mémoli and Needham (2021), a correspondence set between $\mathcal{X}$ and $\mathcal{Y}$ is a set $R \subset \mathcal{X} \times \mathcal{Y}$ whose projections to $\mathcal{X}$ and $\mathcal{Y}$ define surjections on $R$. The set of all such correspondences is denoted by $\mathcal{R}(\mathcal{X}, \mathcal{Y})$. The Gromov-Hausdorff distance can be reformulated as

$$d_{GH}(\mathcal{X}, \mathcal{Y}) = \frac{1}{2} \inf_{R \in \mathcal{R}(\mathcal{X}, \mathcal{Y})} \sup_{(x, x', y, y') \in R} \Gamma_{X, Y}(x, y, x', y'), \quad (2)$$

where $\Gamma_{X, Y}(x, y, x', y') := |d_X(x, x') - d_Y(y, y')|$ is the pointwise distortion between $(x, x') \in \mathcal{X}^2$ and $(y, y') \in \mathcal{Y}^2$. Note that (2) can be written in the following compact form as an $L^\infty$ norm:

$$d_{GH}(\mathcal{X}, \mathcal{Y}) = \frac{1}{2} \inf_{R \in \mathcal{R}(\mathcal{X}, \mathcal{Y})} \|\Gamma_{X, Y}\|_{L^\infty(R \times R)}. \quad (3)$$

**Two mappings reformulation.** Another important reformulation of the Gromov-Hausdorff distance in terms of mappings between spaces is:

$$d_{GH}(\mathcal{X}, \mathcal{Y}) = \frac{1}{2} \inf_{g: \mathcal{Y} \to \mathcal{X}, f: \mathcal{X} \to \mathcal{Y}} \max\{\Delta^X(f), \Delta^Y(g), \Delta_{X, Y}(f, g)\}, \quad (4)$$

where the distortions $\Delta^X, \Delta^Y, \Delta_{X, Y}$ are given by\(^1\)

$$\Delta^\mathcal{X}(f) := \sup_{x, x' \in \mathcal{X}} |d_X(x, x') - d_Y(f(x), f(x'))|,$$

$$\Delta^\mathcal{Y}(g) := \sup_{y, y' \in \mathcal{Y}} |d_X(g(y), g(y')) - d_Y(y, y')|,$$

$$\Delta_{X, Y}(f, g) := \sup_{x \in \mathcal{X}, y \in \mathcal{Y}} |d_X(x, g(y)) - d_Y(f(x), y)|.$$

Formulation (4) thus measures distance by searching for low distortion maps between the two metric spaces, such that the so-called cycle consistency property holds, i.e., the maps are approximate

\(^1\)The superscript $\infty$ indicates that $\Delta^\mathcal{X}, \Delta^\mathcal{Y},$ and $\Delta_{X, Y}$ can be written as $L^\infty$ norms of the appropriate pointwise distortions (e.g., $\Gamma_{X, Y}(x, f(x), x', f(x'))$ for $\Delta^X$).
inverses of one another. More specifically following Mémoli and Sapiro (2005), if \(d_{\text{GH}}(X, Y) \leq \varepsilon\) then there exists \(f : X \to Y\) and \(g : Y \to X\) such that: (1) the induced metric distortions are small, i.e., \(\Delta_{X}^{\infty}(f) \leq 2\varepsilon\) and \(\Delta_{Y}^{\infty}(g) \leq 2\varepsilon\); and (2) these functions are almost inverses one of another, in the sense that \(d_{X}(x, g(f(x))) \leq 2\varepsilon\) and \(d_{Y}(f(g(y)), y) \leq 2\varepsilon\) (which follows from \(|d_{X}(x, g(y)) - d_{Y}(f(x), y)| \leq 2\varepsilon\) by taking \(y = f(x)\) and \(x = g(y)\), respectively). Thus, \(\Delta_{X,Y}^{\infty}\) ensures cycle consistency of the maps.

3 Probability Divergences Across Metric Measure Spaces

We are now ready to present the proposed discrepancy between probability measures on different spaces. In conjunction with the preceding discussion, such a discrepancy can equivalently be viewed as a distance between metric measure (mm) spaces (Mémoli, 2011).

**Definition 1** (Metric measure spaces). A metric measure space is a triple \((X, d_{X}, P)\) where \((X, d_{X})\) is a compact metric space and \(P \in \mathcal{P}(X)\) has full support.

3.1 The Unbalanced Bidirectional Gromov-Monge Divergence

Formulation (4) of \(d_{\text{GH}}\) is computationally appealing and has lead to many algorithmic relaxations that approximate the Gromov-Hausdorff distance (Mémoli and Sapiro, 2004, 2005; Bronstein et al., 2006b). As a stepping stone towards our unbalanced formulation, we first adapt this formulation to an extended metric between two mm spaces \((X, d_{X}, P)\) and \((Y, d_{Y}, Q)\). To that end, we first relax the distortion terms and then restrict the mappings to be measure persevering, as described next.

Let \((X, X') \sim P^{\otimes 2}\) be independent of \((Y, Y') \sim Q^{\otimes 2}\). For \(1 \leq p < \infty\), set

\[
\Delta_{X}^{(p)}(f; P) := \left( \mathbb{E} \left[ |d_{X}(X, X') - d_{X}(f(X), f(X'))|^{p} \right] \right)^{1/p}
\]

\[
\Delta_{Y}^{(p)}(g; Q) := \left( \mathbb{E} \left[ |d_{Y}(g(Y), g(Y')) - d_{Y}(Y, Y')|^{p} \right] \right)^{1/p}
\]

\[
\Delta_{X,Y}^{(p)}(f, g; P, Q) := \left( \mathbb{E} \left[ |d_{X}(X, g(Y)) - d_{Y}(f(X), Y)|^{p} \right] \right)^{1/p},
\]

as the \(L^p\) relaxation of the distortion terms from (4). Restricting the mappings in (4) to be ‘Monge’ measure preserving, i.e., \(f_{1}P = Q\) and \(g_{2}Q = P\), gives rise to \(p\)th order bidirectional Gromov-Monge (BGM) distance, as defined next.

**Definition 2** (Bidirectional Gromov-Monge distance). Fix \(1 \leq p < \infty\). The \(p\)th order BGM distance between \((X, d_{X}, P)\) and \((Y, d_{Y}, Q)\) is

\[
D_{p}(P, Q) := \inf_{\substack{f : X \to Y, f_{1}P = Q \\text{and} \\text{meas-preserving} \\text{on} \ X \ni x \ni f(x) \ni y \ni \mathbb{P}\text{-a.s.}}} \Delta_{p}(f, g; P, Q),
\]

where \(\Delta_{p}(f, g; P, Q) := \Delta_{X}^{(p)}(f; P) + \Delta_{Y}^{(p)}(g; Q) + \Delta_{X,Y}^{(p)}(f, g; P, Q)\). If the set of measure preserving maps is empty, then we set \(D_{p}(P, Q) = \infty\).

This definition follows a reasoning similar to Formulation (4) of \(d_{\text{GH}}\) above: We are looking for measure preserving maps \(f, g\), that are low metric distortion (minimizing \(\Delta_{X}^{(p)}, \Delta_{Y}^{(p)}\)) and satisfy a cycle consistency propriety (minimizing \(\Delta_{X,Y}^{(p)}\), i.e., almost inverses one of another).

The BGM distance defines an extended metric between equivalence classes of mm spaces.

**Definition 3** (Equivalence classes). Two mm spaces \((X, d_{X}, P)\) and \((Y, d_{Y}, Q)\) are called equivalent if and only if (iff) there is an invertible isometry \(f : X \to Y\) such that \(f_{1}P = Q\) (and hence \(f_{2}^{-1}Q = P\)). The set of all such equivalence classes is denoted by \(\mathcal{M}\).
**Proposition 1** (BGM distance metrizes \( \mathfrak{M} \)). For any \( 1 \leq p < \infty \), \( \Delta_p \) defines an extended metric on \( \mathfrak{M} \).

**Remark 1** (Finiteness of BGM). Let \( (\mathcal{X}, d_\mathcal{X}, P) \) be a mm space, with \( \mathcal{X} \) uncountable and \( P \) atomless. If \( C_\infty \) is the subcategory of mm spaces isomorphic to \( (\mathcal{X}, d_\mathcal{X}, P) \) (Mémoli and Needham, 2021), then BGM is a finite metric on \( C_\infty \). This setting is interesting for matching isomorphic mm spaces (of same dimension), in image, shape and text matching applications.

The proof of Proposition 1 is given in Appendix A.1. Positivity, symmetry, and the triangle inequality all follow from elementary calculations. The main challenge is in showing that if \( \Delta_p \) nullifies then the considered spaces are isometrically isomorphic. To that end, we use the following lemma, that may be of independent interest (see Appendix A.2 for the proof).

**Lemma 1** (Existence of isometries). Fix \( P,Q \in \mathcal{P}(\mathcal{X}) \) and let \( \mathcal{F} \) and \( \mathcal{G} \) be arbitrary function classes such that \( \inf_{f \in \mathcal{F}, g \in \mathcal{G}} \Delta_p(f,g;P,Q) = 0 \). Then there exist minimizing sequences \( (f_n)_{n \in \mathbb{N}} \subset \mathcal{F} \) and \( (g_n)_{n \in \mathbb{N}} \subset \mathcal{G} \) that converge almost surely (a.s.) to isometries \( f \) and \( g \), respectively, such that \( f = g^{-1} \).

**Remark 2** (Convergent sequences). By definition of isometry, the limits \( f, g \) are metric preserving, thus continuous and Lipschitz 1. We don’t know if they still live in \( \mathcal{F}, \mathcal{G} \) unless we impose compactness conditions later on. Notice that the convergence stated in the lemma is guaranteed solely by the first two terms of \( \Delta_p(f,g;P,Q) \). If we drop the third term, convergent sequences still exists, but the limits are not guaranteed to be inverse of each other.

While \( \Delta_p \) is a valid extended metric on \( \mathfrak{M} \), its evaluation is computationally challenging as it is unclear how to optimize over bidirectional Monge maps. Following the unbalanced OT framework (Chizat et al., 2018; Frogner et al., 2015), we relax the measure preserving constraint using divergences\(^2 \) \( \Delta_\mathcal{F} \) and \( \Delta_\mathcal{G} \) on measures on \( \mathcal{X} \) and \( \mathcal{Y} \), respectively, and restrict the functions to pre-specified classes. This gives rise to the unbalanced Gromov-Monge formulation.

**Definition 4** (Unbalanced bidirectional Gromov-Monge divergence). Fix \( 1 \leq p < \infty \), let \( \Delta_\mathcal{F} \) and \( \Delta_\mathcal{G} \) be divergences on \( \mathcal{X} \) and \( \mathcal{Y} \), respectively. Further take \( \mathcal{F} \) as a class of mappings from \( \mathcal{X} \) to \( \mathcal{Y} \), and \( \mathcal{G} \) a class of mappings from \( \mathcal{Y} \) to \( \mathcal{X} \). The \( p \)th order UBGM divergence between \( (\mathcal{X}, d_\mathcal{X}, P) \) and \( (\mathcal{Y}, d_\mathcal{Y}, Q) \) is

\[
\text{UD}_p^{\mathcal{F},\mathcal{G}}(P\|Q) := \inf_{f \in \mathcal{F}, g \in \mathcal{G}} \Delta_p(f,g;P,Q) + \lambda_x \Delta_\mathcal{X}(g_Q P\|P) + \lambda_y \Delta_\mathcal{Y}(f_Q P\|Q),
\]

where \( \Delta_p(f,g;P,Q) \) is given in Definition 2, and \( \lambda_x, \lambda_y > 0 \) are fixed regularization coefficients.

Evidently, \( \text{UD}_p^{\mathcal{F},\mathcal{G}} \) no longer requires optimizing over Monge maps, which alleviates the computational difficulty associated with \( \Delta_p \) from Definition 2. The function classes \( \mathcal{F} \) and \( \mathcal{G} \) can also be chosen for computational convenience (e.g., NNs). The following proposition (see Appendix A.3 for the proof) shows that \( \text{UD}_p^{\mathcal{F},\mathcal{G}} \) is a continuous divergence.

**Proposition 2** ( \( \text{UD}_p^{\mathcal{F},\mathcal{G}} \) is a divergence). Suppose that \( \Delta_\mathcal{F} \) and \( \Delta_\mathcal{G} \) are weakly continuous in their arguments, and \( \mathcal{F}, \mathcal{G} \) are rich enough so that they are dense around the isometric bijections if \( \mathcal{X}, \mathcal{Y} \) are isometric. Then

1. \( \text{UD}_p^{\mathcal{F},\mathcal{G}} \) is an upper semi-continuous divergence on \( \mathfrak{M} \), i.e., \( \text{UD}_p^{\mathcal{F},\mathcal{G}}(P\|Q) \geq 0 \) for all \( P \in \mathcal{P}(\mathcal{X}) \) and \( Q \in \mathcal{P}(\mathcal{Y}) \), with equality iff there exists isometries \( f, g \) on the support of \( P, Q \) respectively, such that \( f_Q P = Q, g_Q P = P \), and \( f = g^{-1} \).
2. If further \( \mathcal{F}, \mathcal{G} \) are compact in the sup-metrics \( d_\mathcal{F} \) and \( d_\mathcal{G} \), then \( \text{UD}_p^{\mathcal{F},\mathcal{G}} \) is continuous with respect to (w.r.t.) weak convergence.

\(^2\)A divergence on \( \mathcal{P}(\mathcal{X}) \) is a functional \( D : \mathcal{P}(\mathcal{X}) \times \mathcal{P}(\mathcal{X}) \to \mathbb{R}_{\geq 0} \) such that \( D(P\|Q) = 0 \) iff \( P = Q \).
3.2 Cycle GAN as Unbalanced Gromov-Monge Divergence

If \( D_X \) and \( D_Y \) are integral probability metrics (IPM)\(^3\) (Zolotarev, 1984; Müller, 1997) indexed by the function classes \( F_X \) and \( F_Y \), respectively, then \( \text{UD}_1 \) amounts to a minimax game between the maps \( f, g \) and the witness functions \( \psi \) and \( \phi \) of the IPMs on \( F_X \) and \( F_Y \) respectively, as follows:

\[
\inf_{f: X \to Y} \sup_{g: Y \to X} \Delta_1(f, g; P, Q) + \lambda_x \left( \mathbb{E}[\psi(g(Y))] - \mathbb{E}[\psi(X)] \right) + \lambda_y \left( \mathbb{E}[\phi(f(X))] - \mathbb{E}[\phi(Y)] \right),
\]

where \( X \sim P \) and \( Y \sim Q \).

