Statistical Optimal Transport posed as Learning Kernel Embedding

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Abstract

This work takes the novel approach of posing the statistical Optimal Transport (OT) problem as that of learning the transport plan’s kernel mean embedding. The key advantage is that the estimates for the embeddings of the marginals can now be employed directly, leading to a dimension-free sample complexity for the proposed transport plan and transport map estimators. Also, because of the implicit smoothing in the kernel embeddings, the proposed estimators can perform out-of-sample estimation. Interestingly, the proposed formulation employs an MMD based regularization to avoid overfitting, which is complementary to existing ϕ-divergence (entropy) based regularization techniques. An appropriate representer theorem is presented that leads to a fully kernelized formulation and hence the same formulation can be used to perform continuous/semi-discrete/discrete OT in any non-standard domain (as long as universal kernels in those domains are known). Finally, an ADMM based algorithm is presented for solving the kernelized formulation efficiently. Empirical results show that the proposed estimator outperforms discrete OT based estimator in terms of transport map accuracy.

1 Introduction

Optimal Transport is proving to be an increasingly successful tool in solving diverse machine learning problems. Recent research shows that variants of Optimal Transport (OT) achieve state-of-the-art performance in various machine learning (ML) applications such as domain adaptation \cite{8}, NLP \cite{2, 34, 35}, robust learning \cite{6}, to name a few. It is also shown that OT based metrics serve as good loss functions in both supervised \cite{13} and unsupervised \cite{17} learning. \cite{28} is a comprehensive monologue on the subject with focus on recent developments related to machine learning.

Given two marginal distributions over source and target domains, and a cost function between elements of the domains, the OT problem is that of finding the joint distribution whose marginals are equal to the given marginals, and which minimizes the expected cost with respect to this joint distribution. Since continuous domains are ubiquitous in machine learning applications, the source and target marginals often turn out to be continuous. Moreover, in typical ML applications, only samples from these distributions are given rather than the marginal distributions. This setting is referred to as the statistical continuous OT setting. Also, in applications like domain adaptation \cite{8} and ecological inference \cite{25}, etc., estimates for the optimal solution, which is known as the transport plan, are desirable and merely estimating the optimal objective value is not sufficient. In this work, we focus on the important problem of consistently estimating the transport plan (and thereby estimating the so-called transport map) in the statistical continuous OT setting. A popular estimation strategy is to employ sample based plug-in estimates for the marginals. This reduces the continuous OT problem to a discrete OT problem. Since extremely efficient solvers exist for discrete OT \cite{9, 11}, most existing ML applications employ the discrete OT based estimator. However, the sample complexity of the discrete OT based estimation is plagued with the curse of dimensionality \cite{10}. On the other hand, alternate estimators that have attractive sample complexities are not well-studied \cite{16, 15, 12}. In fact, \cite{15} observes this to be a major bottleneck in applying continuous OT to high-dimensional ML problems and propose appropriate regularization. However, their results (e.g., theorem 3 in \cite{15}) show that the curse of dimensionality is not completely removed, especially if accurate solutions are desired. Empirical results in \cite{11} refer Figures 4 and 5] confirm that the quality of the solution degrades very quickly with entropic regularization, which currently is the most popular regularization scheme.

This work takes the novel approach of posing the statistical OT problem as that of learning the kernel mean embedding \cite{23} of the transport plan using the estimates of the marginal embeddings. This is advantageous because the estimates for the kernel mean embeddings are known to have sample complexities that are dimension-free. Moreover, kernel embeddings also provide implicit smoothness to the marginal estimates. Interestingly, we show that the proposed estimate for the embedding of the transport plan is statistically consistent with a sample complexity that remains dimension-free. The other key aspect of the proposed learning formulation is that it avoids overfitting by regularizing with MMD distances. This nicely complements existing works like \cite{13, 22}, which employ ϕ-divergence based regularization. Lastly, out-of-the-sample estimation for the transport plan and transport map can be performed with the proposed methodology. To the best of our knowledge, existing estimators neither have sample complexities that are completely dimension-free nor can perform out-of-sample estimation.

We present an appropriate representer theorem that guarantees finite characterization for the embedding learning problem and leads to a fully kernelized formulation. Thus the same formulation can be used for all variants of OT: continuous, semi-discrete, and discrete, merely by switching the kernel between the Kronecker delta and the Gaussian kernels. More importantly, it can be used to solve OT problems on non-standard domains using appropriate kernels \cite{7}. On passing we note that though there are existing works that employ kernels in context of OT \cite{16, 36, 26}, none of them use the notion of kernel embedding of distributions.
We also present an alternating direction method of multipliers (ADMM) based algorithm for efficiently solving the proposed formulation. From the optimal solution the transport plan and map can be retrieved. By considering the special cases where analytical solutions for the continuous OT problem are known, it is empirically demonstrated that the proposed estimate for the transport map outperforms the discrete OT based estimate.

We formulate and discuss the main technical results of this work in Section 2 and the empirical results in the Section 3.

We conclude by summarizing in Section 4.

2 Proposed OT Formulations and Estimators

Let \( \mathcal{X}, \mathcal{Y} \) be any two sets that form locally compact Hausdorff topological spaces. We denote the set of all Radon probability measures over \( \mathcal{X} \) by \( \mathcal{M}^1(\mathcal{X}) \); whereas we denote the set of strictly positive measures by \( \mathcal{M}^1_+(\mathcal{X}) \). Let \( c : \mathcal{X} \times \mathcal{Y} \) denote a function that evaluates the cost between elements in \( \mathcal{X}, \mathcal{Y} \) and let \( p_s \in \mathcal{M}^1_+(\mathcal{X}), p_t \in \mathcal{M}^1_+(\mathcal{Y}) \). Then, the Kantorovich’s Optimal Transport (OT) formulation \([20]\) is:

\[
\begin{align*}
\min_{\pi \in \mathcal{M}^1(\mathcal{X}, \mathcal{Y})} & \quad \int c(x, y) \, d\pi(x, y), \\
\text{s.t.} & \quad \pi_X = p_s, \, \pi_Y = p_t,
\end{align*}
\]

where \( \pi_X, \pi_Y \) denote the marginal measures of \( \pi \) over \( \mathcal{X}, \mathcal{Y} \) respectively. An optimal solution of (1) is referred to as an optimal transport plan or optimal coupling. The optimal objective turns out to be the 1-Wasserstein metric between the marginals, provided the cost \( c \) itself is a metric. For reasons discussed earlier, we desire to reformulate (1) in terms of relevant kernel embeddings rather than the measures themselves.

