Entropy Regularized Optimal Transport Independence Criterion

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Abstract

Optimal transport (OT) and its entropy regularized offspring have recently gained a lot of attention in both machine learning and AI domains. In particular, optimal transport has been used to develop probability metrics between probability distributions. We introduce in this paper an independence criterion based on entropy regularized optimal transport. Our criterion can be used to test for independence between two samples. We establish non-asymptotic bounds for our test statistic, and study its statistical behavior under both the null and alternative hypothesis. Our theoretical results involve tools from U-process theory and optimal transport theory. We present experimental results on existing benchmarks, illustrating the interest of the proposed criterion.

1 Introduction

Statistical independence measures have been widely used in machine learning and statistics, ranging from independence component analysis (Bach and Jordan, 2002; Gretton et al., 2005) to causal inference (Pfister et al., 2018; Chakraborty and Zhang, 2019), and recently in self-supervised learning (Li et al., 2021) and representation learning (Ozair et al., 2019). Classical dependence measures such as Pearson’s correlation coefficient, Spearman’s $\rho$, and Kendall’s $\tau$ (Hoeffding, 1948; Kruskal, 1958; Lehmann, 1966) focus on real-valued one dimensional random variables and thus are not suitable for high dimensional data; see also (Schweizer and Wolff, 1981; Nikitin, 1995).

One popular choice of independence measures in high dimension is the Hilbert-Schmidt independence criterion (HSIC) (Gretton et al., 2005). This criterion was used to develop an independence test by Gretton et al. (2007b). Several extensions of HSIC are available, such as a relative dependency measure (Bounliphone et al., 2015) and a joint independence measure among multiple random elements (Pfister et al., 2018). Another choice is the distance covariance (dCov) of Székely et al. (2007). dCov was originally developed in Euclidean spaces using characteristic functions and later generalized to metric spaces (Lyons, 2013). In fact, in their most general form, HSIC and dCov are equivalent as shown by Sejdinovic et al. (2013).

A different line of research explored optimal transport to measure dependence. The Wasserstein distance naturally defines a dependence measure when it is used to quantify the similarity between the joint distribution and the product of marginals; see, e.g., (Cifarelli and Regazzini, 2017). The normalized version—the so-called Wasserstein correlation coefficient—has recently gained attention in (Wiesel, 2021; Mordant and Segers, 2021; Nies et al., 2021). Following the classical rank-based tests such as Pearson’s $\rho$, optimal transport is also used to define multivariate ranks and the subsequent independence tests (Shi et al., 2020; Deb and Sen, 2021). However, these tests can suffer from the curse of dimensionality or high computational complexity, limiting their practical usefulness; see (Peyré and Cuturi, 2019) for a discussion.

A remedy to this challenge is to use the entropy regularized formulation of optimal transport. It is particularly attractive from both a computational viewpoint (Cuturi, 2013) and a statistical viewpoint (Rigollet and Weed, 2018). Genevay et al. (2019); Mena and Weed (2019) showed that its empirical counterpart enjoys as an estimator a parametric rate of convergence and thus overcomes the curse of dimensionality. The Sinkhorn divergence (Feydy et al., 2019), its centered version, defines a semi-metric on probability measures which metrizes weak convergence. Ramdas et al. (2017) used it for two-sample testing and Genevay et al. (2018) for generative modeling; see also (Salimans et al., 2018; Sanjabi et al., 2018).
Outline. In Section 2, we introduce the entropy regularized optimal transport independence criterion (ETIC) and discuss its key properties. We propose the tensor Sinkhorn algorithm with a random feature approximation to compute ETIC, which admits a quadratic scaling in time and space. In Section 3, we give our main theoretical results, i.e., non-asymptotic bounds, characterizing the statistical behavior of the empirical estimator of ETIC under both the null and alternative hypotheses. These results, derived from U-process theory tools, extend previous ones to tensor products of measures. In Section 4, we compare the empirical behavior of ETIC with HSIC on both synthetic and real data.

Related Work. Statistical metrics on the space of probability measures form the backbone of many dependence measures. On the machine learning side, distributions are compared by embedding them into reproducing kernel Hilbert spaces (Gretton et al., 2007a, 2012). The Hilbert-Schmidt independence criterion (HSIC) uses Hilbertian embeddings of probability distributions to compare the joint distribution and the product of marginals (Gretton et al., 2005, 2007b). On the statistics side, distributions defined on Euclidean spaces are compared via their characteristic functions, leading to the so-called energy distance (Székely and Rizzo, 2004). A closely related dependence measure is the distance covariance (Székely et al., 2007). These distances were later generalized to general metric spaces of negative type by Lyons (2013), unifying the two notions via the Barycenter map—a quantity similar to the feature map in kernel methods. In fact, the kernel-based and distance-based approaches are equivalent (Sejdinovic et al., 2013). Their corresponding empirical estimators all admit a U-statistics expression, and enjoy a convergence rate that is independent of the dimension. These results can be established using tools from U-statistics theory; see, e.g., (Serfling, 1980).

On the other hand, Wasserstein distances provide a class of metrics on the space of probability measures with nice geometric properties (Ambrosio et al., 2005). However, it is known that its empirical estimate suffers from the curse of dimensionality (Dudley, 1969; Fournier and Guillin, 2015; Weed and Bach, 2019; Lei, 2020), limiting their usage in high-dimension problems. A remedy to this issue is to introduce the entropic regularization. Genevay et al. (2019) showed that the plug-in estimator of the entropic optimal transport cost possesses a parametric rate of convergence when the measures are compactly supported. Their results can be extended to sub-Gaussian distributions (Mena and Weed, 2019); the main argument relies on empirical process theory. The independence criterion we propose uses entropy regularized optimal transport to compare the joint distribution and the product of marginals. The empirical counterpart involves a product of two empirical measures, leading to a two-sample U-process on paired samples. The resulting U-process requires a sophisticated analysis of its statistical behavior; common tools from empirical processes are ineffective here. Using a decoupling technique from Peña and Giné (1999) and duality theory (Peyré and Cuturi, 2019), we prove a rate of convergence roughly $O(\sigma^2 n^{-1/2})$, where $\sigma$ is the sub-Gaussian parameter, recovering previous results for two sample statistics.

2 Entropy Regularized Optimal Transport Independence Criterion

In this section we introduce the entropy regularized optimal transport independence criterion (ETIC) and discuss its key properties. We design an independence test based on ETIC and develop an efficient algorithm to compute its test statistic.