Written in this form, we see the similarity to the cycle GAN formulation (Zhu et al., 2017; Kim et al., 2017):

\[
\inf_{f: X \to Y} \sup_{g: Y \to X} \mathbb{E}[d_X(X, g \circ f(X))] + \mathbb{E}[d_Y(Y, f \circ g(Y))] + \lambda_x \left( \mathbb{E}[\psi(g(Y))] - \mathbb{E}[\psi(X)] \right) + \lambda_y \left( \mathbb{E}[\phi(f(X))] - \mathbb{E}[\phi(Y)] \right).
\]

The first two terms in (6) encourage \( f \) and \( g \) to be approximate inverses of one another, similar to the role of the distortion \( \Delta_1(f, g; P, Q) \) in \( \text{UD}_1 \) from (5). While the original Cycle GAN formulation did not require \( f \) and \( g \) to be isometries, this constraint was introduced in followup works (Hoshen and Wolf, 2018). We thus see that Cycle GAN, with a relaxed isometry requirement of \( f \) and \( g \), is a particular instantiation of the UBGM divergence.

3.3 Relation to Past Works

We show briefly here the construction of two well-known discrepancies between mm spaces, namely the GW distance (Mémoli, 2011), and the Gromov-Monge (GM) distance (Mémoli and Needham, 2021). The starting point of defining these two distances is the ‘correspondence set formulation’ of \( d_{\text{GH}} \) from (3).

**Gromov-Wasserstein distance.** In a nutshell, the GW distance is an \( L^p \), \( p \geq 1 \) relaxation of the \( L^\infty \) norm in formulation (3) of \( d_{\text{GH}} \), along with a Kantorovich relaxation of the correspondence set using couplings.

**Definition 5** (Gromov-Wasserstein distance (Mémoli, 2011)). The GW distance between \((\mathcal{X}, d_X, P)\) and \((\mathcal{Y}, d_Y, Q)\) is

\[
\text{GW}(P, Q) := \inf_{\pi \in \Pi(P, Q)} \| \Gamma_{X, Y} \|_{L^p(\pi \otimes \pi)}
\]

where \( \Gamma_{X, Y}(x, y, x', y') := |d_X(x, x') - d_Y(y, y')| \), and \( \Pi(P, Q) \) is the set of all couplings of \( P, Q \).

Another closely related formulation is the unbalanced GW distance from Séjourné et al. (2020).

For any divergence\(^4\) \( D_X \) on \( \mathcal{X} \), define its two-fold extension \( D_X^{\otimes 2}(P\|Q) := D_X(P \otimes P \| Q \otimes Q) \).

\(^3\)An IPM indexed by a function class \( \mathcal{F} \) is a pseudometric on \( \mathcal{P}(\mathcal{X}) \) defined as \( d_\mathcal{F}(\mu, \nu) := \sup_{f \in \mathcal{F}} \int_X f d(\mu - \nu) \).

\(^4\)Séjourné et al. (2020) used f-divergences (Csiszar, 1967) for \( D_X \) and \( D_Y \), but we provide a general definition.
**Definition 6** (Unbalanced Gromov-Wasserstein distance (Séjourné et al., 2020)). Let \( \mathcal{M}_+(\mathcal{X}) \) be the set of all nonnegative Borel measures on \( \mathcal{X} \). The unbalanced GW distance between \((\mathcal{X}, d_\mathcal{X}, P)\) and \((\mathcal{Y}, d_\mathcal{Y}, Q)\) is

\[
\text{UGW}(P, Q) := \inf_{\pi \in \mathcal{M}_+(\mathcal{X} \times \mathcal{Y})} \| \Gamma_{\mathcal{X}, \mathcal{Y}} \|_{L^1(\pi \otimes \pi)} + D_{\mathcal{X}}^{\otimes 2}(\pi_1\|P) + D_{\mathcal{Y}}^{\otimes 2}(\pi_2\|Q)
\]

where \( \pi_1, \pi_2 \) are the marginals of \( \pi \) on \( \mathcal{X} \) and \( \mathcal{Y} \).

The unbalanced relaxation of the GW distance is similar to how our UBGMD distance (Definition 4) relaxes the BGM distance. A crucial difference is that both the BGM distance and its unbalanced version explicitly encode bidirectional mappings, which are important in applications as they alleviate the need to recompute the coupling matrix given new datapoints.

**Gromov-Monge distance.** More recently, Mémoli and Needham (2021) presented another extension of \( d_{\text{GH}} \) to a discrepancy between mm spaces. Termed the GM distance, it considers an \( L^p \) Monge relaxation of \( H \) as opposed to the Kantorovich-based approach of GW. Namely, instead of using couplings, the correspondence set now comprises Monge maps, i.e., all measurable maps \( f : \mathcal{X} \to \mathcal{Y} \) s.t. \( f_* P = Q \). Also for arbitrary \( f \), denote \( \pi_f := (\text{id}, f)_\sharp P \). Clearly for Monge maps \( f \) that pushes \( P \) to \( Q \), \( \pi_f \in \Pi(P, Q) \).

**Definition 7** (Gromov-Monge distance (Mémoli and Needham, 2021)). The GM distance between two mm spaces \((\mathcal{X}, d_\mathcal{X}, P)\) and \((\mathcal{Y}, d_\mathcal{Y}, Q)\) is

\[
\text{GM}(P, Q) := \inf_{f : \mathcal{X} \to \mathcal{Y}, f_* P = Q} \| \Gamma_{\mathcal{X}, \mathcal{Y}} \|_{L^p(\pi_f \otimes \pi_f)}
\]

where \( \| \Gamma_{\mathcal{X}, \mathcal{Y}} \|_{L^p(\pi_f \otimes \pi_f)} = \Delta_{\mathcal{X}}^{(p)}(f; P) \).

Comparing \( D_p \) to GM above, we see that while the latter uses a single low metric distortion maps (with a cost of the form \( \Delta_{\mathcal{X}}^{(p)}(f; P) \)), our BGM distance uses two such mappings that are approximately inverses (as enforced by \( \Delta_{\mathcal{X}, \mathcal{Y}}^{(p)}(f, g; P, Q) \)). In a sense our definition is a symmetrized and cycle consistent version of GM.

### 4 Kernelization: Generalized Maximum Mean Discrepancy

Motivated by computational considerations, we now instantiate the divergences \( D_\mathcal{X} \) and \( D_\mathcal{Y} \) in \( \mathcal{U} D_{p, q}^{\mathcal{X}, \mathcal{Y}} \) (see Definition 4) as maximum mean discrepancies (MMDs) (Gretton et al., 2012). We coin the resulting kernelized divergence as the generalized maximum mean discrepancy (GMMD). MMDs can be efficiently computed and offer flexibility in picking the proper kernel for each space. We start by reviewing preliminaries on MMDs (Section 4.1), after which we present the kernelized UBGMD distance (Section 4.2), and explore its empirical convergence rates (Section 4.3).

#### 4.1 Reproducing Kernel Hilbert Spaces

We define reproducing kernel Hilbert spaces (RKHS) and the associated MMD. For a separable space \( \mathcal{X} \) and a continuous, positive definite, real-valued kernel \( k_\mathcal{X} : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \), let \( \mathcal{H}_\mathcal{X} \) denote the corresponding RKHS, in which for any \( f \in \mathcal{H}_\mathcal{X} \), we have \( f(x) = \langle f(\cdot), k(x, \cdot) \rangle_{\mathcal{H}_\mathcal{X}} \), for any \( x \in \mathcal{X} \). See Berlinet and Thomas-Agnan (2011) for existence and uniqueness of \( \mathcal{H}_\mathcal{X} \). There is a natural way to embed \( \mathcal{P}(\mathcal{X}) \) into \( (\mathcal{H}_\mathcal{X}, k_\mathcal{X}) \), given by the kernel mean embedding

\[
\mu_\mathcal{X} P(x) := \int_\mathcal{X} k_\mathcal{X}(x, y) dP(y) = \mathbb{E}[k_\mathcal{X}(x, Y)],
\]
where \( Y \sim P \). This enables defining a discrepancy measure between probability distribution as the RKHS distance between their kernel mean embeddings.

**Definition 8** (Maximum mean discrepancy). Let \( \mathcal{H}_X \) be an RKHS. The MMD between \( P, Q \in \mathcal{P}(X) \) is

\[
\text{MMD}_{X}(P, Q) := \| \mu_X P - \mu_X Q \|_{\mathcal{H}_X} = \left( \int k_X(x, y) d(P - Q)(x) d(P - Q)(y) \right)^{1/2}.
\]

When the kernel \( k_X \) is characteristic, as defined next, MMD \( X \) metrizes the space of distributions \( \mathcal{P}(X) \).

**Definition 9** (Characteristic kernel). The kernel \( k_X \) of an RKHS \( \mathcal{H}_X \) is called characteristic if the mean embedding \( \mu_X : \mathcal{P}(X) \to \mathcal{H}_X \) is injective.

Also recall that characteristic kernels enable defining a metric on the \( X \) space (Sejdnov et al., 2013). Namely, defining \( \rho_{k_X}(x, x') := k_X(x, x) + k_X(x', x') - 2k_X(x, x') \), for \( x, x' \in X \), we have that \((X, \sqrt{\rho_{k_X}})\) is a metric space. To simplify notation, we henceforth denote \( \rho_{k_X} \) by \( \rho_X \).

### 4.2 Generalized MMD

The GMMD is defined as follows. Throughout we assume that \( X \) and \( Y \) are compact with diameters bounded by \( K \), and specialize to the case of \( p = 1 \).

**Definition 10** (Generalized MMD between Metric Measure Spaces). Let \( k_X \) and \( k_Y \) be characteristic kernels on \( X \) and \( Y \), respectively. The GMMD between \((X, d_X, P)\) and \((Y, d_Y, Q)\) is

\[
\text{UD}^{F,G}_{k_X, k_Y}(P||Q) := \inf_{f \in \mathcal{F}, g \in \mathcal{G}} \Delta_1(f, g; P, Q) + \lambda_X \text{MMD}_{X}(P, g_P Q) + \lambda_Y \text{MMD}_{Y}(f_P P, Q).
\]

**Remark 3** (GMMD is a divergence). MMDs w.r.t. characteristic kernels are metrics (in particular, divergences) on the space of Borel probability measures. Proposition 2 thus implies that GMMD is a divergence. Further, under the mild condition that \( k_X, k_Y \) are bounded from above, MMDs are weakly continuous. Hence, weak continuity of GMMD also follows from the proposition, given that \( \mathcal{F}, \mathcal{G} \) are compact.

**Remark 4** (Kernels specify GMMD). GMMD can be fully specified by the kernels if one defines the mm spaces using the kernel induced metrics \( \rho_X \) and \( \rho_Y \).

### 4.3 GMMD Empirical Estimation Rates

We now study the convergence rate of the two-sample plug-in estimator of GMMD. Let \((X_i)_{i=1}^n \) and \((Y_i)_{i=1}^m \) be i.i.d. samples from \( P \) and \( Q \), respectively. Denote by \( P_n := n^{-1} \sum_{i=1}^n \delta_{x_i} \) and \( Q_m := m^{-1} \sum_{i=1}^m \delta_{y_i} \) the empirical measures associated with these samples. Since GMMD is weakly continuous (for compact \( \mathcal{F} \) and \( \mathcal{G} \)), we immediately have \( \text{UD}^{F,G}_{k_X, k_Y}(P_n || Q_m) \to \text{UD}^{F,G}_{k_X, k_Y}(P || Q) \) as \( n, m \to \infty \). The focus of this section is the rate at which this convergence happens.

**Theorem 1.** Suppose \( k_X, k_Y \) are uniformly bounded by a constant \( C \), and the diameters of \( X \) and \( Y \) are bounded by \( K \). Further suppose that \( \mathcal{F} \) and \( \mathcal{G} \) are compact in \( d_F \) and \( d_G \), respectively. Then

\[
\mathbb{E} \left[ \left| \text{UD}^{F,G}_{k_X, k_Y}(P || Q) - \text{UD}^{F,G}_{k_X, k_Y}(P_n || Q_m) \right| \right] \lesssim \lambda_Y \delta_n(\mathcal{G}_{k_Y}) + \lambda_X \delta_m(\mathcal{G}_{k_X}) + \delta_{n,m}(\mathcal{F}, \mathcal{G})
\]
\[ + \lambda_x C^{\frac{1}{\alpha}} n^{-\frac{1}{\alpha}} + \lambda_y C^{\frac{1}{\alpha}} m^{-\frac{1}{\alpha}} + K(n \wedge m)^{-1} \]

where \( \mathcal{F}_{k_y} := \{ k_y \circ (f, f) : f \in \mathcal{F} \} \) and

\[
\delta_n(\mathcal{F}_{k_y}) := \inf_{\alpha > 0} \left( \alpha + \frac{1}{n} \int_{\alpha}^{2\alpha} \log \left( N(\mathcal{F}_{k_y}, \| \cdot \|_\infty, \tau) \right) d\tau \right)^{\frac{1}{2}},
\]

with \( \mathcal{G}_{k_x} \) and \( \delta_m(\mathcal{G}_{k_x}) \) defined analogously, and

\[
\delta_{n,m}(\mathcal{F}, \mathcal{G}) := \inf_{\alpha > 0} \left( \alpha + \frac{1}{\sqrt{n \wedge m}} \int_{\alpha}^{K} \left( \log \left( N(\mathcal{F}, d_{\mathcal{F}}, \tau) \right) + \log \left( N(\mathcal{G}, d_{\mathcal{G}}, \tau) \right) \right)^{\frac{1}{2}} d\tau \right).
\]

Theorem 1 bounds the estimation error for general function classes \( \mathcal{F} \) and \( \mathcal{G} \) in terms of the appropriate entropy integrals. The proof is given in Appendix A.4 and relies on standard chaining arguments and bounds on Rademacher chaos complexity (cf. e.g. Sriperumbudur (2016)). In general, these entropy integrals cannot be further simplified due to the dependence on the arbitrary classes \( \mathcal{F} \) and \( \mathcal{G} \). Nevertheless, as discussed next, Theorem 1 can be instantiated to obtain explicit rates for particular function classes of interest.