2.1 Kernel Embedding based OT

Let \( k_1, k_2 \) be characteristic kernels \([14, 33]\) defined over \( \mathcal{X}, \mathcal{Y} \) respectively. By definition, the key advantage of a characteristic kernel is that the mapping between kernel mean embeddings and \( \mathcal{M}^1 \) becomes one-to-one (injective). For discrete probability measures, the Kronecker Delta kernel is characteristic, while for others, the Gaussian kernel is an example of a characteristic kernel\(^1\) if the underlying topological space is Euclidean. Moreover, the Gaussian is also a universal kernel over Euclidean domains. Let \( \phi_1, \phi_2 \) and \( \mathcal{H}_1, \mathcal{H}_2 \) denote the canonical feature maps and RKHS corresponding to the kernels \( k_1, k_2 \) respectively. Let \( \langle \cdot, \cdot \rangle_{\mathcal{H}_i}, \| \cdot \|_{\mathcal{H}_i} \) denote the default inner-product, norm in the RKHS \( \mathcal{H}_i \). Let \( \mu_s \equiv \mathbb{E}_{X \sim p_s} [\phi_1(X)], \, \mu_t \equiv \mathbb{E}_{Y \sim p_t} [\phi_2(Y)] \) denote the kernel mean embeddings of the marginals \( p_s, p_t \) respectively. Let \( \Sigma_{ss} \equiv \mathbb{E}_{X \sim p_s} [\phi_1(X) \otimes \phi_1(X)] \) and \( \Sigma_{tt} \equiv \mathbb{E}_{Y \sim p_t} [\phi_2(Y) \otimes \phi_2(Y)] \) denote the auto-covariance embeddings of \( p_s, p_t \) respectively.

We now begin re-writing (1) solely in terms of the kernel embeddings. Since the variable, \( \pi \), is a joint measure, the cross-covariance operator, \( \mathcal{U}^T = \mathbb{E}_{(X,Y) \sim \pi} [\phi_1(X) \otimes \phi_2(Y)] \), is the suitable kernel mean embedding to be employed. However, the constraints involve the marginals of \( \pi \), whose embeddings cannot be retrieved from the cross-covariance operator alone. Hence we also employ the conditional embedding operators, \( \mathcal{U}_1^T, \mathcal{U}_2^T \), which embed the conditionals \( \pi_{Y/X}(\cdot|\cdot) \) and \( \pi_{X/Y}(\cdot|\cdot) \) respectively. The relations between these operators and the marginal embeddings are given by \([33]\):

\[
\mathcal{U} = \Sigma_{ss} \mathcal{U}_1^T = \mathcal{U}_2 \Sigma_{tt}, \quad \mathcal{U}_1 \mu_s = \mu_t, \quad \mathcal{U}_2 \mu_t = \mu_s.
\]

\[\text{(2)}\]

The former two equations follow from the definition of conditional embeddings, and the later two equations follow from the kernel sum rule.

In order to re-write the objective using the above operators, we assume that \( c(x, \cdot) \in \mathcal{H}_2 \, \forall \, x \in \mathcal{X} \) and \( c(\cdot, y) \in \mathcal{H}_1 \, \forall \, y \in \mathcal{Y} \). These assumptions are trivially true if the domains are discrete. However, in case of continuous domains they need not be true, in general. Hence we additionally assume that kernel corresponding to a continuous domain is universal and that the cost function is continuous in that variable. Note that these are very mild conditions as universal kernels are well-studied and known for non-standard domains too \([2]\). It then follows that a continuous function like \( c(x, \cdot), c(\cdot, y) \) can be arbitrarily closely approximated\(^2\) by elements in \( \mathcal{H}_2, \mathcal{H}_1 \). Henceforth, we understand that \( c(x, \cdot) \) (or \( c(\cdot, y) \)) denotes either the exact function (if possible) or the (arbitrarily) close approximation of it. With these assumptions\(^3\) the objective in (1) can be written as:

\[
\mathbb{E} \left[ c(X, Y) \right] = \mathbb{E}_{X \sim p_s} \left[ \mathbb{E}_{Y/X} \left[ c(X, Y)/X \right] \right],
\]

by reproducing property is \( = \mathbb{E}_{X \sim p_s} \left[ \mathbb{E}_{Y/X} \left[ c(X, \cdot, \phi_2(Y))_{\mathcal{H}_2}/X \right] \right] \), and using linearity of expectation and the definition of conditional embedding we have it equal to \( \mathbb{E}_{X \sim p_s} \left[ \langle c(X, \cdot), \mathcal{U}_1 \phi_2(Y) \rangle_{\mathcal{H}_1} \right] \).

Like-wise, the objective is also \( \equiv \mathbb{E}_{Y \sim p_t} \left[ \langle c(\cdot, Y), \mathcal{U}_2 \phi_1(X) \rangle_{\mathcal{H}_1} \right] \). This leads to the following kernel embedding formulation for

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\(^1\)For reasons that will be clear later, for continuous domains, we insist on universal kernels rather than characteristic kernels. If a kernel is universal then it is also characteristic, but the converse need not be true.

\(^2\)This follows from the definition of universality of the kernel.

\(^3\)Following \([18]\) these assumptions may be further relaxed.
\[ \min_{\mathbf{U}, \mathbf{U}_1, \mathbf{U}_2} \frac{1}{2} \mathbb{E}_{X \sim p_x} \left[ \langle c(X, \cdot), \mathbf{U}_1 \phi_1(X) \rangle_{\mathcal{H}_2} \right] \\
\quad + \frac{1}{2} \mathbb{E}_{Y \sim p_y} \left[ \langle c(\cdot, Y), \mathbf{U}_2 \phi_2(Y) \rangle_{\mathcal{H}_1} \right] \\
\text{s.t.} \\
\mathbf{U}_1 \mu_s = \mu_s, \quad \mathbf{U}_2 \mu_t = \mu_s, \\
\mathbf{U} = \Sigma_s \mathbf{U}_1^\top = \mathbf{U}_2 \Sigma_t, \\
\mathbf{U} \in \mathcal{E} (\mathcal{H}_2, \mathcal{H}_1), \quad \mathbf{U}_1 \in \mathcal{E} (\mathcal{H}_1, \mathcal{H}_2), \quad \mathbf{U}_2 \in \mathcal{E} (\mathcal{H}_2, \mathcal{H}_1), \]