Notation. For a Euclidean space $\mathcal{Z}$ equipped with the Borel $\sigma$-algebra, let $\mathcal{M}_1(\mathcal{Z})$ be the set of probability measures defined on $\mathcal{Z}$. Let $(X, Y)$ be a pair of random vectors with respective dimension $d_1$ and $d_2$ following some joint distribution $P_{XY} \in \mathcal{M}_1(\mathbb{R}^{d_1})$. Denote $P_X \in \mathcal{M}_1(\mathbb{R}^{d_1})$ and $P_Y \in \mathcal{M}_1(\mathbb{R}^{d_2})$ the marginal distributions of $X$ and $Y$, respectively. Given $Q \in \mathcal{M}_1(\mathbb{R}^{d_1} \times \mathbb{R}^{d_2})$ and a real-valued function $f$ on the same domain, we denote $Q[f]$ the expectation $\mathbb{E}_{(X,Y)\sim Q}[f(X,Y)]$. We adopt the notation from the empirical process theory and write $\|Q\|_{\mathcal{F}} := \sup_{f \in \mathcal{F}} |Q[f]|$ for a real-valued function class $\mathcal{F}$. We say $Q$ is sub-Gaussian with parameter $\sigma^2$, denoted as subG($\sigma^2$), if $\mathbb{E}_Q e^{\|Q(X,Y)\|^2/(2\sigma^2)} \leq 2$; see, e.g., (Vershynin, 2018). We write $\mathbb{E} := \mathbb{E}_{P_{XY}}$ for short.
ETIC-Based Independence Test. Given an i.i.d. sample \( \{(X_i, Y_i)\}_{i=1}^n \) from \( P_{XY} \), we are interested in determining whether \( X \) is independent of \( Y \), which can be formalized as the following hypothesis testing problem:

\[
H_0 : P_{XY} = P_X \otimes P_Y \leftrightarrow H_1 : P_{XY} \neq P_X \otimes P_Y.
\]
For this purpose, we use the empirical estimate of $T(X, Y)$ as the test statistic, that is,

$$ T_n(X, Y) := T_{n,e}(X, Y) := \hat{S}_e(\hat{P}_{XY}, \hat{P}_X \otimes \hat{P}_Y), \quad (6) $$

where $\hat{P}_{XY} := \frac{1}{n} \sum_{i=1}^n \hat{\delta}_{(x_i, y_i)}$ is the empirical measure of the pairs, and $\hat{P}_X := \frac{1}{n} \sum_{i=1}^n \hat{\delta}_x$, and $\hat{P}_Y := \frac{1}{n} \sum_{i=1}^n \hat{\delta}_y$, are the empirical measures of each sample, respectively. Note that this is different from the standard plug-in estimator since the product measure $P_X \otimes P_Y$ is estimated by $n^2$ dependent (rather than independent) pairs $\{(X_i, Y_j)\}_{i,j=1}^n$. It raises challenges in the analysis of its statistical behavior as elaborated in Section 3. The statistical test (or decision rule) is then defined as

$$ \psi(\alpha) := \mathbb{I}\{T_n(X, Y) > H_n(\alpha)\}, \quad (7) $$

where $\alpha$ is a prescribed significance level, e.g., $\alpha = 0.05$, and $H_n(\alpha)$ is a threshold chosen such that the type I error rate $\mathbb{P}(\psi(\alpha) = 1 \mid H_0)$ is bounded by $\alpha$. Here $\{\psi(\alpha) = 1\}$ indicates the rejection the null hypothesis. The (statistical) power of the test is defined as $\mathbb{P}(\psi(\alpha) = 1 \mid H_1)$.

To avoid tuning the regularization parameter $\varepsilon$, we also consider an adaptive version of the test:

$$ \psi_\alpha(\varepsilon) := \mathbb{I}\left\{\max_{\varepsilon \in \mathcal{E}} T_{n,e}(X, Y) > H_{n,\varepsilon}(\alpha)\right\}, \quad (8) $$

where $\mathcal{E}$ is a finite set of positive numbers selected by the user and

$$ T_{n,e}(X, Y) := \frac{T_{n,e}(X, Y) - \mathbb{E}[T_{n,e}(X, Y)]}{\text{Sd}(T_{n,e}(X, Y))} $$

is the studentized version of $T_{n,e}(X, Y)$. In practice, $\mathbb{E}[T_{n,e}(X, Y)]$ and $\text{Sd}(T_{n,e}(X, Y))$ can be estimated from the sample via resampling.

**Tensor Sinkhorn Algorithm.** We then derive an efficient algorithm to compute the test statistic. When $P_{XY}$ admits a density, $P_X \otimes P_Y$ is supported on $n^2$ items $\{x_i\}_{i=1}^n \times \{y_j\}_{j=1}^n$ almost surely. If we compute the ETIC statistic naively using the Sinkhorn algorithm (Cuturi, 2013), each iteration costs $O(n^4)$ time and space due to the matrix-vector product of sizes $n^2 \times n^2$ and $n^2 \times 1$. To speed up its computation, we develop a variant of the Sinkhorn algorithm to solve the EOT between two measures supported on the Cartesian product $\{x_i\}_{i=1}^n \times \{y_j\}_{j=1}^n$.

Let $A$ and $B$ be two probability measures on $\{x_i\}_{i=1}^n \times \{y_j\}_{j=1}^n$, where $x_i \in \mathbb{R}^{d_1}$ and $y_j \in \mathbb{R}^{d_2}$. For convenience, both $A$ and $B$ are represented as a matrix, i.e., $A_{ij} = A(x_i, y_j)$. For instance, if we choose $A = P_{XY}$ and $B = P_X \otimes P_Y$, then, in its matrix form, $A = I_n/n$ and $B = 1_{n \times n}/n^2$. Consider an additive cost function $c$, e.g., the weighted quadratic cost, such that $c((x_i, y_j), (x_i', y_j')) = c_1(x_i, x_i') + c_2(y_j, y_j')$. Let $C_1$ and $C_2$ be the cost matrices of $\{x_i\}_{i=1}^n$ and $\{y_j\}_{j=1}^n$, respectively. Define Gibbs matrices $K_1 := e^{-c_1/\varepsilon}$ and $K_2 := e^{-c_2/\varepsilon}$, where the exponential function is element-wise. We show in Proposition 7 in Appendix A that Algorithm 1 can be used to solve $S_c(A, B)$, where $\otimes$ represents element-wise division. We refer to it as the Tensor Sinkhorn algorithm. Each iteration in the Tensor Sinkhorn algorithm takes $O(n^3)$ time and $O(n^2)$ space, thanks to the additive cost function being used. This algorithm can be generalized to measures supported on the Cartesian product of $p > 2$ sets, which is also noted in (Peyré and Cuturi, 2019, Remark 4.17).