**Remark 5** (Special cases). Corollary 1 in Appendix A.6 instantiates the result for two important cases: when the function classes are (i) Lipschitz and (ii) parametric. We obtain a convergence rate of \( O\left( \frac{1}{n^{1/2d_x}} + \frac{1}{m^{1/2d_y}} \right) \) for the Lipschitz case when \( d_x, d_y > 2 \), and \( O\left( (n \wedge m)^{-1/2} \right) \) for the parametric case. The latter is of particular practical interest, as NNs offer a convenient and trainable model for the bidirectional maps (see next section).

### 5 NUMERICAL EXPERIMENTS

We present applications of GMMD in shape matching. We parametrize the bidirectional maps \( f, g \) as neural networks with parameters \( \theta \) and \( \psi \) respectively. Algorithm 1 (Appendix B) summarizes the optimization of the GMMD objective as function of \( \theta \) and \( \psi \). All experiments are run on the same machine with 4 core CPUs and a Tesla T4 GPU. The examples below highlight the qualitative and quantitative behavior of GMMD, illustrating the fact that GMMD is applicable to the same tasks as classical methods such as GW and UGW for finding correspondences. Further, GMMD amortizes the computational cost, as it results in continuous mappings that generalize to unseen datapoints drawn from the same distributions.

![Heart shape (P)](image1)
(a) Heart shape (P)

![Rotation (Q_b)](image2)
(b) Rotation (Q_b)

![Scaling (Q_s)](image3)
(c) Scaling (Q_s)

![3D embedding (Q_d)](image4)
(d) 3D embedding (Q_d)

Figure 1: Heart shape and its transformations.

#### 5.1 GMMD For Shape Matching

We consider here matching of synthetic shapes, specifically a 2-dimensional heart shape given in Figure 1(a) and its transformations through rotation (b), scaling (c) and isometrically embedding
Figure 2: First row: learned continuous GMMMD Mappings and their cycle consistency in shape matching. Second row: discrete entropic GW Barycentric Mappings. The color code in the heatmaps is coordinate based.

into 3-dimensional space (d). The data is generated via sampling \( n = 4000 \) points for each shape. The distributions for each matching experiment are the empirical measures induced by these samples, with \( P \) corresponding to \( Q_b \), \( Q_c \), and \( Q_d \) corresponding to subfigures (b), (c), and (d), respectively (the subscript is suppressed when we simultaneously refer to several experiments).

For matching experiments, we compute GMMMD using Algorithm 1 for \( \lambda_x = \lambda_y = \lambda^{-1} \), where \( \lambda \in \{2^i \times 10^{-3} : i = 0, \ldots, 9\} \). We use a uniform mixture of Gaussian kernels to define \( \text{MMD}_x \) and \( \text{MMD}_y \) and use kernel induced metrics \( \rho_x \) and \( \rho_y \) in the distortion \( \Delta_1 \). The bandwidths we used for the Gaussian kernels are median of the metric \( \times \{.0001, .001, .01, .05, .25, 1, 4, 20, 100, 1000\} \). The architecture of the bidirectional maps \( f \) and \( g \) is a 3-layer ReLU NN with 200 neurons each, and an output dimension matching the target distribution dimension. We use Adam optimizer (Kingma and Ba, 2014) for 3000 epochs with a learning rate \( 10^{-3} \).

Figure 3: Matching 3D shapes with GMMMD and entropic GW.

In Figure 2, the first row corresponds to GMMMD matching for \( \lambda = 0.064 \). For each case, we see that the learned bidirectional maps of GMMMD successfully perform the matching, i.e., \( f_gP \approx Q \) and \( g_PQ \approx P \). We also confirm that they satisfy the cycle consistency property, i.e., \( f \circ g \approx \text{id}_Y \) and \( g \circ f \approx \text{id}_X \). The second row shows entropic GW matchings (Peyré et al., 2016). We use the POT library (Flamary et al., 2021) to perform discrete entropic GW for an entropic regularization parameter \( \varepsilon = 5e^{-4} \). Note that entropic GW results in a coupling matrix \( \pi \). To
obtain discrete mappings of the points we employ barycentric maps (Ferradans et al., 2014), i.e.,
\( \tilde{f}(x_i) := (\sum_{j=1}^{n} \pi_{ij})^{-1} \sum_{j=1}^{n} \pi_{ij} y_j \) and \( \tilde{g}(y_j) := (\sum_{i=1}^{n} \pi_{ij})^{-1} \sum_{i=1}^{n} \pi_{ij} x_i. \)

We see from Figure 2 that the GMMD continuous maps and the discrete barycentric maps induced by the GW coupling are on par qualitatively in these matching tasks. To confirm this quantitatively, we consider the matching of the heart shape and its rotation (Figure 1(b)) since for this case an isometry exists, i.e., there are \( f^*, g^* \) with \( \Delta_1(f^*, g^*; P, Q_b) = 0. \) Tables 1 and 2 state the values of \( \text{MMD}_Y(f^*, Q_b), \text{MMD}_X(P, g^*Q_b), \) and \( \Delta(f, g; P, Q_b) \) across different regularization parameters for the GMMD and GW-based mappings, respectively. We see that GMMD and GW indeed result in small MMD and distortions values. GMMD yields a smaller distortion than GW. Note that we also have evaluated UGW (Séjourné et al., 2020) with the code provided by the authors and found that it is sensitive to hyper-parameters choice, and did not result in an accurate matching on the considered tasks. We think that more tuning is needed for UGW. Additional results and ablation on regularization parameters and shapes are given in Appendix B.

Figure 3 presents a more complex matching of 3D shapes that consist in two different biplanes models from the Princeton Shape benchmark (Shilane et al., 2004) (for \( n = 8000 \)). We see that GMMD and GW are also on par and that the GMMD bidirectional maps result in less outliers than barycentric GW-based maps. This robustness of GMMD is due to the use of kernel induced metrics. Quantitative evaluation is presented in Appendix B.

Table 1: Evaluating GMMD’s mappings for \( P \) vs. \( Q_b. \)

| \( \lambda \) | GMMD | \( \text{MMD}_X \) | \( \text{MMD}_Y \) | \( \Delta \) |
|---------|------|----------------|----------------|-------|
| 0.256   | 0.0794 | 0.0294 | 0.0294 | 0.0801 |
| 0.128   | 0.00825 | 4.94e-4 | 4.05e-4 | 0.0574 |
| 0.064   | 0.00776 | 0.00227 | 0.00190 | 0.0560 |
| 0.032   | 0.0924 | 2.90e-4 | 0.00386 | 2.76 |

Table 2: GW barycentric maps for \( P \) vs. \( Q_b. \)

| \( \epsilon \) | GW | \( \text{MMD}_X \) | \( \text{MMD}_Y \) | \( \Delta \) |
|-------|----|----------------|----------------|-------|
| 0.0005 | 0.00134 | 0.00420 | 0.00299 | 0.696 |
| 0.005  | 0.00660 | 0.127 | 0.116 | 1.73 |
| 0.05   | 0.0424 | 0.615 | 0.613 | 6.69 |
| 0.5    | 0.0686 | 3.99 | 4.12 | 22.9 |

5.2 GMMD Amortization and Generalization

For the biplane matching experiment with sample size \( n = 8000 \) from each distribution, Table 3 reports the training time for GMMD and the runtime for GW and UGW computations. The computational complexity of training GMMD maps amounts to the complexity of gradient descent in NN training for 3000 epochs, which is \( O(n) \). For entropic GW and UGW, however, the implementations are variants of the Sinkhorn algorithm, whose complexity scales as \( O(n^3) \). The longer training time for GMMD is due to the large number of epochs used in gradient descent (namely, 3000), but at inference time this cost is amortized since we obtain continuous maps that generalize to unseen datapoints (see Appendix B for quantitative evaluation of the generalization). For instance, matching 8000 new datapoints sampled from \( P \) and \( Q \) each using the learned mapping requires 63
ms, while with GW one would incur the cost of recomputing the coupling (26 minutes)—a three order of magnitude speedup.

Table 3: Training Time (in seconds) comparison using 8000 samples from the biplanes data.

| ε | GW       | λ       | GMMMD   |
|---|----------|---------|---------|
| 0.0005 | 1566.86  | 0.002   | 5048.11 |
| 0.1   | UGW 28.7508 | 0.256   | 5026.5  |

6 CONCLUSION

This paper introduced the UBGM divergence—a novel discrepancy measure between distributions across heterogeneous spaces, which employs bidirectional and cycle-consistent mappings. We established structural properties of the UBGM divergence and highlighted its intimate connection to the so-called cycle GAN. We also presented a kernelized variant of this divergence, termed GMMD, and analysed its statistical estimation from samples. Numerical experiments demonstrated the promise of this new divergence and compared it to other known metrics, such as the GW and UGW distances. Appealing future directions include extending the GMMD to allow optimization over kernels, sharper statistical bounds, as well as connections between the UBGM divergence and the UGW distance (in particular, under what conditions they coincide).

References

D. Alvarez-Melis and T. S. Jaakkola. Gromov-Wasserstein alignment of word embedding spaces. arXiv preprint arXiv:1809.00013, 2018.

D. Alvarez-Melis, Y. Mroueh, and T. Jaakkola. Unsupervised hierarchy matching with optimal transport over hyperbolic spaces. In S. Chiappa and R. Calandra, editors, Proceedings of the Twenty Third International Conference on Artificial Intelligence and Statistics (AISTATS-2020), volume 108 of Proceedings of Machine Learning Research, pages 1606–1617, 2020.

A. Berlinet and C. Thomas-Agnan. Reproducing kernel Hilbert spaces in probability and statistics. Springer Science & Business Media, 2011.

P. Bojanowski, E. Grave, A. Joulin, and T. Mikolov. Enriching word vectors with subword information. arXiv preprint arXiv:1607.04606, 2016.

A. M. Bronstein, M. M. Bronstein, and R. Kimmel. Generalized multidimensional scaling: A framework for isometry-invariant partial surface matching. Proceedings of the National Academy of Sciences, 103(5):1168–1172, 2006a.

A. M. Bronstein, M. M. Bronstein, and R. Kimmel. Efficient computation of isometry-invariant distances between surfaces. SIAM Journal on Scientific Computing, 28(5):1812–1836, 2006b.

C. Bunne, D. Alvarez-Melis, A. Krause, and S. Jegelka. Learning generative models across incomparable spaces. In Proceedings of the International Conference on Machine Learning (ICML-2019), pages 851–861, June 2019.
L. Chizat, G. Peyré, B. Schmitzer, and F.-X. Vialard. Unbalanced optimal transport: Dynamic and Kantorovich formulations. *Journal of Functional Analysis*, 274(11):3090–3123, 2018.

C. W. Commander. A survey of the quadratic assignment problem, with applications. *Morehead Electronic Journal of Applicable Mathematics*, 4:MATH–2005–01, 2005.

A. Conneau, G. Lample, M. Ranzato, L. Denoyer, and H. Jégou. Word translation without parallel data. *arXiv preprint arXiv:1710.04087*, 2017.

I. Csiszár. Information-type measures of difference of probability distributions and indirect observation. *Studia Scientiarum Mathematicarum Hungarica*, 2:229–318, 1967.

V. De la Peña and E. Giné. *Decoupling: from dependence to independence*. Springer Science & Business Media, 2012.

S. Ferradans, N. Papadakis, G. Peyré, and J.-F. Aujol. Regularized discrete optimal transport. *SIAM Journal on Imaging Sciences*, 7(3):1853–1882, 2014.

R. Flamary, K. Lounici, and A. Ferrari. Concentration bounds for linear monge mapping estimation and optimal transport domain adaptation. *arXiv preprint arXiv:1905.10155*, 2019.

R. Flamary, N. Courty, A. Gramfort, M. Z. Alayya, A. Boisbunon, S. Chambon, L. Chapel, A. Corenflos, K. Fatras, N. Fournier, L. Gautheron, N. T. Gayraud, H. Janati, A. Rakotomamonjy, I. Redko, A. Rolet, A. Schutz, V. Seguy, D. J. Sutherland, R. Tavenard, A. Tong, and T. Vayer. Pot: Python optimal transport. *Journal of Machine Learning Research*, 22(78):1–8, 2021.

C. Frogner, C. Zhang, H. Mobahi, M. Araya-Polo, and T. Poggio. Learning with a Wasserstein loss. *arXiv preprint arXiv:1506.05439*, 2015.

E. Grave, A. Joulin, and Q. Berthet. Unsupervised alignment of embeddings with Wasserstein procrustes. In *Proceedings of the The 22nd International Conference on Artificial Intelligence and Statistics (AISTATS-2019)*, pages 1880–1890. PMLR, 2019.

A. Gretton, K. M. Borgwardt, M. J. Rasch, B. Schölkopf, and A. Smola. A kernel two-sample test. *The Journal of Machine Learning Research*, 13(1):723–773, 2012.

Y. Hoshen and L. Wolf. Unsupervised correlation analysis. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition (CVPR-2018)*, June 2018.

T. Kim, M. Cha, H. Kim, J. K. Lee, and J. Kim. Learning to discover cross-domain relations with generative adversarail networks. In *Proceedings of the 34th International Conference on Machine Learning (ICML-2017)*, pages 1857–1865. PMLR, 2017.

D. P. Kingma and J. Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.

A. Makkova, A. Taghvaei, S. Oh, and J. Lee. Optimal transport mapping via input convex neural networks. In *Proceedings of the International Conference on Machine Learning (ICML-2020)*, pages 6672–6681. PMLR, 2020.

F. Mémoli. Gromov–Wasserstein distances and the metric approach to object matching. *Foundations of computational mathematics*, 11(4):417–487, 2011.

F. Mémoli and T. Needham. Distance distributions and inverse problems for metric measure spaces. *arXiv preprint arXiv:1810.09646*, 2021.
F. Mémoli and G. Sapiro. Comparing point clouds. In *Proceedings of the 2004 Eurographics/ACM SIGGRAPH symposium on Geometry processing*, pages 32–40, 2004.

F. Mémoli and G. Sapiro. A theoretical and computational framework for isometry invariant recognition of point cloud data. *Foundations of Computational Mathematics*, 5(3):313–347, 2005.

A. Müller. Integral probability metrics and their generating classes of functions. *Advances in Applied Probability*, 29(2):429–443, 1997.