where \( \mathcal{E} (\mathcal{H}_1, \mathcal{H}_2) \) is the set of all linear operators from \( \mathcal{H}_1 \) to \( \mathcal{H}_2 \), and \( \mathcal{E}(\mathcal{H}_2, \mathcal{H}_1) = \{ \mathbf{U} \in \mathcal{E}(\mathcal{H}_2, \mathcal{H}_1) \mid \exists \mathbf{Y} \in \mathcal{M}^t (X, Y) \ni \mathbf{U} = \mathbb{E}_{X,Y} [\phi_1(X) \otimes \phi_2(Y)] \} \) is the set of all valid cross-covariance operators. The equivalence of (3) and (1) follows from the one-to-one correspondence between the measures involved and their kernel embeddings, which is guaranteed by the characteristic kernels and from the crucial embedding characterizing constraint: \( \mathbf{U} \in \mathcal{E} (\mathcal{H}_2, \mathcal{H}_1) \). Without this characterizing constraint, the formulation is not meaningful.

Note that both terms in the objective are equal. Nevertheless both are included to preserve symmetry, which has implications in the statistical estimation setup presented later. More importantly, though it is clear that two of the three operators \( \mathbf{U}, \mathbf{U}_1, \mathbf{U}_2 \) can be eliminated, we critically preserve all of them in (3) as they facilitate efficient regularization in the statistical estimation set-up and lead to efficient algorithms (as will be shown later). However, the characterization of embedding, \( \mathcal{E} (\mathcal{H}_1, \mathcal{H}_2) \), is included only for the cross-covariance as the conditionals are well-defined given the cross-covariance, auto-covariance and marginal embeddings.

The main advantage of the proposed formulation (3) over (1) is that estimates for kernel mean embeddings of the marginals can be employed directly. Since the empirical estimates of kernel embeddings are known to have sample complexities that are independent of dimensions, it is expected that (3) will be more appropriate in the statistical OT setting.

### 2.2 Learning Kernel Embedding for OT

In the setting of statistical OT, the marginals \( p_s, p_t \) are unknown; however, iid samples from them are given: let \( D_x = \{ x_1, \ldots, x_m \} \) denote the set of \( m \) iid samples from \( p_s \) and let \( D_y = \{ y_1, \ldots, y_n \} \) denote \( n \) iid samples from \( p_t \). Also, the cost function is known only at the data sample points.

A popular way to estimate the optimal plan in (1) is to simply employ the sample based plug-in estimates for the marginals: \( \hat{\mu}_s = \frac{1}{m} \sum_{i=1}^m \delta_{x_i} \) and \( \hat{\mu}_t = \frac{1}{n} \sum_{j=1}^n \delta_{y_j} \), in place of the true (unknown) marginals. In such a case, (1) simplifies as the following discrete OT problem:

\[ \min_{\pi \in \mathbb{R}^{m \times n}} \sum_{i=1}^m \sum_{j=1}^n c(x_i, y_j) \pi_{ij}, \]

\[ \text{s.t.} \quad \pi \mathbf{1} = \frac{1}{m} \mathbf{1}, \quad \pi^\top \mathbf{1} = \frac{1}{n} \mathbf{1}, \quad \pi \geq 0, \]

where \( \mathbf{0}, \mathbf{1} \) denote vectors/matrices with all entries as zero, unity respectively (of appropriate dimension). Since it is well-known that the sample complexity of (4) in estimating (1) is not acceptable for high-dimensional domains, alternative estimation methods are sought after.

In this work, we plan to employ the standard estimates for the kernel mean embeddings of the marginals in the proposed formulation (3). Since these estimates are known to have sample complexities that are independent of dimension, we find them more appropriate for statistical OT.

To this end, let estimated marginal kernel mean embeddings be denoted by: \( \hat{\mu}_s = \frac{1}{m} \sum_{i=1}^m \phi_1(x_i) \) and \( \hat{\mu}_t = \frac{1}{n} \sum_{j=1}^n \phi_2(y_j) \). Likewise, the estimates of the auto-covariance embeddings are given by \( \hat{\Sigma}_{ss} = \frac{1}{m} \sum_{i=1}^m \phi_1(x_i) \otimes \phi_1(x_i) \) and \( \hat{\Sigma}_{tt} = \frac{1}{n} \sum_{j=1}^n \phi_2(y_j) \otimes \phi_2(y_j) \). Let \( \hat{c}(x_i, \cdot), \hat{c}(\cdot, y_j) \) denote the sample based approximations of the cost function that are exact at the sample data points, and obtained via the least square solution: \( \hat{c}(x_i, \cdot) = \sum_{j=1}^n \rho_{ij} \phi_2(y_j) \) leads to: \( \rho_{ij} = G_2^{-1} c(x_i, y_j) \), where \( G_2 \) is the gram-matrix induced by \( \mathbf{k}_2 \) over \( D_y \). Like-wise, \( \hat{c}(\cdot, y_j) = \sum_{i=1}^m \sigma_{ji} \phi_1(x_i) \) leads to: \( \sigma_{ji} = G_1^{-1} c(x_i, y_j) \). Employing these estimates in (3) results in:

\[ \min_{\mathbf{U}, \mathbf{U}_1, \mathbf{U}_2} \frac{1}{2m} \sum_{i=1}^m \sum_{j=1}^n \rho_{ij} \langle \phi_2(y_j), \mathbf{U}_1 \phi_1(x_i) \rangle \\
+ \frac{1}{2n} \sum_{j=1}^n \sum_{i=1}^m \sigma_{ji} \langle \phi_1(x_i), \mathbf{U}_2 \phi_2(y_j) \rangle \\
\text{s.t.} \\
\left\| \mathbf{U} - \hat{\Sigma}_{ss} \mathbf{U}_1 \right\|_{\mathcal{H}_2 \oplus \mathcal{H}_1} \leq \epsilon_1, \quad \left\| \mathbf{U} - \hat{\Sigma}_{tt} \mathbf{U}_2 \right\|_{\mathcal{H}_2 \oplus \mathcal{H}_1} \leq \epsilon_2, \\
\mathbf{U} \in \mathcal{E} (\mathcal{H}_2, \mathcal{H}_1), \quad \mathbf{U}_1 \in \mathcal{L} (\mathcal{H}_1, \mathcal{H}_2), \quad \mathbf{U}_2 \in \mathcal{L} (\mathcal{H}_2, \mathcal{H}_1), \]