**ETIC with Random Features.** To further speed up the computation, we apply the random feature technique introduced by Scetbon and Cuturi (2020). Concretely, we approximate $K_1 \approx \xi_1 \xi_1^T$ and $K_2 \approx \xi_2 \xi_2^T$, where $\xi_1, \xi_2 \in \mathbb{R}^{n \times p}$ are the matrices of random features. Replacing $K_1$ and $K_2$ by their random feature approximations in Algorithm 1 leads to an algorithm with $O(p n^2)$ time complexity and $O(n^2)$ space complexity in each iteration. We refer to the statistic computed in this way as the ETIC-RF statistic. Proposition 8 in Appendix A provides a high-probability guarantee for this random feature approximation. We note that if one applies the random feature approximation directly to the original Sinkhorn algorithm, then the resulting algorithm would have the same time complexity as ETIC-RF but $O(n^4)$ space complexity; see Table 1 for a comparison.
Dual Representation. The entropy regularized formulation of OT is known as the Schrödinger bridge problem (Föllmer, 1988; Léonard, 2012, 2014) in continuum and the Sinkhorn distance (Cuturi, 2013; Ferradans et al., 2014) in the discrete case. It admits a dual representation (Genevay et al., 2016):

\[
\sup_{f, g \in C(\mathbb{R}^d \times \mathbb{R}^d)} \left[ \int f dP_{XY} + \int g d(P_X \otimes P_Y) + \varepsilon - \varepsilon \int e^{-D_c(x,y;x',y')} dP_{XY}(x,y) dP_X(x') dP_Y(y') \right],
\]

where \( C \) is the set of real-valued continuous functions and \( D_c(x, y, x', y') = \frac{1}{2}[c_1(x, x') + c_2(y, y') - f(x, y) - g(x', y')] \). Due to (Csiszar, 1975; Rüschendorf and Thomsen, 1993), the optimal potentials \( (f, g, \varepsilon) \), to be called the Schrödinger potentials, satisfy

\[
\int e^{-D_c(x,y;x',y')} dP_X(x') dP_Y(y') \overset{a.s.}{=\rightarrow} 1
\]

\[
\int e^{-D_c(x,y;x',y')} dP_{XY}(x,y) \overset{a.s.}{\approx}= 1.
\]

Connection to Previous Work. As shown in Appendix A, \( T(X, Y) \) tends to the OT-based independence criterion \( OT(P_{XY}, P_X \otimes P_Y) \) as \( \varepsilon \to 0 \). If the cost \( c \) is chosen as the Euclidean distance to the power \( p \geq 1 \), it induces a distance (known as the Wasserstein-\( p \) distance) on the space of probability measures (Villani, 2016). As a result, \( OT(P_{XY}, P_X \otimes P_Y) \) is a valid independence criterion, i.e., \( OT(P_{XY}, P_X \otimes P_Y) = 0 \) iff \( P_{XY} = P_X \otimes P_Y \). The study of this independence criterion can be dated back to Gini; see (Cifarelli and Regazzini, 2017) for a discussion. Its normalized version—the so-called Wasserstein correlation coefficient—has recently gained attention in (Wiesel, 2021; Mordant and Segers, 2021; Nies et al., 2021). When \( \varepsilon \to \infty \), \( T(X, Y) \) tends to 0 if the cost is additive; if the cost is multiplicative, i.e., \( c((x, y), (x', y')) = c_1(x, x') c_2(y, y') \), it recovers the negative of Hilbert-Schmidt Independence Criterion with kernel \( c_1 \) and \( c_2 \).

The quantity \( S_\varepsilon \) is known as the Sinkhorn divergence and has been used in two-sample problems, where the goal is to quantify the distance of two distributions given i.i.d. samples from each of them. In particular, it is applied to two-sample testing (Ramdas et al., 2017) and generative modeling (Genevay et al., 2018). It is shown in (Feydy et al., 2019) that \( S_\varepsilon \) defines a semi-metric (metric without the triangle inequality) on the space of probability measures with bounded support if the Gibbs kernel induced by the cost is positive universal. The limiting behavior of the empirical estimator is to date not known in the literature, though non-asymptotic bounds are attainable using results in (Genevay et al., 2019; Mena and Weed, 2019). Our results also recover the two-sample case.

3 Main Results

We give non-asymptotic bounds for the ETIC statistic with quadratic cost. We present the main results and their proof sketches here. We use \( C \) to denote a constant whose value may change from line to line, where subscripts are used to emphasize the dependency on other quantities. For instance, \( C_d \) represents a constant depending only on the dimension \( d \). The detailed proofs are deferred to Appendices B and C.
Consistency. We first show that the ETIC statistic is a consistent estimator of its population counterpart under both the null and alternative.

Assumption 1. We make the following assumptions:

(i) \( c \) is chosen as the quadratic cost.

(ii) \( P_X \) and \( P_Y \) are \( \text{subG}(\sigma^2) \).

The quadratic cost is chosen for the sake of concision. We extend the results to weighted quadratic cost in Appendices B.

Theorem 2. Under Assumption 1, we have

\[
E |T_n(X, Y) - T(X, Y)| \leq C_d \left( 1 + \frac{\sigma^{[5d/2]+6}}{\varepsilon^{[5d/4]+1}} \right) \frac{\varepsilon}{\sqrt{n}}.
\]

Remark 2. According to Theorem 2, when \( \varepsilon = \varepsilon_n \) is chosen such that \( \varepsilon_n = \omega(n^{-1([5d/2]+4)}) \) and \( \varepsilon_n = o(1) \), we have \( T_n(X, Y) \) converges in \( L^1 \) to \( \text{OT}(P_{XY}, P_X \otimes P_Y) \) as \( n \to \infty \).

We can upper bound the above \( L^1 \) loss by the supremum of an empirical process and a U-process

\[
\begin{align*}
\left\| \hat{P}_{XY} - P_{XY} \right\|_{F^s}^2 & \quad \text{and} \quad \left\| \hat{P}_X \otimes \hat{P}_Y - P_X \otimes P_Y \right\|_{F^s}^2,
\end{align*}
\]

respectively, where \( F^s \) is the set of real-valued functions satisfying

\[
\begin{align*}
|f(x, y)| & \leq C_s,d(1 + \|(x, y)\|^2) \\
|D^\alpha f(x, y)| & \leq C_s,d(1 + \|(x, y)\|^{\alpha}), \quad \forall 1 < |\alpha| \leq s.
\end{align*}
\]

Mena and Weed (2019) used a similar strategy in their proofs. Empirical process theory has a long history in statistics and there are well established tools to control them; see, e.g., (van der Vaart and Wellner, 1996). However, the theory of U-processes is much less well-developed. Moreover, many of the previous works focus on one-sample U-processes; see, e.g., (Peña and Giné, 1999). The second U-process here is a two-sample U-process on a paired sample, bringing about additional challenges in its analysis, compared e.g. to Mena and Weed (2019). In order to control it, we develop the following results.

Remark 3. Proposition 4 can be viewed as a metric entropy bound for the two-sample U-process on a paired sample. In the extreme case when \( Y = X \), it reduces to a bound for the one-sample U-process of order 2.
Exponential Tail Bound. We also prove an exponential tail bound for the ETIC statistic. It follows from Theorem 2 and the McDiarmid inequality.