F.-P. Paty, A. d’Aspremont, and M. Cuturi. Regularity as regularization: Smooth and strongly convex brenier potentials in optimal transport. In *International Conference on Artificial Intelligence and Statistics (AISTATS-2021)*, pages 1222–1232. PMLR, 2020.

M. Perrot, N. Courty, R. Flamary, and A. Habrard. Mapping estimation for discrete optimal transport. In *Advances in Neural Information Processing Systems (NeurIPS-2016)*, pages 4197–4205, 2016.

G. Peyré, M. Cuturi, and J. Solomon. Gromov-Wasserstein averaging of kernel and distance matrices. In M. F. Balcan and K. Q. Weinberger, editors, *Proceedings of The 33rd International Conference on Machine Learning (ICML-2016)*, volume 48 of *Proceedings of Machine Learning Research*, pages 2664–2672, New York, New York, USA, 20–22 Jun 2016. PMLR.

D. Sejdinovic, B. Sriperumbudur, A. Gretton, and K. Fukumizu. Equivalence of distance-based and RKHS-based statistics in hypothesis testing. *The Annals of Statistics*, pages 2263–2291, 2013.

T. Séjourné, F.-X. Vialard, and G. Peyré. The unbalanced Gromov Wasserstein distance: Conic formulation and relaxation. *arXiv preprint arXiv:2009.04266*, 2020.

P. Shilane, P. Min, M. Kazhdan, and T. Funkhouser. The princeton shape benchmark. In *Proceedings of the International Conference on Shape Modeling and Applications (SMI-2004)*, pages 167–178. IEEE, 2004.

B. Sriperumbudur. On the optimal estimation of probability measures in weak and strong topologies. *Bernoulli*, 22(3):1839–1893, 2016.

A. W. van der Vaart and J. A. Wellner. *Weak convergence and empirical processes: with applications to statistics*. Springer Science & Business Media, 1996.

T. Vayer, R. Flamary, R. Tavenard, L. Chapel, and N. Courty. Sliced Gromov-Wasserstein. *arXiv preprint arXiv:1905.10124*, 2019.

M. J. Wainwright. *High-dimensional statistics: A non-asymptotic viewpoint*, volume 48. Cambridge University Press, 2019.

J. Weed and F. Bach. Sharp asymptotic and finite-sample rates of convergence of empirical measures in Wasserstein distance. *Bernoulli*, 25(4A):2620–2648, 2019.

H. Xu, D. Luo, and L. Carin. Scalable Gromov-Wasserstein learning for graph partitioning and matching. *Advances in neural information processing systems (NeurIPS-19)*, 32:3052–3062, 2019.

Y. Yan, W. Li, H. Wu, H. Min, M. Tan, and Q. Wu. Semi-supervised optimal transport for heterogeneous domain adaptation. In *Proceedings of the International Joint Conference on Artificial Intelligence (IJCAI-2018)*, volume 7, pages 2969–2975, 2018.
J.-Y. Zhu, T. Park, P. Isola, and A. A. Efros. Unpaired image-to-image translation using cycle-consistent adversarial networks. In Proceedings of the IEEE international conference on computer vision (CCV-2017), pages 2223–2232, 2017.

V. M. Zolotarev. Probability metrics. Theory of Probability & Its Applications, 28(2):278–302, 1984.
A Proofs

To simplify notation we denote $L_{P,Q}(f,g) := \lambda_x \text{MMD}_X(P,g_2Q)+\lambda_y \text{MMD}_Y(f_2,P,Q)+\Delta_1(f,g;P,Q)$, which is the functional that is optimized in definition of convergence and demonstrate that the limits $X$ of $f_2, g_1, g_2$ (over the appropriate domains) with $(f_1)_P = Q$, $(f_2)_R = P$, $(g_1)_Q = P$, $(g_2)_R = Q$. We only show the derivation for $\Delta^{(p)}_{X,Y}$; a similar argument applies to $\Delta^{(p)}_X$, $\Delta^{(p)}_Y$.

A.1 Proof of Proposition 1

The symmetry and positivity follows directly from definition and Lemma 1, which is proven below. For the triangle inequality, fix 3 mm spaces $(X, d_X, P)$, $(Y, d_Y, Q)$, $(Z, d_Z, R)$ and functions $f_1, f_2, g_1, g_2$ (over the appropriate domains) with $(f_1)_P = Q$, $(f_2)_R = P$, $(g_1)_Q = P$, $(g_2)_R = Q$. We only show the derivation for $\Delta^{(p)}_{X,Y}$; a similar argument applies to $\Delta^{(p)}_X$, $\Delta^{(p)}_Y$.

For $\Delta^{(p)}_{X,Y}$, we have

$$\Delta^{(p)}_{X,Y}(f_1, g_1; P, Q) + \Delta^{(p)}_{X,Y}(f_2, g_2; Q, R)$$

$$= \left( \int |d_X(x, g_1(y)) - d_Y(f_1(x, y))|^p \, dP(x) \, dQ(y) \right)^{\frac{1}{p}}$$

$$+ \left( \int |d_Y(y, g_2(z)) - d_Z(f_2(y, z))|^p \, dQ(y) \, dR(z) \right)^{\frac{1}{p}}$$

$$= \left( \int |d_X(x, g_1(g_2(z))) - d_Y(f_1(x, g_2(z)))|^p \, dP(x) \, dR(z) \right)^{\frac{1}{p}}$$

$$+ \left( \int |d_Y(f_1(x, g_2(z))) - d_Z(f_2(f_1(x), z))|^p \, dP(x) \, dR(z) \right)^{\frac{1}{p}}$$

$$\geq \left( \int |d_X(x, g_1(g_2(z))) - d_Z(f_2(f_1(x), z))|^p \, dP(x) \, dR(z) \right)^{\frac{1}{p}}$$

$$= \Delta^{(p)}_{X,Y}(f_2 \circ f_1, g_1 \circ g_2; P, R).$$

Hence $D_p$ is a metric on $\mathcal{M}$.

A.2 Proof of Lemma 1

Suppose $\{f_n\}_{n \in \mathbb{N}}$ and $\{g_n\}_{n \in \mathbb{N}}$ are sequence such that $\Delta_p(f_n, g_n; P, Q) \to 0$. We will show that up to extracting subsequences, these sequences converge $P \otimes Q$ a.s. to isometries, $f$ and $g$, respectively, such that $f = g^{-1}$. The argument first shows that there is a countable dense $S \subseteq \mathcal{X}$ such that the distortion function $\phi_n$ (defined below) converges on $S \times S$ to 0. Then we take a subsequence of $f_n$ that converges on $S$, and show that this subsequence also converges $P$-a.s. on $\mathcal{X}$, and the limit is an isometry. After applying the same to $\{g_n\}_{n \in \mathbb{N}}$, we conclude the desired convergence and demonstrate that the limits $f$ and $g$ satisfy $f = g^{-1}$.

We first consider the term $\Delta^{(p)}_X(f_n; P)$. Since

$$\int |d_X(x, x') - d_Y(f_n(x), f_n(x'))|^p \, dP(x) \, dP(x') \to 0,$$

we may assume that, up to extraction of subsequences, we have

$$\phi_n(x, x') := |d_X(x, x') - d_Y(f_n(x), f_n(x'))| \to 0, \quad P^{\otimes 2} - a.s.$$

Set $\Omega = \{(x, x') : \phi_n(x, x') \to 0\}$ as the set of pairs for which the convergence occurs, and let $\Omega_x = \{x' : (x, x') \in \Omega\}$ be the slice at $x \in \mathcal{X}$ in the first coordinate. Then $P^{\otimes 2}(\mathcal{X} \times \mathcal{X} - \Omega) = 0$, and by Fubini’s theorem

$$\int_{\mathcal{X}} P(\Omega_x) \, dP(x) = P^{\otimes 2}(\Omega) = 1.$$
Denoting $A = \{x : P(\Omega_x) = 1\}$, we thus have $P(A) = 1$, and hence $A$ is dense. We next construct $S$ as a countable dense subset of $A$.

Step 1 – Separability of convergence points: We present an inductive construction of a countable dense subset $S \subseteq X$ such that $\tilde{\phi}_n$ converges to 0 on $S \times S$. First take any $x_0 \in A$ and define

$$S_0 := \{x' : \phi_n(x_0, x') \text{ does not converge to } 0\} = X - \Omega_{x_0},$$

then $P(S_0) = 0$ since $x_0 \in A$. Suppose we have points $x_0, \ldots, x_k \in A$, such that $\phi(x_i, x_j) \to 0$ for $i, j = 0, \ldots, k$, and define $S_i = X - \Omega_{x_i}$ for $i = 0, \ldots, k$. Define function

$$\psi_k(x) := \min_{0 \leq i \leq k} \{d_X(x, x_i)\},$$

and set $w_k = \arg\max \psi_k(x)$. Suppose $\psi_k(w_k) > 0$, otherwise $x_0, \ldots, x_k$ is already dense. Since $\psi_k(x)$ is continuous, $B_k = \{\psi_k(x) > \psi_k(w_k)/2\}$ is a nonempty open set on $X$. Notice that set $C_k = A - \bigcup_{0 \leq l \leq k} S_l$ still have probability 1, and any point $x' \in C_k$ satisfies that $\phi_n(x', x_i)$ converges for all $i = 0, \ldots, k$. Since $P$ has full support, $B_k \cap C_k$ is not empty, hence we pick $x_{k+1} \in B_k \cap C_k$. Inductively we have sequence $\{x_k\}_{k \in \mathbb{N}}$ such that $\phi_n(x_i, x_j)$ converges for any $i, j \in \mathbb{N}$. Denote $S = \{x_k\}_{k \in \mathbb{N}}$.

Now we prove that $S$ is dense in $X$. Suppose it is not, then there is an $\epsilon > 0$ and an $\tilde{x} \in X$ such that $d_X(\tilde{x}, x_k) > \epsilon$, for all $k \in \mathbb{N}$. So $\psi_k(w_k) \geq \psi_k(\tilde{x}) > \epsilon$. By construction, $d_X(x_{k+1}, x_k) \geq \psi_k(w_k)/2 \geq \epsilon/2$, for all $i \leq k$, so $d_X(x_i, x_j) \geq \epsilon/2$ for any $i \neq j$. This is a contradiction since $X$ is compact.

Step 2 – Convergence to isometry: Next we find a subsequence of $\{f_n\}_{n \in \mathbb{N}}$ such that it converges on $S$ to an isometry $f$, and extend this convergence to a.s. on $X$. Now we have a countable set $S \subseteq A$ that is dense in $X$ such that $\phi_n(s, t) \to 0$, $\forall s, t \in S$. We can thus take a subsequence of $\{f_n\}_{n \in \mathbb{N}}$ such that it converges on $S$ pointwise to a mapping $f$. Without loss of generality (WLOG) we assume $f_n$ converges, for any $s \in S$, as any subsequence still approaches infimum and the subsequence $\phi_n$ still converges to 0 on $S \times S$. Since $\lim_{n \to \infty} \{d_X(s, t) - d_Y(f_n(s), f_n(t))\} = 0$, by continuity we have $d_X(s, t) = d_Y(f(s), f(t))$. For any $x \notin S$, fix a sequence $\{s_{\ell}\}_{\ell \in \mathbb{N}} \subseteq S$ with $s_{\ell} \to x$, and define

$$f(x) := \lim_{\ell \to \infty} f(s_{\ell}).$$

So

$$d_Y(f(x), f(x')) = \lim_{\ell \to \infty} d_Y(f(s_{\ell}), f(t_{\ell})) = \lim_{\ell \to \infty} d_X(s_{\ell}, t_{\ell}) = d_X(x, x')$$

for $x, x' \in X$, and $s_{\ell} \to x, t_{\ell} \to x'$. So $f$ is extended to an isometry on $X$.

Now consider any $x \in C = \cap_{s \in S} \Omega_s$, where $P(C) = 1$. Clearly for all $s \in S$,

$$\lim_{n \to \infty} d_Y(f_n(x), f_n(s)) = d_X(x, s).$$

We have a sequence $\{s_{\ell}\}_{\ell \in \mathbb{N}}$ in $S$ such that $s_{\ell} \to x$, and

$$d_Y(f_n(x), f(x)) \leq d_Y(f_n(x), f_n(s_{\ell})) + d_Y(f_n(s_{\ell}), f(s_{\ell})) + d_Y(f(s_{\ell}), f(x)),$$

which is true for all $\ell$. Fix $\ell$, and take upper limit in $n$, we have

$$\lim_{n} \sup d_Y(f_n(x), f(x)) \leq 2d_X(s_{\ell}, x),$$

which holds for all $\ell$. Then we can take $\ell \to \infty$ which shows that $\lim_{n \to \infty} f_n(x) = f(x)$, i.e. $f_n$ converges on $C$. So $f_n$ converges to $f$ P-a.s. Similarly, via subsequence extraction, we can find $g_n$ that also converges Q-a.s. to an isometry $g$. As $\mathcal{X}, \mathcal{Y}$ are compact, the limits $f$ and $g$ are both surjective and have inverses.
Now consider the third term, i.e., \( \int |d_x(x, g_n(y)) - d_x(f_n(x), y)|^p \, dP(x) \, dQ(y) \to 0 \). Since \( \mathcal{X}, \mathcal{Y} \) are bounded, by dominated convergence theorem we have

\[
\lim_n \int |d_x(x, g_n(y)) - d_x(f_n(x), y)|^p \, dP(x) \, dQ(y) = 0.
\]

Thus \( d_x(x, x') = d_x(g \circ f(x), x') \) holds \( P \otimes g \circ f \)-a.s., hence holds densely on \( \mathcal{X} \times \mathcal{X} \). By continuity this holds for all \( \mathcal{X} \times \mathcal{X} \). So \( g \circ f(x) = x \), i.e. \( f = g^{-1} \).