\[ \text{Typical formulae in embedding literature write } \hat{\mu}_i, \hat{\mu}_j \text{ in terms of } \mu. \]

\[ \text{Here, } \delta \text{ denotes the Dirac delta function.} \]

\[ \text{One may also employ other sophisticated estimates like } [24] \text{ and carry out derivations accordingly.} \]

\[ \text{Universal kernels are strictly pd, and hence any gram-matrix induced by them is invertible. Also, gram-matrices induced by the Kronecker delta are invertible, as the induced gram-matrices are always Identity matrices.} \]
where $\| \cdot \|_{\mathcal{H}_2 \otimes \mathcal{H}_1}$ is the Hilbert-Schmidt operator norm, $\Delta_1, \Delta_2, \epsilon_1, \epsilon_2$ are regularization hyper-parameters introduced to prevent overfitting to the estimates. As, $\Delta_i$ decreases, the regularization decreases and $\Delta_i = 0$ recovers the case where estimates of marginal mean embeddings and auto-covariances are exactly matched, which may lead to overfitting. Efficient estimates are possible with the right amount of regularization. Also, as mentioned earlier, $\mathcal{U}_1, \mathcal{U}_2$ are guaranteed to be valid conditional embeddings only as $\Delta_i, \epsilon_i \to 0$. Hence, we suggest $\Delta_i, \epsilon_i = o\left( \frac{1}{\sqrt{\min(m,n)}} \right)$, following known sample complexities for the marginal embedding estimates, which are $O \left( \frac{1}{\sqrt{m}} \right)$, $O \left( \frac{1}{\sqrt{n}} \right)$ respectively. Since the kernel embedding estimates have sample complexities that are independent of dimension, it is expected that the statistical estimation error with the proposed formulation $\mathcal{E}$ is also independent of dimensionality, which is formalized in the following theorem:

**Theorem 1.** Let $g(\tilde{\mu}_s, \tilde{\mu}_t, \tilde{\Sigma}_{ss}, \tilde{\Sigma}_{tt})$ denote the optimal objective of $\mathcal{E}$. Let us assume that there exist some $m_0 \in \mathbb{N}, n_0 \in \mathbb{N}$ such that the feasible $\mathcal{U}_1, \mathcal{U}_2$ are valid conditional embeddings, for all $m \geq m_0, n \geq n_0$. Since $\mathcal{U} \in \mathcal{E}(\mathcal{H}_2, \mathcal{H}_1)$ such $m_0, n_0$ should exist for low enough regularization hyper-parameters $\epsilon_1, \epsilon_2$. For any fixed set of such low enough hyper-parameters, with high probability, $\left| g(\tilde{\mu}_s, \hat{\mu}_t, \hat{\Sigma}_{ss}, \hat{\Sigma}_{tt}) - g(\mu_s, \mu_t, \Sigma_{ss}, \Sigma_{tt}) \right| \leq O \left( \frac{1}{\sqrt{\min(m,n)}} \right)$.

Thus by appropriate regularization one can obtain consistent estimators by solving $\mathcal{E}$. Note that the proposed regularization in $\mathcal{E}$ is based on the so-called MMD distances between the kernel embeddings, which is in strict contrast with the popular entropic regularization $\mathcal{B}$, or $\phi$-divergence based regularization $\mathcal{D}$ [22]. While the dependence on dimensionality is adversely exponential with entropic regularization, if accurate solutions are desired [15], MMD based regularization leads to dimension-free estimation.

Interestingly, $\mathcal{E}$ admits a finite parameterization (see theorem 2). Consequently, $\mathcal{E}$ is equivalent to $\mathcal{B}$, which is completely kernelized:

$$\begin{align*}
\min_{\alpha, \beta, \gamma} & \sum_{i=1}^{m} \frac{1}{2m} \text{tr}(\mathcal{C} \beta G_1) + \frac{1}{2n} \text{tr}(\mathcal{C}^T \gamma G_2), \\
\text{s.t.} & \frac{1}{m^2} \mathbf{1}^T \beta \mathbf{1}^T G_2 \beta \mathbf{1} - \frac{2}{mn} \mathbf{1}^T G_2 \beta \mathbf{1} + \frac{1}{m^2} \mathbf{1}^T G_2 \mathbf{1} \leq \Delta_1^2, \\
& \frac{1}{n^2} \mathbf{1}^T \gamma \mathbf{1}^T G_2 \gamma \mathbf{1} - \frac{2}{mn} \mathbf{1}^T \gamma \mathbf{1}^T G_2 \mathbf{1} + \frac{1}{m^2} \mathbf{1}^T \gamma \mathbf{1} \leq \Delta_2^2, \\
& \langle \alpha G_1 - \frac{1}{m} \gamma G_2, \alpha G_2 - \frac{1}{m} \beta G_2 \rangle_F \leq \epsilon_1^2, \\
& \langle \alpha G_2 - \frac{1}{n} \gamma G_2, \alpha G_1 - \frac{1}{n} \beta G_2 \rangle_F \leq \epsilon_2^2,
\end{align*}$$

where $\mathcal{C}_{m \times n}$ is the cost matrix with $i j^{th}$ entry as $c(x_i, y_j)$. The proof of this theorem follows from representation theorem kind of arguments and is detailed in $\mathcal{B}$.

**Theorem 2.** Whenever $\mathcal{E}$ is solvable, there exists an optimal solution, $\mathcal{U}^*, \mathcal{U}_1^*, \mathcal{U}_2^*$, of $\mathcal{E}$ such that $\mathcal{U}^* = \sum_{i=1}^{m} \sum_{j=1}^{n} \alpha_{ij} \phi_1(x_i) \phi_2(y_j), \mathcal{U}_1^* = \sum_{i=1}^{m} \sum_{j=1}^{n} \beta_{ij} \phi_2(y_j) \phi_1(x_i), \mathcal{U}_2^* = \sum_{i=1}^{m} \sum_{j=1}^{n} \gamma_{ij} \phi_1(x_i) \phi_2(y_j)$, for some $\alpha, \beta, \gamma \in \mathbb{R}^{m \times n}$.