**Theorem 5.** Let \( c \) be the quadratic cost. Assume that \( P_X \) and \( P_Y \) are supported on a bounded domain of radius \( D \). Then we have, with probability at least \( 1 - \delta \),

\[
|T_n(X, Y) - T(X, Y)| \leq C_d \left( 1 + \frac{D^{5d+16}}{\varepsilon^{5d/2+8}} \sqrt{\log \frac{6}{\delta}} \right) \frac{\varepsilon}{\sqrt{n}}.
\]

Under \( H_0 \), we have \( T(X, Y) = 0 \), so Theorem 5 implies that

\[
T_n(X, Y) > C_d \left( 1 + \frac{D^{5d+16}}{\varepsilon^{5d/2+8}} \sqrt{\log \frac{6}{\delta}} \right) \frac{\varepsilon}{\sqrt{n}}
\]

with probability at most \( \delta \). It gives an estimate of the tail behavior of \( T_n(X, Y) \) which suggests that the critical value \( H_n(\alpha) \) in (7) should be of order \( O(n^{-1/2}) \). Under \( H_1 \), Theorem 5 implies that

\[
T_n(X, Y) > T(X, Y) - C_d \left( 1 + \frac{D^{5d+16}}{\varepsilon^{5d/2+8}} \sqrt{\log \frac{6}{\delta}} \right) \frac{\varepsilon}{\sqrt{n}}
\]

with probability at least \( 1 - \delta \). When \( T(X, Y) > 0 \), it is clear that the right hand side in the above inequality exceeds the threshold \( H_n(\alpha) \) for large \( n \). Hence, the ETIC test has power converging to 1 as \( n \to \infty \).

4 Experiments

We examine the empirical behavior of the proposed ETIC test for independence testing on both synthetic and real data. We consider synthetic benchmarks from (Gretton et al., 2007b; Jitkrittum et al., 2017; Zhang
We focus on the weighted quadratic cost
\[
c((x, y), (x', y')) = \frac{1}{\lambda_1} \| x - x' \|^2 + \frac{1}{\lambda_2} \| y - y' \|^2.
\]
For convenience, we absorb the regularization parameter \( \varepsilon \) into the weights and set \( \varepsilon = 1 \). It then induces two Gibbs kernels
\[
k_1(x, x') = e^{-\frac{\| x - x' \|^2}{\lambda_1}} \quad \text{and} \quad k_2(y, y') = e^{-\frac{\| y - y' \|^2}{\lambda_2}}
\]
with \( \lambda_i \) being the parameter of kernel \( k_i \) for \( i \in \{1, 2\} \). To select the weights, we apply the median heuristic (Gretton et al., 2007b) widely used for HSIC, i.e.,
\[
\lambda_1 = r_1 M_x \quad \text{and} \quad \lambda_2 = r_2 M_y
\]
with \( r_1 \) and \( r_2 \) ranging from 0.25 to 4, where \( M_x \) and \( M_y \) are the medians of the costs \( \{\| X_i - X_j \|^2 \} \) and \( \{\| Y_i - Y_j \|^2 \} \), respectively. We also examine its variant ETIC-RF discussed in Section 2, where the number of random features is set to be 100 unless otherwise noted. As for the adaptive ETIC test, we defer its results to Appendix E. We compare them with the HSIC statistic with kernels \( k_1 \) and \( k_2 \). For a fair comparison, we calibrate these tests by a Monte Carlo resampling technique (Feuerverger, 1993) with 200 permutations.

For each of the experiment, we repeat the whole procedure 200 times and report the rejection frequency as either the type I error rate (when the null is true) or power (when the null is not true). Note that, even though we are using the same \( \lambda_1 \) and \( \lambda_2 \) in the cost and kernels, that does not mean we should compare ETIC and HSIC under the same hyperparameters. Our goal is to explore their performance over a range of hyperparameters.

Our main findings are: 1) Both ETIC and ETIC-RF are consistent in power as the sample size approaches infinity. 2) In some scenarios, ETIC and ETIC-RF outperforms HSIC significantly; in the linear dependency model and Gaussian convolution model in particular, their power is much more robust than HSIC to the value of the hyperparameters. 3) ETIC-RF performs reasonably good compared to ETIC with a moderate number (i.e., 100) of random features. 4) All three tests benefit from large hyperparameters in detecting simple linear dependency, but smaller values lead to higher power when the dependency is more complicated.

**Hilbert-Schmidt Independence Criterion.** Before we present our results, let us recall the definition of HSIC. Let \( k : \mathbb{R}^{d_1} \times \mathbb{R}^{d_1} \rightarrow \mathbb{R} \) and \( l : \mathbb{R}^{d_2} \times \mathbb{R}^{d_2} \rightarrow \mathbb{R} \) be two positive semi-definite kernels. The Hilbert-Schmidt independence criterion (HSIC) between \( X \) and \( Y \), HSIC(\( X, Y \)), is defined as
\[
E[k(X, X')l(Y, Y')] + E[k(X, X')E[l(Y, Y') | X]] - 2 E[E[k(X, X') | X]E[l(Y, Y') | Y]],
\]
where \( (X', Y') \) is an independent copy of \( (X, Y) \). Given an i.i.d. sample \( \{(X_i, Y_i)\}_{i=1}^n \) from \( P_{XY} \), we can estimate HSIC(\( X, Y \)) by
\[
\frac{1}{n^2} \sum_{i,j=1}^n k_{ij} l_{ij} + \frac{1}{n^4} \sum_{i,j,s,t=1}^n k_{ij} l_{st} - \frac{2}{n^3} \sum_{i,j,s=1}^n k_{ij} l_{is},
\]
where \( k_{ij} := k(X_i, X_j) \) and \( l_{ij} := l(Y_i, Y_j) \). We refer to it as the HSIC statistic.

### 4.1 Synthetic Data

We first compare their performance on synthetic data. We consider synthetic benchmarks from (Zhang et al., 2018), (Jitkrittum et al., 2017), and (Gretton et al., 2007b). We also consider two synthetic examples that are related to the Schrödinger bridge problem. To facilitate the exhibition, we set \( r_1 = r_2 = r \in \{0.25, 0.5, 1, 2, 4\} \) in this section.
Linear Dependency. We begin with a simple linear dependency model. Concretely,

\[ X \sim \mathcal{N}_d(0, I_d) \quad \text{and} \quad Y = X_1 + Z, \quad (10) \]

where \( X_1 \) is the first coordinate of \( X \), and \( Z \sim \mathcal{N}(0, 1) \) is independent with \( X \). We fix \( n = 50 \) and plot the power versus \( d \in [1, 10] \) in Figure 1. All the tests have decaying power as the dimension increases. This is as expected since larger dimension results in weaker dependency between \( X \) and \( Y \). It is clear that the power of both ETIC and HSIC increases as \( r \) increases, with the former more robust than the latter. While the performance of HSIC is similar to ETIC when \( r \) is large, it is much worse than ETIC when \( r \) is small. As for ETIC-RF, it has similar power curves as ETIC.