### A.3 Proof of Proposition 2

Non-negativity of \( \text{UD}_P^{F,G}(P\|Q) \) is immediate. The fact that it nullifies when the mm spaces are equivalent, as specified in Definition 3, is also straightforward. For the opposite implication, let \( (\mathcal{X}, d_x, P) \) and \( (\mathcal{Y}, d_y, Q) \) be mm spaces such that \( \text{UD}_P^{F,G}(P\|Q) = 0 \). Since all summands in the definition of \( \text{UD}_P^{F,G}(P\|Q) \) are non-negative we have that

\[
\inf_{f \in F, g \in G} \Delta_p(f, g; P, Q) = 0.
\]

By Lemma 1, there exist infimizing sequences \( \{f_n\}_{n \in \mathbb{N}} \subset \mathcal{F} \) and \( \{g_n\}_{n \in \mathbb{N}} \subset \mathcal{G} \) that converge \( P, Q \)-a.s. to isometries \( f : \mathcal{X} \to \mathcal{Y} \) and \( g : \mathcal{Y} \to \mathcal{X} \), respectively. This further implies weak convergence of the pushforward measures, i.e., \( (f_n)_*P \xrightarrow{w} f_*P \) and \( (g_n)_*Q \xrightarrow{w} g_*Q \). In fact, for any bounded continuous function \( \phi \) on \( \mathcal{Y} \), \( \phi \circ f_n \) converges to \( \phi \circ f \) \( P \)-a.s. Consequently, we have

\[
\int \phi(f_n(x)) \, dP(x) \to \int \phi(f(x)) \, dP(x),
\]

and hence \( (f_n)_*P \xrightarrow{w} f_*P \) (the argument for \( g_n \) is analogous). Since \( D_x \) and \( D_y \) are weakly continuous in their arguments, we have

\[
0 = \lim_{n \to \infty} \Delta_p(f_n, g_n; P, Q) = D_x((g_n)_*Q\|P) + D_y((f_n)_*P\|Q),
\]

which further implies that \( D_x(g_nQ\|P) = D_y(f_nP\|Q) = 0 \). We conclude that \( f_*P = Q \) and \( g_*Q = P \) for the isometries \( f \) and \( g \) that are inverses of each other, which establishes equivalence of the mm space.

We next prove continuity. Suppose \( P_n \xrightarrow{w} P \) and \( Q_n \xrightarrow{w} Q \). For any fixed \( f \in \mathcal{F} \) and \( g \in \mathcal{G} \),

\[
\text{UD}_P^{F,G}(P_n\|Q_n) \leq \Delta_p(f, g; P_n, Q_n) + \lambda_x D_x(g_nQ_n\|P_n) + \lambda_y D_y(f_nP_n\|Q_n),
\]

and by infimizing over \( \mathcal{F} \) and \( \mathcal{G} \), we have

\[
\limsup_{n \to \infty} \text{UD}_P^{F,G}(P_n\|Q_n) \leq \inf_{f \in \mathcal{F}, g \in \mathcal{G}} \lim_{n \to \infty} \Delta_p(f, g; P_n, Q_n) + \lambda_x D_x(g_nQ_n\|P_n) + \lambda_y D_y(f_nP_n\|Q_n) = \text{UD}_P^{F,G}(P\|Q).
\]

Thus \( \text{UD}_P^{F,G} \) is upper semi-continuous. If further \( \mathcal{F}, \mathcal{G} \) are both compact, let \( f_n^+, g_n^+ \) be minimizers for \( \text{UD}_P^{F,G}(P\|Q_n) \). Suppose \( \{k_n\}_{n \in \mathbb{N}} \) is the index sequence of a \( \liminf \) subsequence of the sequence \( \{\text{UD}_P^{F,G}(P\|Q_n)\}_{n \in \mathbb{N}} \). Since \( \mathcal{F}, \mathcal{G} \) are both compact, we may also assume that \( \{f_{k_n}\}_{n \in \mathbb{N}} \) converges in \( \mathcal{F} \), and \( \{g_{k_n}\}_{n \in \mathbb{N}} \) converges in \( \mathcal{G} \). Denote by \( f^+ \) and \( g^+ \) the limits of \( \{f_{k_n}\}_{n \in \mathbb{N}} \) and \( \{g_{k_n}\}_{n \in \mathbb{N}} \), respectively. Also by Prokhorov’s theorem, WLOG we can suppose that \( (f_{k_n})_*P_{k_n} \) and
Lemma 2: For mapping class $\mathcal{F}$, recall that $\mathcal{F}_{\kappa y} := \{\kappa y \circ (f, g) : f \in \mathcal{F}\}$. Under the same condition of Theorem 1, we have

$$
\mathbb{E} \left[ \sup_f \| \mu_y f_z P_n - \mu_y f_z P \|_{H_{\mathcal{Y}}} \right] \leq \inf_{\alpha > 0} \left( \alpha + \frac{1}{n} \int_{\alpha}^{2C} \log \left( N(\mathcal{F}_{\kappa y}, \cdot, \|\cdot\|_{\infty}, \tau) \right) d\tau \right)^{1/2} + \sqrt{\frac{C}{n}}.
$$
Lemma 3 (Convergence of $\Delta_1$). Under the same condition of Theorem 1, we have

$$
\mathbb{E} \left[ \sup_{f,g} \left| \Delta_1(f,g; P_n, Q_m) - \Delta_1(f,g; P) \right| \right] \\
\lesssim \inf_{\alpha > 0} \left( \alpha + \frac{1}{n \wedge m} \int_{\alpha}^{K} \sqrt{\log(N(F,d_F, \tau))} + \log(N(G,d_G, \tau)) \ d\tau \right) + \frac{K}{n \wedge m}.
$$

Proceeding from (7) and using the lemmas, we obtain the desired bound:

$$
\mathbb{E} \left[ \left| \text{UD}_{\mathbb{F} F_{k_x,k_y}}(P) - \text{UD}_{\mathbb{F} F_{k_x,k_y}}(P_n\|Q_m) \right| \right] \\
\lesssim \frac{K}{n \wedge m} + \lambda_y \inf_{\alpha > 0} \left( \alpha + \frac{1}{n} \int_{\alpha}^{2C} \log\left(N(F_{k_y}, \| \cdot \|_\infty, \tau)\right) \ d\tau \right)^{1/2} + \lambda_y \sqrt{\frac{C}{m}} \\
+ \lambda_x \inf_{\alpha > 0} \left( \alpha + \frac{1}{m} \int_{\alpha}^{2C} \log\left(N(G_{k_x}, \| \cdot \|_\infty, \tau)\right) \ d\tau \right)^{1/2} + \lambda_x \sqrt{\frac{C}{n}} \\
+ \inf_{\alpha > 0} \left( \alpha + \frac{1}{n \wedge m} \int_{\alpha}^{K} \sqrt{\log(N(F,d_F, \tau))} + \log(N(G,d_G, \tau)) \ d\tau \right).
$$

\[\Box\]

A.5 Complementary Proofs for Theorem 1

A.5.1 Proof of Lemma 2

First observe that $\|\mu_Y f_x P_n - \mu_Y f_P\|_{\mathcal{H}_Y} = \|n^{-1} \sum_{i=1}^{n} k_y(\cdot, f(X_i)) - \mu_Y f_P\|_{\mathcal{H}_Y}$. Let $\{\epsilon_i\}_{i \in \mathbb{N}}$ be a sequence of i.i.d. Rademacher random variables and consider the following symmetrization. Suppose $X'_1, \cdots, X'_n$ are another i.i.d sequence from $P$ that is independent of $X_1, \cdots, X_n$. By Jensen’s inequality we have

$$
\mathbb{E} \left[ \sup_{f} \left\| \frac{1}{n} \sum_{i=1}^{n} k_y(\cdot, f(X_i)) - \mu_Y f_P \right\|_{\mathcal{H}_Y} \right] \\
= \mathbb{E} \left[ \sup_{f} \left( \mathbb{E} \left[ \frac{1}{n} \sum_{i=1}^{n} k_y(\cdot, f(X_i)) - \frac{1}{n} \sum_{i=1}^{n} k_y(\cdot, f(X'_i)) \bigg| X_1, \ldots, X_n \right] \right) \right] \\
\leq \mathbb{E} \left[ \sup_{f} \left\| \frac{1}{n} \sum_{i=1}^{n} k_y(\cdot, f(X_i)) - \frac{1}{n} \sum_{i=1}^{n} k_y(\cdot, f(X'_i)) \right\|_{\mathcal{H}_Y} \right] \\
= \mathbb{E} \left[ \sup_{f} \left\| \frac{1}{n} \sum_{i=1}^{n} \epsilon_i \left( k_y(\cdot, f(X_i)) - k_y(\cdot, f(X'_i)) \right) \right\|_{\mathcal{H}_Y} \right] \\
\leq \frac{2}{n} \mathbb{E} \left[ \sup_{f} \left\| \sum_{i=1}^{n} \epsilon_i k_y(\cdot, f(X_i)) \right\|_{\mathcal{H}_Y} \bigg| X_1, \ldots, X_n \right]. \quad (8)
$$

The RKHS norm inside the conditional expectation can be further bounded as

$$
\left\| \sum_{i=1}^{n} \epsilon_i k_y(\cdot, f(X_i)) \right\|_{\mathcal{H}_Y} = \left( \sum_{i=1}^{n} \epsilon_i \epsilon_j k_y( f(X_i), f(X_j)) \right)^{1/2}
$$

20
Inserting this back into (8), we obtain

\[
\mathbb{E} \left[ \sup_f \| \mu y f_1 P_n - \mu y f_1 P \|_{\mathcal{H}_y} \right] 
\leq \frac{2}{n} \mathbb{E} \left[ \left( 2 \mathbb{E} \left[ \sup_f \sum_{i<j}^n \epsilon_i \epsilon_j k_y(f(X_i), f(X_j)) \right] X_1, \ldots, X_n \right)^{1/2} \right] + 2 \sqrt{\frac{C}{n}}. \tag{9}
\]

Recall that the Rademacher chaos complexity (Sriperumbudur, 2016) of a kernel class \( \mathcal{G} \) is define as

\[
U(\mathcal{G}, x_1, \ldots, x_n) := \mathbb{E} \left[ \sup_{g \in \mathcal{G}} \left| \sum_{i<j}^n \epsilon_i \epsilon_j g(x_i, x_j) \right| \right].
\]

Evidently, the inner expectation of the right-hand side (RHS) of 9 corresponds to the Rademacher chaos complexity of the class \( \mathcal{F}_{k_y} \), and using Lemma A.2 from Sriperumbudur (2016) we have

\[
U(\mathcal{F}_{k_y}, X_1, \ldots, X_n) \lesssim n^2 \inf_{\alpha > 0} \left( \alpha + \frac{1}{n} \int_0^{2C} \log \left( N(\mathcal{F}_{k_y}, \| \cdot \|_\infty, \tau) \right) d\tau \right) + nC.
\]

Combining all previous bounds we have that

\[
\sup_f \| \mu y f_1 P_n - \mu y f_1 P \|_{\mathcal{H}_y} \leq \frac{2}{n} \mathbb{E} \left[ \left( 2 \mathbb{E} \left[ U(\mathcal{F}_{k_y}, X_1, \ldots, X_n) \right] X_1, \ldots, X_n \right)^{1/2} \right] + 2 \sqrt{\frac{C}{n}} 
\lesssim \inf_{\alpha > 0} \left( \alpha + \frac{1}{n} \int_0^{2C} \log \left( N(\mathcal{F}_{k_y}, \| \cdot \|_\infty, \tau) \right) d\tau \right)^{1/2} + \sqrt{\frac{C}{n}}.
\]

\[\square\]

**A.5.2 Proof of Lemma 3**

Recalling the definition of \( \Delta_1 \) from Definition 2, to prove the lemma we separately bound the terms \( \sup_f |\Delta_{\mathcal{X}}^{(1)}(f; P_n) - \Delta_{\mathcal{Y}}^{(1)}(f; P)|, \sup_g |\Delta_{\mathcal{Y}}^{(1)}(g; Q_m) - \Delta_{\mathcal{Y}}^{(1)}(g; P)| \), and \( \sup_{f,g} |\Delta_{\mathcal{X,Y}}^{(1)}(f, g; P_n, Q_m) - \Delta_{\mathcal{X,Y}}^{(1)}(f, g; P, Q)| \). For the first, we have

\[
\mathbb{E} \left[ \sup_f \left| \Delta_{\mathcal{X}}^{(1)}(f; P_n) - \Delta_{\mathcal{X}}^{(1)}(f; P) \right| \right] 
\leq \frac{2K}{n} + \mathbb{E} \left[ \sup_f \left| \frac{1}{n(n-1)} \sum_{i \neq j}^n d\mathcal{X}(X_i, X_j) - d\mathcal{Y}(f(X_i), f(X_j)) - \Delta(f; P) \right| \right],
\]

which follows because the summands with \( i = j \) are all 0. Also recall that \( K \) is the bound of diameters of \( \mathcal{X}, \mathcal{Y} \). Denote

\[
h_f(x, x') := |d\mathcal{X}(x, x') - d\mathcal{Y}(f(x), f(x'))| - \Delta_{\mathcal{X}}^{(1)}(f; P),
\]
and note that it is a bounded, symmetric, and centered (w.r.t. $P$) kernel. By Theorem 3.5.3 in (De la Peña and Giné, 2012), we have

$$\mathbb{E} \left[ \sup_f \left| \frac{1}{n(n-1)} \sum_{i \neq j} h_f(X_i, X_j) \right| \right] \leq \mathbb{E} \left[ \sup_f \left| \frac{1}{n(n-1)} \sum_{i \neq j} \epsilon_i h_f(X_i, X_j) \right| \right]$$

where $\{\epsilon_i\}_{i \in \mathbb{N}}$ is a sequence of i.i.d. Rademacher variables, independent of the samples $X_1, \ldots, X_n$. To control the RHS above, we shall apply Dudley’s entropy integral bound to sub-Gaussian processes (see, for example, Theorem 5.22 from Wainwright (2019)). To that end we need a handle on the covering number of the function class $\{h_f : f \in F\}$ w.r.t. the sup-norm. Specifically, we next bound this covering number in terms of that of the original class $\mathcal{F}$. Define

$$A_f := \frac{1}{\sqrt{n(n-1)}} \sum_{i \neq j} \epsilon_i h_f(X_i, X_j),$$

Observe that, conditioned on the samples $X_1, \ldots, X_n$, $A_f$ is sub-Gaussian in $L^2(\hat{P})$ norm where

$$\hat{P} := \frac{1}{n(n-1)} \sum_{i \neq j} \delta_{X_i, X_j},$$

since for any function $h$,

$$\sum_{i=1}^{n} \left( \frac{1}{\sqrt{n(n-1)}} \sum_{j \neq i} h(X_i, X_j) \right)^2 = \sum_{i=1}^{n} \frac{1}{n(n-1)^2} \left( \sum_{j \neq i} h(X_i, X_j) \right)^2 \leq \frac{1}{n(n-1)} \sum_{i \neq j} h(X_i, X_j)^2.$$