The key challenge now is to characterize the set $\mathcal{S} = \{ \alpha \in \mathbb{R}^{m \times n} \mid \mathcal{U}^* \in \mathcal{E}(\mathcal{H}_2, \mathcal{H}_1) \}$ leading to computationally tractable constraints. If both the domains are discrete, then the characterization is very easy, leading to $\alpha \geq 0, \mathbf{1}^T \alpha \mathbf{1} \leq 1$. Unfortunately, when domains are continuous, computationally efficient characterization is indeed very challenging. For example, a necessary constraint for $\alpha \in \mathcal{S}$ is $\langle \phi_1(x) - \mu_1, \mathcal{U}^* \phi_2(y) \rangle \geq 0, \forall x, y \in \mathcal{X}_1, \mathcal{Y}_1$. This is because $\langle \phi_1(x), \mathcal{U}^* \phi_2(y) \rangle = \mathbb{E}_{(x,y) \sim \mathcal{P}} [k_1(x, X)k_2(y, Y)] \geq \min_{x', y' \in \mathcal{X}_1, \mathcal{Y}_1} k_1(x, x')k_2(y, y') = 0$. The last equality is true for normalized Universal kernels (like Gaussian). Characterizing non-negative functions in Gaussian RKHS in a computationally tractable way is itself known to be a difficult problem [3, 27]. Hence, usually relaxation based techniques are employed, which ensure non-negative functions are induced; however some non-negative functions may be missed.

We critically note here that the characterizing conditions for the discrete case, $\alpha \geq 0, \mathbf{1}^T \alpha \mathbf{1} = 1$, turn out to be asymptotically necessary. This follows from arguments detailed in section $\mathcal{C}$. Also, it is easy to see that these conditions are always sufficient for inducing valid joint embeddings. Thus we replace $\mathcal{U}^* \in \mathcal{E}(\mathcal{H}_2, \mathcal{H}_1)$ by $\alpha \geq 0, \mathbf{1}^T \alpha \mathbf{1} = 1$. To summarize the above discussion, the approximation error with this substitution may not be zero at finite samples, but asymptotically it is guaranteed that the approximation error is zero. This leads to our final kernel embedding learning formula for $\text{OT}$.

\[\text{[22]}\] show that MMD and $\phi$-divergence based regularization have completely different properties.
which is one of the key technical contributions of this work:

\[
\begin{align*}
\min_{\alpha, \beta, \gamma \in \mathbb{R}^{m \times n}} & \quad \frac{1}{2m} tr(C\beta G_1) + \frac{1}{2n} tr(C^T \gamma G_2), \\
\text{s.t.} & \quad \frac{1}{m^2} 1^T G_1 \beta G_2 \beta G_1 1 - \frac{2}{mn} 1^T G_2 \beta G_1 1 + \frac{1}{m^2} 1^T G_2 1 \leq \Delta_1^2 , \\
& \quad \frac{1}{n^2} 1^T G_2 \gamma G_1 \gamma G_2 1 - \frac{2}{mn} 1^T G_1 \gamma G_2 1 + \frac{1}{n^2} 1^T G_1 1 \leq \Delta_2^2 , \\
& \quad \langle G_1 \alpha - \frac{1}{m} G_1^2 \beta^T, \alpha G_2 - \frac{1}{m} G_1 \beta^T \rangle_F \leq \epsilon_1^2 , \\
& \quad \langle \alpha G_2 - \frac{1}{n} \gamma G_2^2, \alpha G_1 - \frac{1}{n} \gamma G_1 \gamma G_2 \rangle_F \leq \epsilon_2^2 , \\
& \quad \alpha \geq 0, 1^T \alpha 1 = 1, \beta \geq 0, \gamma \geq 0.
\end{align*}
\]

We additionally include the constraints \( \beta \geq 0, \gamma \geq 0 \) so that \( \beta, \gamma \) are less prone to inducing invalid conditional eddentials in the finite sample case. Note that the additional constraints do not effect the estimation and approximation errors.

Once the proposed formulation (7) is solved, it can be either used to (consistently) estimate the optimal transport plan using methods like [19, 29]. Or more importantly, one can estimate the transport map at any \( x \in \mathcal{X} \) as \( \arg\min_{y \in \mathcal{Y}} \mathbb{E}[c(y, Y) / x] = \arg\min_{y \in \mathcal{Y}} \langle c(y, \cdot), U_1^T \phi_1 (x) \rangle = \arg\min_{y \in \mathcal{Y}} \sum_{j=1}^n \left( c(y, y_j) \sum_{j=1}^n (\beta_{yj}^T k_1(x_i, x_j)) \right) \) (8)

The additional constraints \( \beta \geq 0, \gamma \geq 0 \) in (7) also ensure that the inference problem (8) turns out to be that of finding the Karcher mean [21], whenever the cost is a metric etc. More importantly, unlike existing estimators, (8) can be used to infer the optimal map at out-of-sample data points too.

As discussed earlier, the objective of the proposed formulation can be made as low or high as possible by changing the regularization parameters. Hence the quality of the transport map computed using the inference formula (8) is a better way of evaluating the goodness of our proposed estimator than by merely evaluating the objective (7).

We summarize the key features of the proposed estimator that make it especially attractive for machine learning applications. As far as we know, all these features are unique to our estimator: (i) (7) provides statistically consistent estimators with a sample complexity that is independent of dimensionality. (ii) Our estimator can perform out-of-sample inference using (8). We empirically show that out-of-sample performance is very competitive. (iii) The same formulation (7) can be used to solve any OT variant: continuous, semi-discrete, and discrete by merely choosing the right kernel. Moreover, in the special case where \( k_1, k_2 \) are Kronecker Delta, and all regularization hyper-parameters are zero, (7) is exactly same as (4). (iv) Using universal kernels on non-standard domains [7], the proposed formulation can be used to solve OT problems in such domains too.