Gaussian Sign. We then consider a Gaussian sign model, i.e.,

\[ X \sim \mathcal{N}_d(0, I_d) \quad \text{and} \quad Y = |Z| \prod_{i=1}^{d} \text{sgn}(X_i), \quad (11) \]

where \( \text{sgn}(\cdot) \) is the sign function and \( Z \sim \mathcal{N}(0, 1) \) is independent with \( X \). This problem is challenging since \( Y \) is independent with any strict subset of \( \{X_1, \ldots, X_d\} \). We fix \( d = 3 \) and plot the power versus \( n \in [100, 500] \) in Figure 2. All the tests have improved power as the sample size increases. Additionally, they all benefit from a small regularization parameter, with HSIC performs the best and the other two perform similarly.

Subspace Dependency. One important application of independence testing is independent component analysis (Gretton et al., 2005), which involves separating random variables from their linear mixtures. We construct our data by i) generating \( n \) i.i.d. copies of two random variables following independently \( 0.5\mathcal{N}(0.98, 0.04) + 0.5\mathcal{N}(-0.98, 0.04) \), ii) mixing the two random variables by a rotation matrix parameterized by \( \theta \in [0, \pi/4] \) (larger \( \theta \) leads to stronger dependency), iii) appending \( \mathcal{N}_{d-1}(0, I_{d-1}) \) to each of the two mixtures, and iv) multiplying each vector by an independent random \( d \)-dimensional orthogonal matrix. We
refer to it as the \textit{subspace dependency model}. We fix $n = 64$, $d = 2$, and plot the power versus $\theta \in [0, \pi/4]$ in Figure 3. As expected, the power of all three tests improves as $\theta$ becomes closer to $\pi/4$. Moreover, they all have improved power as $r$ decreases. ETIC and ETIC-RF performs similarly, and they are outperformed by HSIC.

\textbf{Gaussian Convolution.} Finally, we consider a Gaussian convolution model, i.e.,

$$X \sim \frac{1}{2}N_d(\mathbf{1}_d, 0.2I_d) + \frac{1}{2}N_d(-\mathbf{1}_d, 0.2I_d) \quad \text{and} \quad Y = X + \sqrt{\frac{\tau}{2}}Z,$$

where $Z \sim N_d(\mathbf{0}_d, I_d)$ and $\tau > 0$ controls the dependency between $X$ and $Y$, i.e., the larger $\tau$ is the less dependent $X$ and $Y$ are. It can be shown that the joint distribution of $(X, Y)$ is the solution to the entropy regularized optimal transport problem with regularization parameter $\tau$ (del Barrio and Loubes, 2020, Theorem 2.4). We fix $n = 64$, $d = 2$, and plot the power versus $\tau \in [0, 50]$ in Figure 4. As expected, all tests have decaying power as $\tau$ increases. The power curves of ETIC and ETIC-RF are fairly robust to the value of $r$, while the performance of HSIC deteriorates significantly as $r$ decreases.

\subsection*{4.2 Dependency between Bilingual Text}

Inspired by Gretton et al. (2007b), we now investigate the performance of the proposed tests on bilingual data using recent developments in natural language processing. Our dataset is taken from the parallel European Parliament corpus (Koehn, 2005) which consists of a large number of documents of the same content in different languages. Note that it is also used in (Bounliphone et al., 2015) to test for relative dependency. For the hyperparameters, we consider different values of $r_1$ and $r_2$ ranging from 0.25 to 4.

To be more specific, we randomly select $n = 64$ English documents and a paragraph in each document from the corpus. We then 1) pair each paragraph with the corresponding paragraph in French to form the dependent sample, 2) pair each paragraph with a random paragraph in the same document in French to form the partially dependent sample, and 3) pair each paragraph with a random paragraph in French to form the independent sample.

Finally, we use LaBSE (Feng et al., 2020) to embed all the paragraphs into a common feature embedding space of dimension 768 and perform independence testing on these feature vectors. LaBSE is a state-of-the-art, language agnostic, sentence embedding model based on Bidirectional Encoder Representations from Transformers (BERT). This allows us to revisit the idea of Gretton et al. (2007b) yet with more modern feature embeddings.

Both ETIC and HSIC perform perfectly on the dependent sample (with power 1) and the independent sample (with low type I error) across all values of $r_1$ and $r_2$ considered. The results on the partially dependent sample is shown in Figure 5. ETIC performs better than HSIC when one of $r_1$ and $r_2$ is large; while HSIC has larger power when $r_1$ or $r_2$ is small.
Figure 6: Heatmaps of power for ETIC-RF with \(d'\) PCs and \(p\) random features on the partially dependent sample of the bilingual data (Top: \(p = 700\) and \(d' \in \{10, 20\}\); bottom: \(d' = 10\) and \(p \in \{700, 1500\}\)). The \(x\)-axis is for \(r_1\) and \(y\)-axis is for \(r_2\). The indices from 0 to 11 correspond to equally spaced values from 0.25 to 4. Lighter color indicates larger power.

**ETIC-RF.** Since the feature embeddings are of high dimension (i.e., 768), which imposes challenges on the random feature approximation. Hence, we first use dimension reduction (principal component analysis) on the English embeddings and French embeddings separately to reduce the dimension to \(d' \ll 768\), and then perform ETIC-RF on the low-dimensional embeddings. Since the dimension reduction step does not utilize information about the joint distribution \(P_{XY}\), it will not violate the level consistency of the test. This is also validated in our experimental results, i.e., all the tests have type I error rate close to 0.05 as expected.

As shown in the top row of Figure 6, the number of principal components (PC) \(d'\) has an interesting effect on the power. Intuitively, the larger \(d'\) is the less information we lose, and thus the larger power the test has. This can be seen at the lower right corner where both \(r_1\) and \(r_2\) are large. However, larger \(d'\) also suggests that the random feature approximation is harder, especially when \(r_1\) and \(r_2\) are small. This is reflected at the upper left corner where the power decreases as \(d'\) increases. We then investigate the effect of \(p\) — the number of random features. As shown in the bottom row of Figure 6, the power increases with the number of random features. Overall, the ETIC-RF demonstrates similar performance as the exact ETIC with enough random features.