Also

$$|A_f - A_{f'}| \leq \frac{1}{n-1} \left( \sum_{i=1}^{n} \left( \sum_{j \neq i} (h_f - h_{f'})(X_i, X_j) \right)^2 \right)^{1/2} \leq \frac{1}{\sqrt{n-1}} \left( \sum_{j \neq i} (h_f - h_{f'})(X_i, X_j)^2 \right)^{1/2} = \sqrt{n} \|h_f - h_{f'}\|_{L^2(\hat{P})}.$$

Further note that $\|h_f - h_{f'}\|_{\infty} \leq 4d_F(f, f')$, hence we see that the covering number of $\{h_f : \mathcal{F}\}$ is bounded by that of $\mathcal{F}$ in $d_F$: $N\{h_f : f \in \mathcal{F}\}, \| \cdot \|_{\infty}, \tau \leq N(\mathcal{F}, d_F, \tau/4)$. By Dudley’s entropy integral bound we have

$$\mathbb{E} \left[ \sup_f \left| \frac{1}{n(n-1)} \sum_{i \neq j} \epsilon_i h_f(X_i, X_j) \right| X_1, \ldots, X_n \right] = \mathbb{E} \left[ \sup_f \frac{A_f}{\sqrt{n}} \left| X_1, \ldots, X_n \right| \right] \leq \inf_{\alpha > 0} \left( \alpha + \frac{1}{\sqrt{n}} \int_{\alpha}^{4K} \sqrt{\log \left( N\{h_f : f \in \mathcal{F}\}, \| \cdot \|_{\infty}, \tau \right)} \, d\tau \right).$$

So

$$\mathbb{E} \left[ \sup_f \left| \frac{1}{n(n-1)} \sum_{i \neq j} h_f(X_i, X_j) \right| \right]$$
we now have
\[
\mathbb{E} \left[ \sup_f \left| \frac{1}{n(n-1)} \sum_{i \neq j}^n \epsilon_i h_f(X_i, X_j) \right| \right]
\]
\[
\leq \inf_{\alpha > 0} \left( \alpha + \frac{1}{\sqrt{n}} \sqrt{\log \left( N \left( \{h_f : f \in \mathcal{F} \}, \|\cdot\|_{\infty, \tau} \right) \right)} \right)
\]
By a similar argument, we also have
\[
\mathbb{E} \left[ \sup_g \left| \Delta^{(1)}_{X,Y}(g; Q_m) - \Delta^{(1)}_{X,Y}(g; Q) \right| \right]
\]
\[
\leq \frac{2K}{m} + \inf_{\alpha > 0} \left( \alpha + \frac{1}{\sqrt{m}} \int_{\alpha}^K \sqrt{\log \left( N(\mathcal{G}, d_{\mathcal{G}}, \tau) \right)} \right).
\]
For the third term, we decouple the samples into several stacks that have the same distribution, and within each stack the points are i.i.d. samples from \( P \otimes Q \). This allows us to apply again the entropy integral bound to each stack of samples. Suppose \( n \leq m \), and consider the samples sets \( \{(X_i, Y_{i+j-1})\}_{i=1}^n \), for \( j = 1, \ldots, m \), where the index of \( Y_{i+j-1} \) is modulo \( m \). Denote \( Z_i^j := (X_i, Y_{i+j-1}) \), for \( i = 1, \ldots, n \) and \( j = 1, \ldots, m \), and further set \( Z^n_j := \{Z_i^j\}_{i=1}^n \). Note that for each \( j = 1, \ldots, m \), the \( Z_j \) comprises \( n \) i.i.d. samples from \( P \otimes Q \). Denoting
\[
h_{f,g}(x,y) := |d_X(x,g(y)) - d_Y(f(x),y)| - \Delta^{(1)}_{X,Y}(f,g; P,Q),
\]
we now have
\[
\mathbb{E} \left[ \sup_{f,g} \left| \Delta^{(1)}_{X,Y}(f,g; P_n, Q_m) - \Delta^{(1)}_{X,Y}(f,g; P,Q) \right| \right] = \mathbb{E} \left[ \sup_{f,g} \left| \frac{1}{nm} \sum_{i=1}^n \sum_{j=1}^m h_{f,g}(X_i, Y_j) \right| \right]
\]
\[
\leq \mathbb{E} \left[ \sup_{f,g} \left| \frac{1}{m} \sum_{j=1}^m \frac{1}{n} \sum_{i=1}^n h_{f,g}(Z_i^j) \right| \right]
\]
\[
\leq \frac{1}{m} \sum_{j=1}^m \mathbb{E} \left[ \sup_{f,g} \left| \frac{1}{n} \sum_{i=1}^n h_{f,g}(Z_i^j) \right| \right]
\]
\[
= \mathbb{E} \left[ \sup_{f,g} \left| \frac{1}{n} \sum_{i=1}^n h_{f,g}(Z_i^1) \right| \right].
\]
Notice that up to a factor of \( \sqrt{n} \), the quantity within the absolute value is an empirical process of \( n \) i.i.d. samples \( \{Z_i^1\}_{i=1}^n \) from \( P \otimes Q \), that is indexed by function class \( \{h_{f,g} : f \in \mathcal{F}, g \in \mathcal{G}\} \). Further note that \( ||h_{f,g} - h_{f,g'}||_{\infty} \leq 2d_F(f, f') + 2d_G(g, g') \), hence the covering number of this function class is bounded as \( N(\{h_{f,g} : f \in \mathcal{F}, g \in \mathcal{G}\}, ||\cdot||_{\infty, \tau}) \leq N(\mathcal{F}, d_F, \tau/4)N(\mathcal{G}, d_G, \tau/4) \). Applying the entropy integral bound (see Lemma 2.14.3 in van der Vaart and Wellner (1996)), we have
\[
\mathbb{E} \left[ \sup_{f,g} \left| \Delta^{(1)}_{X,Y}(f,g; P_n, Q_m) - \Delta^{(1)}_{X,Y}(f,g; P,Q) \right| \right]
\]
\[
\leq \mathbb{E} \left[ \sup_{f,g} \left| \frac{1}{n} \sum_{i=1}^n h_{f,g}(Z_i^1) \right| \right].
\]
\[
\begin{align*}
\lesssim \inf_{\alpha > 0} \left( \alpha + \frac{1}{\sqrt{n}} \int_{\alpha}^{4K} \sqrt{\log (N(\{ h_{f,g} : f \in \mathcal{F}, g \in \mathcal{G} \}, \| \cdot \|_{\infty}, \tau)})} \, d\tau \right) \\
\lesssim \inf_{\alpha > 0} \left( \alpha + \frac{1}{\sqrt{n}} \int_{\alpha}^{K} \sqrt{\log (N(\mathcal{F}, d_\mathcal{F}, \tau)) + \log (N(\mathcal{G}, d_\mathcal{G}, \tau))} \, d\tau \right).
\end{align*}
\]

Combining all 3 terms we have
\[
\mathbb{E} \left[ \sup_{f,g} \| \Delta_1(f, g; P_n, Q_m) - \Delta_1(f, g; P, Q) \| \right] \lesssim \frac{K}{n \wedge m} + \inf_{\alpha > 0} \left( \alpha + \frac{1}{\sqrt{n \wedge m}} \int_{\alpha}^{K} \sqrt{\log (N(\mathcal{F}, d_\mathcal{F}, \tau)) + \log (N(\mathcal{G}, d_\mathcal{G}, \tau))} \, d\tau \right).
\]

\section*{A.6 Special Cases of Theorem 1}

\textbf{Corollary 1} (Special cases). Under the same condition of Theorem 1, further suppose that $\mathcal{X} \subset \mathbb{R}^{d_x}, \mathcal{Y} \subset \mathbb{R}^{d_y}$ are compact, and $k_{\mathcal{X}}, k_{\mathcal{Y}}$ are $L$-Lipschitz in both slots$^5$.

1. For $\mathcal{F} = \text{Lip}_{L_\mathcal{F}}(\mathcal{X}, \mathcal{Y}), \mathcal{G} = \text{Lip}_{L_\mathcal{G}}(\mathcal{Y}, \mathcal{X})$, and $d_x, d_y > 2$, we have
   \[
   \mathbb{E} \left[ \sup_{f,g} \| \Delta_1(f, g; P_n, Q_m) - \Delta_1(f, g; P, Q) \| \right] \lesssim \frac{1}{\mathcal{L}^{2}} + \left( \frac{1}{m} \right)^\frac{1}{2s}.
   \]

2. Consider parametrized classes $\mathcal{F}, \mathcal{G}$. Namely, let $\Theta \subset \mathbb{R}^{k_1}, \Phi \subset \mathbb{R}^{k_2}$ be compact parameter sets with diameters bounded by $K'$. Take $\mathcal{F} = \{ f_\theta : \theta \in \Theta \}$, with $d_{\mathcal{F}}(f_{\theta_1}, f_{\theta_2}) \leq L_\Theta \| \theta_1 - \theta_2 \|$, for some constant $L_\Theta$ and all $\theta_1, \theta_2 \in \Theta$. Suppose analogously for $\mathcal{G} = \{ g_\phi : \phi \in \Phi \}$ and $L_\Phi$. Then
   \[
   \mathbb{E} \left[ \sup_{f,g} \| \Delta_1(f, g; P_n, Q_m) - \Delta_1(f, g; P, Q) \| \right] \lesssim \frac{1}{\mathcal{L}^{2}} + \left( \frac{1}{m} \right)^\frac{1}{2s}.
   \]

The proof of Corollary 1 employs the 1-Wasserstein distance, as defined next.

\textbf{Definition 11} (1-Wasserstein distance). The 1-Wasserstein distance between $P, Q \in \mathcal{P}(\mathcal{X})$ is
\[
\mathcal{W}_1(P, Q) := \inf_{\pi \in \Pi(P, Q)} \int_{\mathcal{X} \times \mathcal{X}} \| x - y \| \, d\pi(x, y),
\]
where $\Pi(P, Q)$ is the set of couplings of $P$ and $Q$.

We also make use of the following technical lemma.

\textbf{Lemma 4}. Under the assumptions of Corollary 1, and take $\mathcal{F} = \text{Lip}_{L_\mathcal{F}}(\mathcal{X}, \mathcal{Y}), \mathcal{G} = \text{Lip}_{L_\mathcal{G}}(\mathcal{Y}, \mathcal{X})$, we have
\[
\mathbb{E} \left[ \sup_{f,g} \| \Delta_1(f, g; P_n, Q_m) - \Delta_1(f, g; P, Q) \| \right] \lesssim (L_{\mathcal{F}} + 1) \mathbb{E}[\mathcal{W}_1(P, P_n)] + (L_{\mathcal{G}} + 1) \mathbb{E}[\mathcal{W}_1(Q, Q_m)],
\]
\[
\mathbb{E} \left[ \sup_{g} \| \mu_x g_{\tau} Q - \mu_x g_{\tau} Q_m \|_{\mathcal{H}_x} \right] \leq \sqrt{2LL_\mathcal{G}} \mathbb{E}[\mathcal{W}_1(Q, Q_m)],
\]
\[
\mathbb{E} \left[ \sup_{f} \| \mu_y f_{\tau} P - \mu_y f_{\tau} P_n \|_{\mathcal{H}_y} \right] \leq \sqrt{2LL_\mathcal{F}} \mathbb{E}[\mathcal{W}_1(P, P_n)].
\]

$^5$Namely, $|k_{\mathcal{X}}(x_1, x'_1) - k_{\mathcal{X}}(x_2, x'_2)| \leq L(d_{\mathcal{F}}(x_1, x_2) + d_{\mathcal{F}}(x'_1, x'_2))$, and similarly for $k_{\mathcal{Y}}.
Proof. We first give bounds for $\Delta_{X,Y}^{(1)}$, $\Delta_{X,Y}^{(1)}$, $\Delta_{X,Y}^{(1)}$, using the coupling trick, i.e. we treat integration of different variables as marginals of a joint distribution, and optimize over all such choice with the chosen marginals. This leads to the 1-Wasserstein distance in the resulting bound. For any $\pi \in \Pi(P_m^{\otimes 2}, P^{\otimes 2})$ we have

$$\Delta_{X,Y}^{(1)}(f; P_m) - \Delta_{X,Y}^{(1)}(f; P) = \int |d_X(x, x') - d_Y(f(x), f(x'))| - |d_X(w, w') - d_Y(f(w), f(w'))| \, d\pi(x, x', w, w').$$

Consequently, we may infimize over $\pi \in \Pi(P_m^{\otimes 2}, P^{\otimes 2})$ to obtain

$$\Delta_{X,Y}^{(1)}(f; P_m) - \Delta_{X,Y}^{(1)}(f; P) = \inf_{\pi} \int |d_X(x, x') - d_Y(f(x), f(x'))| - |d_X(w, w') - d_Y(f(w), f(w'))| \, d\pi(x, x', w, w')$$

$$\leq \inf_{\pi} \int |d_X(x, x') - d_X(w, w')| + |d_Y(f(x), f(x')) - d_Y(f(w), f(w'))| \, d\pi(x, x', w, w')$$

$$\leq \inf_{\pi} \int d_X(x, w) + d_X(x', w') + d_Y(f(x), f(w)) + d_Y(f(x'), f(w')) \, d\pi(x, x', w, w')$$

$$\leq \inf_{\pi} \int d_X(x, w) + d_X(x', w') + L_F d_X(x, w) + L_F d_X(x', w') \, d\pi(x, x', w, w')$$

$$= 2(L_F + 1)W_1(P, P_m),$$

where $W_1$ is the 1-Wasserstein distance. The last line is because the minimum is achieved by $\pi^{\otimes 2}$ where $\pi$ is the 1-Wasserstein optimal coupling between $P_m$ and $P$, hence

$$\mathbb{E}\left[|\Delta_{X,Y}^{(1)}(f; P_m) - \Delta_{X,Y}^{(1)}(f; P)|\right] \leq 2(L_F + 1)\mathbb{E}[W_1(P, P_m)].$$