2.3 Algorithms

The proposed formulation (7) turns out to be a convex quadratically constrained linear program, which can be solved using existing solvers. Also, in the special case \( \epsilon_1 = 0, \epsilon_2 = 0 \) simplifies as (9), which can be solved by existing solvers more efficiently:

\[
\begin{align*}
\min_{\alpha \in \mathbb{R}^{m \times n}} & \quad tr(\alpha C^T), \\
\text{s.t.} & \quad 1^T \alpha^T G_1 \alpha 1 - \frac{2}{m} 1^T \alpha^T G_1 1 + \frac{1}{m^2} 1^T G_1 1 \leq \Delta_1^2 , \\
& \quad 1^T \alpha G_2 \alpha^T 1 - \frac{2}{n} 1^T \alpha G_2 1 + \frac{1}{n^2} 1^T G_2 1 \leq \Delta_2^2 , \\
& \quad (G_1^{-1} \alpha) \geq 0, 1^T \alpha 1 = 1 \\
& \quad (\alpha G_2^{-1}) \geq 0, \alpha \geq 0.
\end{align*}
\]

Interestingly, it turns out that the structure in (7) can be further exploited to derive extremely fast ADMM based solvers. We begin by noting that \( \epsilon_1 = 0 \) leads to the constraints \( \alpha = \frac{1}{m} \gamma G_2 = \frac{1}{m} G_1 \beta^T \). Replacing the corresponding regularization terms in (7) by these equations and re-writing in Tikhonov form leads to:

\[
\begin{align*}
\min_{\alpha \in \mathbb{A}_{m \times n}, \beta, \gamma \in \mathbb{R}^{m \times n} \geq 0} & \quad F_1(\beta) + F_2(\gamma) \\
\text{s.t.} & \quad \alpha = \frac{1}{m} G_1 \beta^T, \alpha = \frac{1}{n} \gamma G_2
\end{align*}
\]

9Consider the special regularization, \( \epsilon_1 = 0, \Delta_1 = \Delta_2, \) and the Tikhonov regularized form: \( \min_{U \in \mathcal{U}_2} \mathbb{E}[c(\cdot, \cdot), U] + \lambda \|U \Sigma_u^{-1} \mu_\beta - \mu\|_{\mathcal{H}_2} + \lambda \|U \Sigma_u^{-1} \mu_\gamma - \mu\|_{\mathcal{H}_2} \). Since this resembles the Hillinger-Kantorovich metrics [22] (when cost is squared-Euclidean), we conjecture that our optimal objective in this special case/form may be more meaningful than in the current form. However, we postpone such connections (if any) to future work.
We evaluate the performance of our estimator for transport map (8) on the problem of learning the optimal transport map between two multivariate Gaussian distributions. The optimal transport map between two Gaussian distributions $g_{\text{source}} = N(m_1, \Sigma_1)$ and $g_{\text{target}} = N(m_2, \Sigma_2)$ with squared Euclidean cost is given by

$$T : x \mapsto m_2 + A(x - m_1).$$  

where $A_n = \{x \in \mathbb{R}^n \mid x \geq 0, 1^T x 1 = 1\}$, $F_1(\beta) \equiv \frac{1}{2m} tr(C\beta G_1) + \lambda_1 \left( \frac{1}{m^2} 1^T G_1 \beta^T G_2 \beta G_1 1 - \frac{2}{m^2} 1^T G_2 \beta G_1 1 \right)$, where $\lambda_1$ is the regularization hyper-parameter corresponding to $\lambda_1$, $F_2(\gamma) \equiv \frac{1}{2n} tr(C^T \gamma G_2) + \lambda_2 \left( \frac{1}{n^2} 1^T G_2 \gamma G_1 \gamma G_2 1 - \frac{2}{n^2} 1^T G_1 \gamma G_2 1 \right)$, where $\lambda_2$ is the regularization hyper-parameter corresponding to $\lambda_2$. The above form makes it very attractive for employing the ADMM algorithm for three reasons: i) the natural consensus form, ii) the constraints in terms of $\alpha, \beta, \gamma$ variables (apart from the consensus constraints) are simple and motivate efficient mirror descent based solvers for the ADMM updates iii) the consensus in [10] needs to be applied only via regularization (and not an exact match), which is naturally facilitated in the ADMM updates. The updates for the ADMM are summarized below:

$$\beta^{(k+1)} \equiv \arg\min_{\beta \geq 0} F_1(\beta) + tr(D_1^{(k)^T} \beta) + \frac{\rho}{2} \|\alpha^{(k)} - \frac{1}{m} G_1 \beta^T \|^2$$  

(11)

$$\gamma^{(k+1)} \equiv \arg\min_{\gamma \geq 0} F_2(\gamma) + tr(D_2^{(k)^T} \gamma) + \frac{\rho}{2} \|\alpha^{(k)} - \frac{1}{n} \gamma \|^2$$  

(12)

$$\alpha^{(k+1)} \equiv \arg\min_{\alpha \in A_{mn}} - tr \left( \left(D_1^{(k)} + D_2^{(k)}\right) \alpha \right) + \frac{\rho}{2} \left( \|\alpha - \frac{1}{m} G_1 \beta^{(k+1)^T} \|^2 + \|\alpha - \frac{1}{n} \gamma^{(k+1)} G_2 \|^2 \right)$$  

(13)

\[D_1^{(k+1)} = D_1^{(k)} + \rho \left( \frac{1}{m} G_1 \beta^{(k+1)^T} - \alpha^{(k+1)} \right)\]

\[D_2^{(k+1)} = D_2^{(k)} + \rho \left( \frac{1}{n} \gamma^{(k+1)} G_2 - \alpha^{(k+1)} \right)\]

Note that (11) can be efficiently solved using the mirror descent algorithm.

### 3 Experiments

We evaluate the performance of our estimator for transport map (8) on the problem of learning the optimal transport map between two multivariate Gaussian distributions. The optimal transport map between two Gaussian distributions $g_{\text{source}} = N(m_1, \Sigma_1)$ and $g_{\text{target}} = N(m_2, \Sigma_2)$ with squared Euclidean cost is given by

$$T : x \mapsto m_2 + A(x - m_1).$$  

(14)
average out-of-sample MSE

where $A = \Sigma_1^{-\frac{1}{2}}(\Sigma_1^\dagger \Sigma_2 \Sigma_1^\dagger)^\frac{1}{2} \Sigma_1^{-\frac{1}{2}}$. We compare the proposed estimator \( (8) \) in terms of the deviation from the optimal transport map \( (14) \).

**Data generation:** We consider mean zero Gaussian distributions with unit-trace covariances in our experiments. The covariance matrices are computed as $\Sigma_1 = V_1 V_1^T/\|V_1\|_F$ and $\Sigma_2 = V_2 V_2^T/\|V_2\|_F$, where $V_1 \in \mathbb{R}^{d \times d}$ and $V_2 \in \mathbb{R}^{d \times d}$ are generated randomly from uniform distribution. We next sample $m$ and $n$ data points from $g_{\text{source}}$ and $g_{\text{target}}$ distributions, respectively. In our experiments, we consider $d \in \{5, 10, 50, 100, 500, 1000\}$, $m \in \{10, 20, 50, 100, 150, 200\}$, and set $n = m$ for simplicity.