**Conclusion.** We introduced a new independence criterion ETIC based on entropy regularized optimal transport. The proposed criterion can be approximated using a random features based approximation. We established non-asymptotic bounds using U-process theory and optimal transport theory. The experimental results show that ETIC can exhibit stable behavior w.r.t. its hyperparameters. The extension of ETIC to multi-way dependence is an interesting venue for future work.
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A Properties of ETIC

In this section, we prove the properties of ETIC discussed in Section 2. For the sake of generality, we state the problem for general notations $P$ and $Q$ while keeping in general that $P, Q \in \{P_{XY}, P_X \otimes P_Y\}$ in our case. Let $P \in \mathcal{M}_1(\mathbb{R}^{d_1} \times \mathbb{R}^{d_2})$ and $P_X$ and $P_Y$ be the marginals on $\mathbb{R}^{d_1}$ and $\mathbb{R}^{d_2}$, respectively. Define $Q$, $Q_X$, and $Q_Y$ similarly. We are interested in the EOT cost between $P$ and $Q$ under the cost function $c$:

$$ S_\varepsilon(P, Q) := \inf_{\gamma \in \Pi(P, Q)} \left[ \int cd\gamma + \varepsilon \text{KL}(\gamma \| P \otimes Q) \right]. \tag{13} $$

When $\varepsilon = 0$, $S_0(P, Q)$ is the optimal transport cost between $P$ and $Q$. When $\varepsilon > 0$, it admits a dual representation:

$$ S_\varepsilon(P, Q) := \sup_{f, g \in C(\mathbb{R}^{d_1} \times \mathbb{R}^{d_2})} \left[ \int f dP + \int g dQ + \varepsilon - \varepsilon \int e^{\frac{1}{\varepsilon} \left[ f(z) + g(z') - c(z, z') \right]} dP(z) dQ(z') \right]. \tag{14} $$

The Schrödinger bridge potentials $(f_\varepsilon, g_\varepsilon)$ satisfy the optimality conditions:

$$ \int e^{\frac{1}{\varepsilon} [f_\varepsilon(z) + g_\varepsilon(z') - c(z, z')]} dQ(z') \overset{\text{a.s.}}{=} 1, \tag{15} $$

$$ \int e^{\frac{1}{\varepsilon} [f_\varepsilon(z) + g_\varepsilon(z') - c(z, z')]} dP(z) \overset{\text{a.s.}}{=} 1. $$

We first derive the limit ETIC as $\varepsilon \to 0$ and $\varepsilon \to \infty$.

**Proposition 6.** Let $c$ be a continuous cost function. If either $c$ is bounded or $P$ and $Q$ have compact support, it holds that

$$ T_\varepsilon(X, Y) \to \begin{cases} 0 & \text{if } c = c_1 \oplus c_2 \\ -\frac{1}{2} \text{HSIC}_{c_1, c_2}(X, Y) & \text{if } c = c_1 \otimes c_2, \end{cases} \text{ as } \varepsilon \to \infty. \tag{16} $$

Moreover, if both $P$ and $Q$ are densities (or discrete measures), then

$$ T_\varepsilon(X, Y) \to S_0(P_{XY}, P_X \otimes P_Y), \text{ as } \varepsilon \to 0. \tag{17} $$

**Proof.** To show (16), we claim that, for all $P, Q \in \mathcal{M}_1(\mathbb{R}^d)$,

$$ S_0(P, Q) \leq S_\varepsilon(P, Q) \leq (P \otimes Q)[c], \tag{18} $$

and

$$ \lim_{\varepsilon \to \infty} S_\varepsilon(P, Q) = (P \otimes Q)[c]. \tag{19} $$

In fact, for any $\varepsilon_1 < \varepsilon_2$, we have

$$ \int cd\gamma + \varepsilon_1 \text{KL}(\gamma \| P \otimes Q) \leq \int cd\gamma + \varepsilon_2 \text{KL}(\gamma \| P \otimes Q), \text{ for all } \gamma \in \Pi(P, Q). $$

This yields that

$$ S_{\varepsilon_1}(P, Q) \leq S_{\varepsilon_2}(P, Q), \text{ for all } \varepsilon_1 \leq \varepsilon_2, $$

and thus (18) follows.

We then study the limit of $S_\varepsilon$ as $\varepsilon \to \infty$. By the assumption that $c$ is bounded or $P$ and $Q$ have compact support, there exists $M > 0$ such that $\sup_{\gamma \in \Pi(P, Q)} \int cd\gamma \leq M < \infty$. As a result,

$$ \sup_{\gamma \in \Pi(P, Q)} \left| \frac{1}{\varepsilon} \int cd\gamma + \text{KL}(\gamma \| P \otimes Q) - \text{KL}(\gamma \| P \otimes Q) \right| \leq \frac{M}{\varepsilon}, $$

16
which implies that
\[
\inf_{\gamma \in \Pi(P, Q)} \left[ \frac{1}{\varepsilon} \int cd\gamma + \text{KL}(\gamma \| P \otimes Q) \right] \rightarrow \inf_{\gamma \in \Pi(P, Q)} \text{KL}(\gamma \| P \otimes Q) = 0, \quad \text{as} \quad \varepsilon \rightarrow \infty.
\]

By the strict convexity of KL, the problem on the LHS has a unique minimizer $\gamma_\varepsilon$ and the problem on the RHS has a unique minimizer $\gamma_* = P \otimes Q$. Now, by the tightness of $\Pi(P, Q)$ (e.g., (Santambrogio, 2015, Theorem 1.7)), every sequence of $\{\gamma_\varepsilon\}$ has a weakly converging subsequence whose limit must be $\gamma_*$. Therefore, the claim (19) holds true.

Let $c = c_1 \oplus c_2$. According to (19), we have
\[
\lim_{\varepsilon \to \infty} S_\varepsilon(P_{XY}, P_X \otimes P_Y) = (P_{XY} \otimes P_X \otimes P_Y)[c] = (P_X \otimes P_X)[c_1] + (P_Y \otimes P_Y)[c_2].
\]

Similarly, it holds that
\[
\lim_{\varepsilon \to \infty} S_\varepsilon(P_{XY}, P_{XY}) = (P_X \otimes P_X)[c_1] + (P_Y \otimes P_Y)[c_2]
\]
\[
\lim_{\varepsilon \to \infty} S_\varepsilon(P_X \otimes P_Y, P_X \otimes P_Y) = (P_X \otimes P_X)[c_1] + (P_Y \otimes P_Y)[c_2].
\]

Consequently, $\lim_{\varepsilon \to \infty} T_\varepsilon(X, Y) = 0$. An analogous argument implies that, when $c = c_1 \otimes c_2$
\[
\lim_{\varepsilon \to \infty} T_\varepsilon(X, Y) = \mathbb{E}_{P_{XY}} \mathbb{E}_{P_X} [c_1(X, X') | X] \mathbb{E}_{P_Y} [c_2(Y, Y') | Y] - \frac{1}{2} \frac{\mathbb{E}_{P_{XY}} [c_1(X, X')c_2(Y, Y')]}{\mathbb{E}_{P_X} [c_2(Y, Y')] - \frac{1}{2} \frac{\mathbb{E}_{P_{XY}} [c_1(X, X')c_2(Y, Y')]}{\mathbb{E}_{P_X} [c_2(Y, Y')]}} = -\frac{1}{2} \text{HSIC}_{c_1, c_2}(X, Y).
\]

Note that
\[
\lim_{\varepsilon \to 0} S_\varepsilon(P, Q) = S_0(P, Q)
\]
when both $P$ and $Q$ are densities (Léonard, 2012) and when both of them are discrete measures (Peyré and Cuturi, 2019, Proposition 4.1). The statement (17) follows immediately from the fact that $S_0(P, P) = 0$ for all $P$.