A similar derivation applies to $\Delta_{Y}^{(1)}$. For $\Delta_{X,Y}^{(1)}$, abbreviate the coupling set notation as $\Pi_{n,m} := \Pi(P_n \otimes Q_m, P \otimes Q)$ and consider:

$$\Delta_{X,Y}^{(1)}(f, g; P_m, Q_m) - \Delta_{X,Y}^{(1)}(f, g; P, Q) = \inf_{\pi \in \Pi_{n,m}} \int |d_X(x, g(y)) - d_Y(f(x), y)| - |d_X(x', g(y')) - d_Y(f(x'), g(y'))| \, d\pi(x, x', y, y')$$

$$\leq \inf_{\pi \in \Pi_{n,m}} \int d_X(x, x') + d_Y(y, y') + d_X(g(y), g(y')) + d_Y(f(x), f(x')) \, d\pi(x, x', y, y')$$

$$\leq \inf_{\pi \in \Pi_{n,m}} \int d_X(x, x') + d_Y(y, y') + L_G d_Y(y, y') + L_F d_X(x, x') \, d\pi(x, x', y, y')$$

$$= (L_F + 1)W_1(P, P_m) + (L_G + 1)W_1(Q, Q_m).$$

So we have

$$\mathbb{E}\left[\sup_{f,g} |\Delta_1(f, g; P_m, Q_m) - \Delta_1(f, g; P, Q)|\right] \lesssim (L_F + 1)\mathbb{E}[W_1(P, P_m)] + (L_G + 1)\mathbb{E}[W_1(Q, Q_m)].$$

For the MMD terms we use the same method:

$$\|\mu_X g_{\sharp} Q - \mu_X g_{\sharp} Q_m\|_{H_X}^2 = \int k_X(x, x') \, d(g_{\sharp} Q - g_{\sharp} Q_m)(x) \, d(g_{\sharp} Q - g_{\sharp} Q_m)(x')$$

$$= \int k_X(g(y), g(y')) \, dQ(y) \, dQ(y')$$
\[ + \int k_X(g(w), g(w')) \, dQ_m(w) \, dQ_m(w') - \int 2k_X(g(y), g(w)) \, dQ(y) \, dQ_m(w) \leq \inf_{\pi \in \Pi(Q, Q_m)} \int 2Ld_X(g(y), g(w)) \, d\pi(y, w) \leq 2LL_{\pi} \inf_{\pi \in \Pi(Q, Q_m)} \int dy(y, w) \, d\pi(y, w) = 2LL_{\pi}W_1(Q, Q_m). \]

Similarly we have \[ \sup \| \mu_y f_z P - \mu_y f_z P_n \|_{\tilde{W}_1}^2 \leq 2LL_{\pi}W_1(P, P_n), \] which concludes the proof. \hfill \Box

**Proof of Corollary 1.** We still adopt the same decomposition in proof of Theorem 1, but bound each term explicitly. We first prove part 1. For simplicity we apply Lemma 4 instead of the general claim in Theorem 1. Combined with the fact that \( \mathbb{E}[W_1(P, P_n)] \leq n^{-1/d_x} \) for \( d_x > 2 \) (see, e.g., Weed and Bach 2019), we have the overall rate of convergence is

\[ \mathbb{E} \left[ \| \text{UD}_{k_y, k_X}^P(P) - \text{UD}_{k_y, k_X}^P(P_n) \|_{Q_m} \right] \leq \lambda_y \sqrt{\mathcal{L}_x} \left( \frac{1}{n} \right)^{\frac{1}{\alpha}} + \lambda_x \sqrt{\mathcal{L}_y} \left( \frac{1}{m} \right)^{\frac{1}{\alpha}} + (\mathcal{L}_x + 1) \left( \frac{1}{m} \right)^{\frac{1}{\alpha}} \]

\[ + (\mathcal{L}_y + 1) \left( \frac{1}{m} \right)^{\frac{1}{\alpha}} + \lambda timeStamp \sqrt{\mathcal{C}} \frac{\sqrt{\mathcal{C}}}{n} + \lambda_y \sqrt{\mathcal{C}} \frac{\sqrt{\mathcal{C}}}{m}. \]

For part 2, notice that the entropy integral is finite when taking \( \alpha = 0 \). Following Theorem 1, we know that the rate in terms of \( m, n \) is bounded by \( (n \wedge m)^{-1/2} \), with a multiplicative constant depending on \( \lambda_x, \lambda_y, \mathcal{L}_x, \mathcal{L}_y, \mathcal{C}, \mathcal{K}, \mathcal{K}', k_1, k_2 \). \hfill \Box

**Remark 6.** For part one in Corollary 1, recall that Weed and Bach 2019 claims

\[ \mathbb{E}[W_1(P, P_n)] \lesssim \begin{cases} n^{-1/2}, & d_x = 1 \\ n^{-1/2} \log(1 + n), & d_x = 2. \end{cases} \]

One can easily adapt the bound to the case where \( d_x \) or \( d_y \) is no larger than 2. The bounds obtained in Corollary 1 for Lipschitz classes, although they use different proof techniques, they essentially lead to similar rates in \( m, n \) to the ones obtained by simply applying the general bound in Theorem 1.

### A.7 Continuity of the Functional \( \mathcal{L} \)

Recall that \( \mathcal{L}_{P, Q}(f, g) := \lambda_x \mathbb{MMD}_X(P, g_t Q) + \lambda_y \mathbb{MMD}_Y(f_z P, Q) + \Delta_1(f, g; P, Q) \).

**Proposition 3.** Suppose \( \mathcal{F}, \mathcal{G} \) are Lipschitz subclasses with Lipschitz constants \( \mathcal{L}_x, \mathcal{L}_y \) respectively, and kernels \( k_X, k_Y \) are Lipschitz on both slots with constant \( L \). We have the continuity of \( \mathcal{L} \) in all of its arguments:

\[ |\mathcal{L}_{P, Q}(f, g) - \mathcal{L}_{P', Q'}(f', g')| \leq \lambda_x \mathbb{MMD}_X(P, P') + \lambda_y \mathbb{MMD}_Y(Q, Q') + \lambda_z \mathbb{MMD}_X(g_t P, Q) + \lambda_y \mathbb{MMD}_Y(f_z P, f_z P') + 3(1 + \mathcal{L}_x)W_1(P, P') + 3(1 + \mathcal{L}_y)W_1(Q, Q') + (2L \lambda_x + 3)d_{\mathcal{F}}(f, f') + (2L \lambda_y + 3)d_{\mathcal{G}}(g, g'). \]
Proof of Proposition 3. We prove separately for the MMD and $\Delta$.

$$\left| \text{MMD}_X(P, g_\sharp Q) - \text{MMD}_X(P', g'_\sharp Q') \right|$$

$$= \left| \| \mu_X P - \mu_X g_\sharp Q \|_{H_X} - \| \mu_X P' - \mu_X g'_\sharp Q' \|_{H_X} \right|$$

$$\leq \text{MMD}_X(P, P') + \| \mu_X g_\sharp Q' - \mu_X g_\sharp Q \|_{H_X}$$

$$\leq \text{MMD}_X(P, P') + 2d_G(g, g') + \text{MMD}_X(g_\sharp Q, g'_\sharp Q').$$

Also for any coupling $\pi(x, x', w, w')$ of $P \otimes P$ and $P' \otimes P'$

$$\left| \Delta^{(1)}_X(f; P) - \Delta^{(1)}_X(f'; P') \right|$$

$$\leq \int d_X(x, w) + d_X(x', w') + d_Y(f(x), f'(w)) + d_Y(f(x'), f'(w')) \, d\pi(x, x', w, w')$$

$$\leq 2d_F(f, f') + \int (1 + L_F)d_X(x, w) + (1 + L_F)d_X(x', w') \, d\pi(x, x', w, w').$$

And similarly for any coupling $\eta(x, y, x', y')$ of $P \otimes Q$ and $P' \otimes Q'$

$$\left| \Delta^{(1)}_{X,Y}(f, g; P, Q) - \Delta^{(1)}_{X,Y}(f', g'; P', Q') \right|$$

$$\leq \int d_X(x, x') + d_Y(y, y') + d_X(g(y), g'(y')) + d_Y(f(x), f'(x')) \, d\eta(x, y, x', y')$$

$$\leq d_F(f, f') + d_G(g, g') + \int (1 + L_F)d(x, x') + (1 + L_G)d(y, y') \, d\eta(x, y, x', y').$$

Apply the same coupling trick as in the previous section, we have

$$\left| \Delta_1(f, g; P, Q) - \Delta_1(f', g'; P', Q') \right|$$

$$\leq \left| \Delta^{(1)}_X(f; P) - \Delta^{(1)}_X(f'; P') \right| + \left| \Delta^{(1)}_Y(f; P) - \Delta^{(1)}_Y(f'; P') \right|$$

$$+ \left| \Delta^{(1)}_{X,Y}(f, g; P, Q) - \Delta^{(1)}_{X,Y}(f', g'; P', Q') \right|$$

$$\leq 3d_F(f, f') + 3d_G(g, g') + 3(1 + L_F)W_1(P, P') + 3(1 + L_G)W_1(Q, Q'),$$

which concludes the proof. \qed
B Experiments

B.1 Algorithm

Algorithm 1 Cycle consistent Monge map computation

Require: $X \in \mathbb{R}^{n \times d}$, $Y \in \mathbb{R}^{m \times d}$. $\alpha$, the learning rate. $\theta$, the batchsize.

while $\theta$ has not converged do
  Sample $\{x_i\}_{i=1}^b$ a batch from the rows of $X$, forming $P_b$.
  Sample $\{y_i\}_{i=1}^b$ a batch from the rows of $Y$, forming $Q_b$.
  $v \leftarrow \nabla_{\theta} \mathcal{L}_{P_b, Q_b}(f_{\theta}, g_w)$
  $u \leftarrow \nabla_w \mathcal{L}_{P_b, Q_b}(f_{\theta}, g_w)$
  $\theta \leftarrow \text{Adam}(v, \theta, \alpha)$
  $w \leftarrow \text{Adam}(u, w, \alpha)$
end while

return $(f_{\theta}, g_w)$.

B.2 Additional High Dimensional Experiments on Unaligned Word Embeddings

We present here an additional experiment for alignment of word embedding spaces (see Alvarez-Melis and Jaakkola (2018) for experiment details), which demonstrates the applicability of GMMD method to higher dimensional scenarios. Specifically, we consider words from English and French that are embedded into 300 dimensional spaces. We apply our GMMD method to obtain mappings between these two spaces, and obtain correspondence by searching for the nearest neighbor. We verify how well the learned mappings align these spaces by checking how many words in the English-French dictionary are correctly matched. The word embedding data sets are from Bojanowski et al. (2016), and dictionaries are from Conneau et al. (2017).

For training we use the 20k most frequent words, and learning rate 0.01. The kernel is a single Gaussian kernel with bandwidth 1, and $\lambda = 0.01$. Batchsize is 500, and we train the NNs for 1000 epochs. The NNs are both single linear layer without bias. See Table 4 for comparison with the GW method (Alvarez-Melis and Jaakkola, 2018) and the MUSE method (Conneau et al., 2017). The MUSE method outperforms GMMD and GW on this task. GMMD matching is not far behind the GW method.

Note that the MUSE method uses a linear orthonomal mapping that maps only in one direction as follows:

$$\min_{U, U^\top = I_d} \sup_{f \in \mathcal{F}} \mathbb{E}_P f(UX) - \mathbb{E}_Q f(x).$$

(in fact MUSE uses a GAN objective to learn the witness function $f$ and not an IPM objective as we present it here). Mémoli and Needham (2021) showed that this form of the MUSE algorithm is related to the Gromov-Monge distance (Section A.3 in Mémoli and Needham (2021)). As Conneau et al. (2017) pointed out, learning the kernel or the discriminator is advantageous for the word alignment task. We believe that GMMD will benefit from learning the kernels similar to MUSE in order to further improve its performance. The min-max formulation of GMMD with learned kernels (Equation (5)) is left for future work in terms of analysis and practical implementations.

B.3 Comparison to GW and UGW

We present full results of the comparison between continuous GMMD mappings and discrete GW Barycentric Mappings. In Figure 4 we illustrate the results for different $\lambda$ and 4 cases: heart vs.
rotated/scaled/embedded heart, and biplanes. For each test case we present both the image of the learned mappings and the cycle consistency of the mappings. Figure 5 contains results for the same test cases, using barycentric mapping from entropic GW. The parameter $\epsilon$ in Figure 5 corresponds to the entropic regularizer.

We also provide full tables of the quantitative behavior of GMMD and GW on the test cases. In Table 5 to 16, the marginal MMDs and $\Delta$ for GMMD, GW and UGW are computed across different parameters respectively. For GMMD we use $\lambda = 10^{-3} \times 2^{0,1,\ldots,9}$; for GW we use entropic regularizer $\epsilon = 5 \times 10^{0,1,2,3,4}$; for UGW we use entropic regularizer $10^{\{-2,-1,0,1\}}$. For GW and UGW we only list results for hyperparameters that don’t fail using POT Flamary et al. (2021) and UGW’s code of Séjourné et al. (2020).

Table 4: Word matching performance comparison.

|            | EN to FR | FR to EN |
|------------|----------|----------|
| GMMD       | 76.1%    | 74.5%    |
| GW ($\epsilon = 10^{-4}$) | 79.3%    | 78.3%    |
| Alvarez-Melis and Jaakkola (2018) | 81.3%    | 78.9%    |
| GW ($\epsilon = 10^{-5}$) | 82.3%    | 82.1%    |
| MUSE       | 82.3%    | 82.1%    |
| Conneau et al. (2017) | 82.3%    | 82.1%    |

Figure 4: Learned continuous GMMD Mappings and their cycle consistency in shape matching. First row: heart ($P$) and rotated heart ($Q_b$). Second row: heart ($P$) and scaled heart ($Q_c$). Third row: heart ($P$) and embedded heart ($Q_d$). Last row: biplanes.
Figure 5: GW Barycentric Mappings. First row: heart ($P$) and rotated heart ($Q_b$). Second row: heart ($P$) and scaled heart ($Q_b$). Third row: heart ($P$) and embedded heart ($Q_b$). Last row: biplanes.