**Algorithm details:** We employ Gaussian kernels, $k(x, z) = \exp(-\|x - z\|^2/2\sigma^2)$, in our approach and experiment with different bandwidth $\sigma$. Our initial experiments indicate that suitable values of $\sigma$ include those that does not yield very high condition number of the Gram matrices (i.e., the Gram matrices are not ill-conditioned). In our setup, in general, the condition number of the Gram matrices increase with $\sigma$ for a fixed $d$ and decrease with $d$ for a fixed $\sigma$. The regularization parameters are set to $\Delta_1^2 = (1^T G_1 1)/100m^2$ and $\Delta_2^2 = (1^T G_2 1)/100m^2$. As a baseline, we also report the results obtained from the discrete OT estimator, henceforth referred to as EMD, learned via the discrete OT problem \( (4) \).

**Evaluation:** For a given data point $x_i$ from the source distribution, a transport map estimator maps $x_i$ to a data point $x_t$ in the target distribution. Such a mapping obtained from the optimal transport map \( (14) \) is considered as the ground truth. The proposed estimator \( (8) \) and the EMD are evaluated in terms of the mean squared error from the ground truth. For each $(d, m)$, we randomly sample five sets of data points from the same source-target distribution pair, learn the estimators on each of the five sets, evaluate the estimators on the corresponding set, and report the average MSE over the five sets.

**Results:** The results are reported in Figure 1. We observe that the proposed estimator obtains lower average MSE (and hence better estimation of the transport map) than EMD across different number of samples $m$ and dimensions $d$. The advantage of the proposed estimator over EMD is more pronounced at higher dimension.

**Out-of-sample prediction:** We also evaluate our estimator’s ability to learn the mapping for out-of-sample data points by sampling additional $m_{\text{out}} = 200$ data points from the source distributions in the above experiments. These data points are not used to learn the estimator and are only used for evaluation during the inference stage. As before, we evaluate the mean squared error (MSE) with respect to the optimal estimator \( (14) \). The baseline EMD cannot perform inference on out-of-sample data points.

The results are reported in Figure 2. We observe that the performance on out-of-sample data points are similar to the
corresponding in-sample data points (reported in Figure 1). In addition, the average out-of-sample MSE generally decreases with increasing number of samples since a better estimator is learned with more number of samples. Overall, the results illustrate the utility of the proposed approach for out-of-sample inference.

4 Summary

The idea of employing kernel embeddings of distributions in OT seems promising, especially in the continuous case. It not only leads to sample complexities that are dimension-free, but also provides a new regularization scheme based on MMD distances, which is complementary to existing ϕ-divergence based regularization. Empirical results show that the improvement over discrete OT based estimator in terms of MSE in the induced transport map can be as high as around 40%.

A Proof for Theorem 1

Proof. We begin by noting that the feasibility set of (5) is bounded. This is because: i) the set $E(\mathcal{H}_2, \mathcal{H}_1)$ is bounded. This is true as $\mathcal{U} \in E(\mathcal{H}_2, \mathcal{H}_1) \Rightarrow$ there exists $p \in M^1(\mathcal{X} \times \mathcal{Y})$ such that $\|\mathcal{U}\| = \|E(\mathcal{X}, Y) \rightarrow p \|\phi_1(\mathcal{X}) \otimes \phi_2(Y)\| \leq E(\mathcal{X}, Y) \rightarrow p \|\phi_1(\mathcal{X}) \otimes \phi_2(Y)\| = 1$. The first inequality follows from Jensen's inequality and the second equality is true for any bounded kernel like Gaussian and the Kronecker Delta. ii) By triangle inequality, $||\mathcal{U}|| - ||\hat{\Sigma}_{ss}\mathcal{U}_1|| \leq ||\mathcal{U} - \hat{\Sigma}_{ss}\mathcal{U}_1^\top|| \leq \epsilon_i^2$. This shows that the set of all feasible $\mathcal{U}$ is bounded, since $\mathcal{U}$ is itself bounded in the feasibility set. Now, since $\text{maxeig}(\hat{\Sigma}_{ss}) = \text{maxeig}(G) / n \leq \text{tr}(G) / n = 1$ (again true for Kronecker and Gaussian kernels), we obtain that set of all feasible $\mathcal{U}_1$ is bounded. Similarly, set of all feasible $\mathcal{U}_2$ is bounded. Now consider the Tikhonov regularized form of (5). Then, one of the term in the objective is $\|\hat{\Sigma}_{ss}\mathcal{U}_1 - \hat{\mu}\| \leq \|\mathcal{U}_1 (\hat{\mu}_s - \hat{\mu}_t)\| + \|\mu_t - \mu_t\| + \|\mathcal{U}_1 \hat{\mu}_s - \hat{\mu}_t\|$, which is less than $\|\mathcal{U}_1 \hat{\mu}_s - \hat{\mu}_t\| + \Omega(\frac{1}{\sqrt{n}})$ with high probability. Hence, $p = \text{min}(m, n)$. The first inequality is by triangle inequality and the second is the crucial one that follows from sample complexity of kernel mean embeddings (see theorem 2 in [30]). Also, the constants in $\Omega(\frac{1}{\sqrt{n}})$ are independent of samples, variables and dimensions. By symmetry, we also have with high probability that $\|\mathcal{U}_1 \hat{\mu}_s - \hat{\mu}_t\| \leq \|\mathcal{U}_1 \hat{\mu}_s - \hat{\mu}_t\| + O(\frac{1}{\sqrt{n}})$. Hence, with high probability, uniformly over the feasibility set, $\|\mathcal{U}_1 \hat{\mu}_s - \hat{\mu}_t\| \leq \|\mathcal{U}_1 \hat{\mu}_s - \hat{\mu}_t\| \leq O(\frac{1}{\sqrt{n}})$. Analogous arguments hold for the other quadratic terms too. Now, recall that the first linear term is nothing but the sample average version of $E_{Y \sim p} \|\hat{\epsilon}^{(X, Y) \rightarrow \mathcal{U}_1} (\hat{\epsilon}^{(X, Y)})/Y\|$. Also, this estimate remains the same with the true (unknown) cost function, $c$, also. This is because the sample-based cost function, $\hat{c}$, is exactly same as $c$ at the samples. Also, since the true cost is arbitrarily well approximated by functions in the RKHS, the sample average of cost values converges (again uniformly) to the true expected cost with sample complexity $O(\frac{1}{\sqrt{n}})$ (Refer theorem 3.2 in [30]). Like-wise the other term also has sample complexity $O(\frac{1}{\sqrt{n}})$.