We then prove the validity of ETIC as a dependence measure as stated in Proposition 1.

Proof of Proposition 1. Due to Blanchard et al. (2011, Lemma 5.2), the Gibbs kernel
\[
k_\varepsilon(z, z') := e^{-c(z, z')/\varepsilon} = k_1(x, x')k_2(y, y')
\]
is universal since both $k_1$ and $k_2$ are. It is also clear that $k_\varepsilon$ is positive since both $k_1$ and $k_2$ are. Consequently, the Sinkhorn divergence $S_\varepsilon$ defines a semi-metric on $\mathcal{M}_1(\mathcal{X} \times \mathcal{Y})$ according to Feydy et al. (2019, Theorem 1). Hence, if $P_{XY}, P_X \otimes P_Y \in \mathcal{M}_1(\mathcal{X} \times \mathcal{Y})$, then $T_\varepsilon(X, Y) := S_\varepsilon(P_{XY}, P_X \otimes P_Y) = 0$ iff $P_{XY} = P_X \otimes P_Y$.  

Finally, we analyze the computational complexity of the Tensor Sinkhorn algorithm for additive cost functions, i.e.,
\[
c(z, z') := c_1(x, x') + c_2(y, y'),
\]
where $z = (x, y)$ and $z' = (x', y')$.

Let $\{x_i\}_{i=1}^n$ and $\{y_j\}_{j=1}^n$ be two sets of atoms. Note that the two sets are assumed to be of the same size for convenience. Let $A$ and $B$ be two probability measures on $\{x_i\}_{i=1}^n \times \{y_j\}_{j=1}^n$. For convenience, both $A$ and $B$ are represented as a matrix, i.e., $A_{ij} = A(x_i, y_j)$. For instance, if we choose $A = P_{XY}$ and $B = P_X \otimes P_Y$, then, in its matrix form, $A = I_n/n$ and $B = 1_{n \times n}$. Denote $C_1$ and $C_2$ as the cost matrices of $\{x_i\}_{i=1}^n$ and $\{y_j\}_{j=1}^n$, respectively. Define Gibbs matrices $K_1 := e^{-C_1/\varepsilon}$ and $K_2 := e^{-C_2/\varepsilon}$, where the exponential function is applied element-wisely. Let $K := K_2 \otimes K_1 \in \mathbb{R}^{n^2 \times n^2}$ be the Gibbs matrix associated with the cost matrix on the pairs $\{(x_1, y_1), (x_2, y_1), \ldots, (x_n, y_n)\}$, where $\otimes$ is the Kronecker product.
Proof. Let \( a := \text{Vec}(A) \in \mathbb{R}^{n^2} \) and \( b := \text{Vec}(B) \in \mathbb{R}^{n^2} \) be the probability vectors corresponding to \( A \) and \( B \), respectively. Denote \( u := \text{Vec}(U) \in \mathbb{R}^{n^2} \) and \( v := \text{Vec}(V) \in \mathbb{R}^{n^2} \). The Sinkhorn algorithm to solve \( S_c(a,b) \) has the following two update steps:

\[
u = a \otimes K v \quad \text{and} \quad v = b \otimes K^\top u.
\]

By the identity \( \text{Vec}(MNL) = (L^\top \otimes M) \text{Vec}(N) \) for matrices \( M, N, \) and \( L \) of compatible dimensions, we obtain

\[
\text{Vec}(K_1 VK_2^\top) = (K_2 \otimes K_1) \text{Vec}(V) = K v.
\]

Thus, the update \( U = A \otimes (K_1 VK_2^\top) \) is equivalent to \( u = a \otimes K v \). Similarly, the updated \( V = B \otimes (K_1^\top UK_2) \) is equivalent to \( v = b \otimes K^\top u \). Due to Dvurechensky et al. (2018, Theorem 1), the Tensor Sinkhorn algorithm therefore outputs an \( \delta \)-accurate estimate in \( O(\log(\kappa_1 \kappa_2 \kappa_3)/\delta) \) iterations. Since each iteration costs \( O(n^3) \) time, it has overall time complexity \( O(n^3 \log(\kappa_1 \kappa_2 \kappa_3)/\delta) \).

Remark 4. A direct application of the Sinkhorn algorithm leads to \( O(n^4 \log(\kappa_1 \kappa_2 \kappa_3)/\delta) \) time complexity, which is \( n \) times slower than the Tensor Sinkhorn algorithm.

We then characterize the convergence of the Tensor Sinkhorn algorithm with the random feature approximation. Let \( \rho_1 \) and \( \rho_2 \) be two probability measures on metric spaces \( \mathcal{U} \) and \( \mathcal{V} \), respectively. Following Scetbon and Cuturi (2020, Section 3), we focus on Gibbs kernels of the form

\[
k_1(x,x') = \int \varphi(x,u)^\top \varphi(x',u) d\rho_1(u) \quad \text{and} \quad k_2(y,y') = \int \psi(y,v)^\top \psi(y',v) d\rho_2(v),
\]

where \( \varphi : \{x_i\}_{i=1}^n \times \mathcal{U} \to \mathbb{R}^q_+ \) and \( \psi : \{y_i\}_{i=1}^n \times \mathcal{V} \to \mathbb{R}^q_+ \). Note that the Gibbs kernels induced by the weighted quadratic cost admit this expression. For \( p \in \mathbb{N}_+ \), we obtain two i.i.d. samples \( \{u_i\}_{i=1}^p \) and \( \{v_i\}_{i=1}^p \) from \( \rho_1 \) and \( \rho_2 \), respectively. We denote \( u := (u_1, \ldots, u_p) \) and approximate \( k_1(x,x') \) by

\[
k_{1,u}(x,x') := \frac{1}{p} \sum_{k=1}^p \varphi(x,u_k)^\top \varphi(x',u_k).
\]

This new kernel induces the cost \( c_{1,u}(x,x') := -\varepsilon \log k_{1,u}(x,x') \). Similarly, we define \( v := (v_1, \ldots, v_p) \), \( k_{2,v}(y,y') \), and \( c_{2,v}(y,y') \). It is clear that Algorithm 1 with inputs \( A, B, K_{1,u}, \) and \( K_{2,v} \) solves the entropy-regularized optimal transport problem with cost \( c_{u,v}(z,z') := c_{1,u}(x,x') + c_{2,v}(y,y') \). Let \( S_{c,c,u,v}(A,B) \) be the entropic cost. The next proposition characterizes the approximation error \( |S_{c,c,u,v}(A,B) - S_{c,c}(A,B)| \).