Table 5: Evaluation of GMMD mappings between heart ($P$) and rotated heart ($Q_b$).

| $\lambda$ | GMMMD | $\text{MMD}_Y$ | $\text{MMD}_X$ | $\Delta$ |
|-----------|-------|----------------|----------------|-------|
| 0.512     | 1.33  | 0.0524         | 0.00207        | 2.50  |
| 0.256     | 0.0794| 0.0294         | 0.0294         | 0.0801|
| 0.128     | 0.00825| 4.94e-4        | 4.05e-4        | 0.0574|
| 0.064     | 0.00776| 0.00227        | 0.00190        | 0.0560|
| 0.032     | 0.0924| 2.90e-4        | 0.00386        | 2.76  |
| 0.016     | 0.0579| 0.00137        | 3.33e-4        | 3.51  |
| 0.008     | 0.0136| 0.00188        | 0.00181        | 1.24  |
| 0.004     | 8.04e-4| 2.85e-4        | 2.55e-4        | 0.0661|
| 0.002     | 0.00624| 0.00149        | 0.00147        | 1.64  |
| 0.001     | 0.00378| 0.00118        | 0.00114        | 1.47  |

B.4 Amortization

To illustrate the performance of the trained GMMD maps on unseen data, we push 8000 new datapoints through the learned networks. Note that GMMD was trained on only 4000 points. The output of the pushforward maps on unseen data points during training is shown in Figure 6. We see that GMMD maps successfully generalizes to unseen data. We also quantitatively demonstrate the amortization in Table 17 to 20, where for the same set of parameters $\lambda$ as previously, we push the 8000 new points through the NNs (trained with 4000 points), and compute the resulting marginal MMDs and $\Delta$. As is shown in the tables, the MMDs remain small which means the marginals are well matched.
Table 6: GW and its induced MMDs and $\Delta$ between heart ($P$) and rotated heart ($Q_b$).

| $\epsilon$ | GW   | MMD$_X$ | MMD$_Y$ | $\Delta$ |
|------------|------|---------|---------|---------|
| 0.0005     | 0.00134 | 0.00420 | 0.00299 | 0.696   |
| 0.005      | 0.00660 | 0.127   | 0.116   | 1.73    |
| 0.05       | 0.0424  | 0.615   | 0.613   | 6.69    |
| 0.5        | 0.0686  | 3.99    | 4.12    | 22.9    |
| 5          | 0.0699  | 4.86    | 4.89    | 26.2    |

Table 7: UGW and its induced MMDs and $\Delta$ between heart ($P$) and rotated heart ($Q_b$).

| $\epsilon$ | UGW  | MMD$_X$ | MMD$_Y$ | $\Delta$ |
|------------|------|---------|---------|---------|
| 10         | 0.277856 | 5.00562 | 5.00562 | 25.8038 |
| 1          | 0.199544  | 4.96044 | 4.96038 | 25.6224 |
| 0.1        | 0.189629  | 4.57678 | 4.57691 | 24.0855 |
| 0.01       | 0.178746  | 3.34716 | 3.34713 | 19.1421 |

Table 8: Evaluation of GMMD mappings between biplanes.

| $\lambda$ | GMMD | MMD$_X$ | MMD$_Y$ | $\Delta$ |
|-----------|------|---------|---------|---------|
| 0.512     | 0.315 | 0.124   | 0.124   | 0.131   |
| 0.256     | 0.284 | 0.125   | 0.125   | 0.134   |
| 0.128     | 0.0270 | 0.00704 | 0.00669 | 0.104   |
| 0.064     | 0.0166 | 0.00594 | 0.00619 | 0.0691  |
| 0.032     | 0.127 | 0.00891 | 0.00947 | 3.40    |
| 0.016     | 0.0267 | 0.00892 | 0.00812 | 0.602   |
| 0.008     | 0.0357 | 0.00637 | 0.00548 | 2.98    |
| 0.004     | 0.0243 | 0.00305 | 0.00532 | 3.98    |
| 0.002     | 0.0115 | 0.00343 | 0.00252 | 2.79    |
| 0.001     | 0.0116 | 0.00397 | 0.00409 | 3.58    |

Table 9: GW and its induced MMDs and $\Delta$ between biplanes.

| $\epsilon$ | GW   | MMD$_X$ | MMD$_Y$ | $\Delta$ |
|------------|------|---------|---------|---------|
| 5          | 0.0699 | 4.86    | 4.89    | 26.2    |
| 0.5        | 0.0686 | 3.99    | 4.12    | 22.9    |
| 0.05       | 0.0424 | 0.615   | 0.613   | 6.68    |
| 0.005      | 0.00660 | 0.127  | 0.116   | 1.73    |
| 0.0005     | 0.00134 | 0.00420 | 0.00299 | 0.696   |

31
Table 10: UGW and its induced MMDs and $\Delta$ between biplanes.

| $\epsilon$ | UGW  | $\text{MMD}_X$ | $\text{MMD}_Y$ | $\Delta$  |
|------------|------|----------------|----------------|----------|
| 10         | 0.277856 | 5.00562       | 5.00562       | 25.8038  |
| 1          | 0.199544 | 4.96044       | 4.96038       | 25.6224  |
| 0.1        | 0.189629 | 4.57678       | 4.57691       | 24.0855  |
| 0.01       | 0.178746 | 3.34716       | 3.34713       | 19.1421  |

Table 11: Evaluation of GMMD mappings between heart ($P$) and scaled heart ($Q_c$).

| $\lambda$ | GMMD | $\text{MMD}_X$ | $\text{MMD}_Y$ | $\Delta$  |
|-----------|------|----------------|----------------|----------|
| 0.512     | 0.0362 | 0.00145       | 0.00150       | 0.0649   |
| 0.256     | 0.0148 | 0.00144       | 0.00147       | 0.0464   |
| 0.128     | 0.0675 | 0.0247        | 0.0251        | 0.139    |
| 0.064     | 0.00640 | 0.00139    | 0.00145       | 0.0556   |
| 0.032     | 0.0961 | 0.000462      | 0.000444      | 2.85     |
| 0.016     | 0.000201 | 0.000612   | 0.000598      | 0.0500   |
| 0.008     | 0.0281 | 0.00137       | 0.00137       | 2.96     |
| 0.004     | 0.00869 | 0.00108      | 0.00215       | 1.36     |
| 0.002     | 0.0104 | 0.00106       | 0.00128       | 4.03     |
| 0.001     | 0.00506 | 0.000304    | 0.00159       | 3.17     |

Table 12: GW and its induced MMDs and $\Delta$ between heart ($P$) and scaled heart ($Q_c$).

| $\epsilon$ | GW  | $\text{MMD}_X$ | $\text{MMD}_Y$ | $\Delta$  |
|------------|-----|----------------|----------------|----------|
| 5          | 0.0776 | 5.00          | 5.00          | 25.8     |
| 0.5        | 0.0770 | 4.93          | 4.93          | 25.5     |
| 0.05       | 0.0498 | 0.483         | 0.483         | 5.89     |
| 0.005      | 0.00483 | 0.00307     | 0.00307       | 0.378    |
| 0.0005     | 0.000470 | 0.000227   | 0.000227      | 0.0833   |

Table 13: UGW and its induced MMDs and $\Delta$ between heart ($P$) and scaled heart ($Q_c$).

| $\epsilon$ | UGW | $\text{MMD}_X$ | $\text{MMD}_Y$ | $\Delta$  |
|------------|-----|----------------|----------------|----------|
| 10         | 2.47 | 4.09           | 4.84           | 23.6     |
| 1          | 1.79 | 3.02           | 4.28           | 20.4     |
| 0.1        | 1.50 | 2.90           | 4.22           | 20.0     |
Table 14: Evaluation of GMMD mappings between heart ($P$) and embedded heart ($Q_d$).

| $\lambda$ | GMMD | $\text{MMD}_{X^*}$ | $\text{MMD}_{Y^*}$ | $\Delta$ |
|-----------|-------|---------------------|---------------------|---------|
| 0.512     | 0.0532 | 0.00157             | 0.00151             | 0.0979  |
| 0.256     | 0.0625 | 0.0256              | 0.0255              | 0.0446  |
| 0.128     | 0.0146 | 0.00177             | 0.00154             | 0.0881  |
| 0.064     | 0.00612| 0.00145             | 0.00148             | 0.0500  |
| 0.032     | 0.0942 | 0.00179             | 0.00338             | 2.78    |
| 0.016     | 0.0204 | 0.00222             | 0.00213             | 1.00    |
| 0.008     | 0.0345 | 0.00152             | 0.00194             | 3.88    |
| 0.004     | 0.0186 | 0.00152             | 0.00117             | 3.97    |
| 0.002     | 0.00229| 0.000984            | 0.000964            | 0.172   |
| 0.001     | 0.00683| 0.00143             | 0.00131             | 4.09    |

Table 15: GW and its induced MMDs and $\Delta$ between heart ($P$) and embedded heart ($Q_d$).

| $\epsilon$ | GW    | $\text{MMD}_{X^*}$ | $\text{MMD}_{Y^*}$ | $\Delta$ |
|-------------|-------|---------------------|---------------------|---------|
| 5           | 0.0776| 5.00                | 5.00                | 25.8    |
| 0.5         | 0.0770| 4.93                | 4.93                | 25.5    |
| 0.05        | 0.0498| 0.483               | 0.483               | 5.89    |
| 0.005       | 0.00483| 0.00307             | 0.00307             | 0.378   |
| 0.0005      | 0.000470| 0.000227            | 0.000227            | 0.0833  |

Table 16: UGW and its induced MMDs and $\Delta$ between heart ($P$) and embedded heart ($Q_d$).

| $\epsilon$ | UGW   | $\text{MMD}_{X^*}$ | $\text{MMD}_{Y^*}$ | $\Delta$ |
|-------------|-------|---------------------|---------------------|---------|
| 10          | 0.278 | 5.01                | 5.01                | 25.8    |
| 1           | 0.200 | 4.96                | 4.96                | 25.6    |
| 0.1         | 0.190 | 4.58                | 4.58                | 24.1    |
| 0.01        | 0.179 | 3.35                | 3.35                | 19.1    |

Figure 6: GMMD amortization. Each pair shows the image through the learned GMMD mapping. The pairs from left to right: heart ($P$) vs. rotated/scaled/embedded heart ($Q_b/Q_c/Q_d$), and biplanes. All 4 cases here are trained with $\lambda = 0.064$. 
Table 17: GMMD amortization between heart ($P$) and rotated heart ($Q_b$).

| $\lambda$ | GMMD | $\text{MMD}_X$ | $\text{MMD}_Y$ | $\Delta$ |
|-----------|------|----------------|----------------|---------|
| 0.512     | 1.33 | 5.43e-02       | 1.67e-03       | 2.49    |
| 0.256     | 0.0731 | 0.0262       | 0.0262         | 0.0809  |
| 0.128     | 0.00790 | 0.000276     | 0.000215       | 0.0579  |
| 0.064     | 0.00711 | 0.00199      | 0.00152        | 0.0564  |
| 0.032     | 9.34e-02 | 1.46e-04     | 4.86e-03       | 2.76    |
| 0.016     | 5.72e-02 | 7.75e-04     | 1.82e-04       | 3.51    |
| 0.008     | 0.0148 | 0.00242       | 0.00243        | 1.24    |
| 0.004     | 0.000568 | 0.000162     | 0.000141       | 0.0660  |
| 0.002     | 0.00675 | 0.00174       | 0.00173        | 1.64    |
| 0.001     | 4.91e-03 | 1.70e-03     | 1.73e-03       | 1.47    |

Table 18: GMMD amortization between heart ($P$) and scaled heart ($Q_c$).

| $\lambda$ | GMMD | $\text{MMD}_X$ | $\text{MMD}_Y$ | $\Delta$ |
|-----------|------|----------------|----------------|---------|
| 0.512     | 0.0347 | 0.000555      | 0.000856       | 0.0650  |
| 0.256     | 0.0133 | 0.000599      | 0.000787       | 0.0466  |
| 0.128     | 0.0708 | 0.0261        | 0.0268         | 0.139   |
| 0.064     | 0.00488 | 0.000577     | 0.000716       | 0.0561  |
| 0.032     | 9.68e-02 | 3.00e-04     | 5.05e-03       | 2.86    |
| 0.016     | 0.00153 | 0.000366      | 0.000361       | 0.0501  |
| 0.008     | 2.83e-02 | 1.60e-03     | 3.23e-03       | 2.94    |
| 0.004     | 0.00952 | 0.00210       | 0.00196        | 1.37    |
| 0.002     | 1.19e-02 | 1.76e-03     | 2.01e-03       | 4.05    |
| 0.001     | 4.89e-03 | 1.75e-04     | 1.59e-03       | 3.12    |

Table 19: GMMD amortization between heart ($P$) and embedded heart ($Q_d$).

| $\lambda$ | GMMD | $\text{MMD}_X$ | $\text{MMD}_Y$ | $\Delta$ |
|-----------|------|----------------|----------------|---------|
| 0.512     | 0.0518 | 0.000721      | 0.000717       | 0.0985  |
| 0.256     | 0.0657 | 0.0272        | 0.0271         | 0.0446  |
| 0.128     | 0.0133 | 0.00126       | 0.000716       | 0.0885  |
| 0.064     | 0.00431 | 0.000566     | 0.000516       | 0.0504  |
| 0.032     | 9.38e-02 | 1.52e-03     | 3.98e-03       | 2.76    |
| 0.016     | 0.0198 | 0.00199       | 0.00194        | 0.990   |
| 0.008     | 3.52e-02 | 1.62e-03     | 2.77e-03       | 3.85    |
| 0.004     | 1.96e-02 | 1.92e-03     | 1.93e-03       | 3.95    |
| 0.002     | 0.00287 | 0.00131       | 0.00122        | 0.173   |
| 0.001     | 6.89e-03 | 1.48e-03     | 1.34e-03       | 4.07    |
Table 20: GMMD amortization between biplanes.

| $\lambda$ | GMD  | MMD$_X$ | MMD$_Y$ | $\Delta$ |
|-----------|------|---------|---------|---------|
| 0.512     | 0.316| 0.123   | 0.124   | 0.134   |
| 0.256     | 0.283| 0.124   | 0.124   | 0.137   |
| 0.128     | 0.0274| 0.00664| 0.00660| 0.111   |
| 0.064     | 0.0165| 0.00596| 0.00636| 0.0658  |
| 0.032     | 0.127 | 0.00852| 0.00953| 3.40    |
| 0.016     | 0.0291| 0.00995| 0.00953| 0.600   |
| 0.008     | 0.0367| 0.00666| 0.00627| 2.97    |
| 0.004     | 2.33e-02| 2.83e-03| 4.58e-03| 3.98   |
| 0.002     | 1.13e-02| 3.31e-03| 2.30e-03| 2.83    |
| 0.001     | 1.21e-02| 3.96e-03| 4.51e-03| 3.60    |