Now, again by triangle inequality, $\left| g(\hat{\mu}_s, \hat{\mu}_t, \hat{\Sigma}_{ss}, \hat{\Sigma}_{tt}) - g(\mu_s, \mu_t, \Sigma_{ss}, \Sigma_{tt}) \right|$ is less than the sum of deviations in each of the terms detailed above. Since each of these deviations is upper bounded uniformly by $O(\frac{1}{\sqrt{n}})$, the theorem is proved. One technicality though is that the above argument (for the linear term in objective) assumes that the $\mathcal{U}_1, \mathcal{U}_2$ are valid conditional embeddings. While this is obviously true for $\epsilon_i = 0$, it need not hold for higher $\epsilon_i$. Hence we insist on the technical condition in the theorem. This technicality could have been avoided by equivalently taking estimate of expected cost using $\mathcal{U}$ itself (it is guaranteed to be a valid embedding). However, that form is less attractive for the proposed ADMM algorithm presented in section 2.3.

B Proof of representer theorem

Proof. Without loss of generality, we consider the parameterization: $\mathcal{U}^x = \sum_{i=1}^{m} \sum_{j=1}^{n} \alpha_{ij} \phi_1(x_i) \otimes \phi_2(y_j) + \mathcal{U}^1, \mathcal{U}^2 = \sum_{i=1}^{m} \sum_{j=1}^{n} \beta_{ij} \phi_2(y_j) \otimes \phi_1(x_i) + \mathcal{U}_1^1, \mathcal{U}_2^1$ where $\mathcal{U}_1^1, \mathcal{U}_1^2, \mathcal{U}_2^1, \mathcal{U}_2^2$ are the respective orthogonal complements. It is easy to see that the objective as well as the first two inequalities in (5) do not involve the orthogonal complements. Also the term $\left\| \mathcal{U} - \hat{\Sigma}_{ss} \mathcal{U}_1^\top \right\|^2_{H_{\mathcal{H}} \otimes H_{\mathcal{I}}} \mathcal{H}$ can be written as sum of a term not involving the orthogonal complements and $\left\| \mathcal{U}^1 - \hat{\Sigma}_{ss} \mathcal{U}_1^1 \right\|^2_{H_{\mathcal{H}} \otimes H_{\mathcal{I}}} \mathcal{H}$. Like-wise $\left\| \mathcal{U} - \hat{\Sigma}_{tt} \right\|^2_{H_{\mathcal{H}} \otimes H_{\mathcal{I}}} \mathcal{H}$ can be written as sum of a term not involving the orthogonal complements as $\left\| \mathcal{U}^1 - \mathcal{U}_1^1 \right\|^2_{H_{\mathcal{H}} \otimes H_{\mathcal{I}}} \mathcal{H}$. Now re-writing (5), where all the norm constraints are equivalently replaced by the norm-squared constraints, in Tikhonov regularization form reads as: $\min_{f \in S \subseteq \mathcal{H}} \mathcal{R}[f] + \Omega[f]$, where $f = (U, U_1, U_2), \mathcal{H} = (\mathcal{H}_2 \otimes \mathcal{H}_1) \otimes (\mathcal{H}_2 \otimes \mathcal{H}_1)$, $S = E(\mathcal{H}_2, \mathcal{H}_1) \times L(\mathcal{H}_1, \mathcal{H}_2) \times L(\mathcal{H}_2, \mathcal{H}_1), \Omega[f] = \left\| \mathcal{U}^1 - \hat{\Sigma}_{ss} \mathcal{U}_1^1 \right\|^2_{H_{\mathcal{H}} \otimes H_{\mathcal{I}}} \mathcal{H} + \left\| \mathcal{U}^1 - \mathcal{U}_1^1 \right\|^2_{H_{\mathcal{H}} \otimes H_{\mathcal{I}}} \mathcal{H}$ and $\mathcal{R}[f]$ is the remaining objective that does not involve the orthogonal complements. Also, let $\hat{\mathcal{S}} \subset S$ denote $\{ f = (U, U_1, U_2) \in S | \mathcal{U}^1 = 0, \mathcal{U}_1^1 = 0, \mathcal{U}_2^1 = 0 \}$ and let $\Pi_{\hat{\mathcal{S}}}$ denote the projection onto $\hat{\mathcal{S}}$. Now, for any $f \in \mathcal{H}$, we have that: $\mathcal{R}[\Pi_{\hat{\mathcal{S}}}[f]] = \mathcal{R}[f]$ and more importantly, $0 = \Omega[\Pi_{\hat{\mathcal{S}}}[f]] \leq \Omega[f]$. The following argument concludes the proof:

---

10See also [8] for similar a argument.
\[
\min_{f \in S \subset H} \hat{\mathcal{R}}[f] + \Omega[f] \leq \min_{f \in \mathcal{S} \subset H} \mathcal{R}[f] + \Omega[f] = \min_{f \in \mathcal{S} \subset H} \mathcal{R}[\Pi_S(f)] + \Omega[\Pi_S(f)] \leq \min_{f \in \mathcal{S} \subset H} \hat{\mathcal{R}}[f] + \Omega[f].
\]

\[\square\]

**C Characterization of constraints**

On the contrary, let us assume that the condition \(\alpha \geq 0\) is not asymptotically necessary. Then, \(\exists f \in \mathcal{H}_2 \otimes \mathcal{H}_1 \ni f \geq 0\) but \(f \notin \mathcal{P}\), where \(\mathcal{P}\) is conic closure of \(\{\phi_1(x) \otimes \phi_2(y) \mid x \in \mathcal{X}, y \in \mathcal{Y}\}\). Recall that marginals are assumed to be positive measures and hence all \(x \in \mathcal{X}, y \in \mathcal{Y}\) will be sampled for large enough \(m,n\). Now, by separation theorem, there will exist at least one \(x' \in \mathcal{X}, y' \in \mathcal{Y}\) such that \(\langle \phi_1(x') \otimes \phi_2(y'), f \rangle < 0 \Rightarrow f(x', y') < 0\), which is a contradiction. Similarly, the condition \(1^\top \alpha 1 = 1\) (together with \(\alpha \geq 0\)) is always a sufficient condition, but asymptotically necessary because all embeddings are nothing but limits of averages.

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