Assumption 2. There exists a constant \( C > 0 \) such that

\[
\varphi(x,u)^\top \varphi(x',u)/k_1(x,x') \leq C \quad \text{and} \quad \psi(y,v)^\top \psi(y',v)/k_2(y,y') \leq C
\]

for all \( x,x' \in \{x_i\}_{i=1}^n \), \( y,y' \in \{y_j\}_{j=1}^n \), \( u \in \mathcal{U} \), and \( v \in \mathcal{V} \).

Proposition 8. Let \( \delta > 0 \), \( \tau > 0 \), and \( p = \Omega \left( \frac{C^2}{\delta \tau} \log \frac{n}{\tau} \right) \). Under Assumption 2, with probability at least \( 1 - \tau \), it holds that

\[
|S_{c,c,u,v}(A,B) - S_{c,c}(A,B)| \leq \delta.
\]

Proof of Proposition 8. The proof is heavily inspired by Scetbon and Cuturi (2020, Proof of Theorem 3.1). In consideration of the space, we only present the part that is significantly different from theirs, i.e., a counterpart of Scetbon and Cuturi (2020, Proposition 3.1). This proposition gives a uniform tail bound for
the ratio between the approximated kernel and the original kernel. In our case, we are approximating the kernel $K := K_2 \otimes K_1$ by $K_{u,v} := K_2,v \otimes K_1,u$. Hence, it suffices to bound

$$\sup_{x,x' \in \{i\}_{i=1}^{p}, y,y' \in \{i\}_{i=1}^{p}} \left| \frac{k_{1,u}(x,x')k_{2,v}(y,y')}{k_1(x,x')k_2(y,y')} - 1 \right|.$$ 

Note that

$$\frac{k_{1,u}(x,x')}{k_1(x,x')} = \frac{1}{p} \sum_{k=1}^{p} \frac{\varphi(x, u_k)^{T}\varphi(x', u_k)}{k_1(x,x')}$$

is a sum of nonnegative i.i.d. random variables with mean 1. Due to Assumption 2, they are also bounded. It follows from the Hoeffding inequality that

$$\mathbb{P}\left( \left| \frac{k_{1,u}(x,x')}{k_1(x,x')} - 1 \right| \geq t \right) \leq 2 \exp\left( -\frac{pt^2}{C^2} \right).$$

The same inequality holds for the ratio $k_{2,v}(y,y')/k_2(y,y')$. Since

$$\left| \frac{k_{1,u}(x,x')k_{2,v}(y,y')}{k_1(x,x')k_2(y,y')} - 1 \right| \leq \left| \frac{k_{1,u}(x,x')}{k_1(x,x')} - 1 \right| \left| \frac{k_{2,v}(y,y')}{k_2(y,y')} - 1 \right| + \left| \frac{k_{1,u}(x,x')}{k_1(x,x')} - 1 \right| + \left| \frac{k_{2,v}(y,y')}{k_2(y,y')} - 1 \right|,$$

it follows that

$$\mathbb{P}\left( \left| \frac{k_{1,u}(x,x')k_{2,v}(y,y')}{k_1(x,x')k_2(y,y')} - 1 \right| \leq t^2 + 2t \right) \geq \mathbb{P}\left( \left\{ \left| \frac{k_{1,u}(x,x')}{k_1(x,x')} - 1 \right| \leq t \right\} \cap \left\{ \left| \frac{k_{2,v}(y,y')}{k_2(y,y')} - 1 \right| \leq t \right\} \right)$$

$$= \mathbb{P}\left( \left| \frac{k_{1,u}(x,x')}{k_1(x,x')} - 1 \right| \leq t \right) \mathbb{P}\left( \left| \frac{k_{2,v}(y,y')}{k_2(y,y')} - 1 \right| \leq t \right)$$

$$\geq 1 - 4 \exp\left( -\frac{pt^2}{C^2} \right).$$

Equivalently,

$$\mathbb{P}\left( \left| \frac{k_{1,u}(x,x')k_{2,v}(y,y')}{k_1(x,x')k_2(y,y')} - 1 \right| \geq t \right) \leq 4 \exp\left( -\frac{p(\sqrt{t}+1-1)^2}{C^2} \right).$$

A uniform bound yields

$$\mathbb{P}\left( \sup_{x,x' \in \{i\}_{i=1}^{p}, y,y' \in \{i\}_{i=1}^{p}} \left| \frac{k_{1,u}(x,x')k_{2,v}(y,y')}{k_1(x,x')k_2(y,y')} - 1 \right| \geq t \right) \leq 4n^4 \exp\left( -\frac{p(\sqrt{t}+1-1)^2}{C^2} \right).$$

\[ \square \]

**Remark 5.** Let $\hat{S}_{e,cu,v}(A,B)$ be the cost computed from Algorithm 1. Following Dvurechensky et al. (2018, Theorem 1), we can get that

$$\left| \hat{S}_{e,cu,v}(A,B) - S_{e,cu,v}(A,B) \right| \leq \delta$$

in $O\left( pn^2 \log(k_1k_2k_3)/\delta \right)$ arithmetic operations, where $k_1 := \max_{i,i'} k_1^{-1}(x_i,x_{i'})$, $k_2 := \max_{j,j'} k_2^{-1}(y_j,y_{j'})$, and $k_3 := \max_{i,j} \{a_{ij}^{-1}, b_{ij}^{-1} \}$.

**B Consistency of ETIC**

In this section, we prove the main results in Section 3. For the sake of generality, we start by considering the formulation in (13). We focus on the weighted quadratic cost function

$$c(z, z') := w_1 \|x - x'\|^2 + w_2 \|y - y'\|^2,$$

where $z = (x,y)$, $z' = (x',y')$ and $w_1, w_2 \in \mathbb{R}_+$. Denote $w := \max\{w_1, w_2\}$. Due to Lemma 23, we assume, w.l.o.g., that $\varepsilon = 1$ and write $S(P,Q) := S_1(P,Q)$.

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B.1 Smoothness Properties of the Schrödinger Potentials

We start by deriving some smoothness properties of the Schrödinger potentials. Our proofs are deeply inspired by Mena and Weed (2019). Our results generalize theirs to weighted quadratic cost functions.

Assumption 3. We assume that $P_X$, $P_Y$, $Q_X$, and $Q_Y$ are all sub-$G(\sigma^2)$.

Proposition 9. Under Assumption 3, there exist smooth Schrödinger potentials $(f, g)$ for $S(P, Q)$ such that the optimality conditions (15) hold for all $z, z' \in \mathbb{R}^d$. Moreover, we have

$$f(z) \geq -d\sigma^2 \left[ 2w_1 + 2w_2 + 4w_2^2 (\sqrt{2d_1 \sigma} + ||x||)^2 + 4w_2^2 (\sqrt{2d_2 \sigma} + ||y||)^2 \right] - 1$$

$$f(z) \leq w_1(||x|| + \sqrt{2d_1 \sigma})^2 + w_2(||y|| + \sqrt{2d_2 \sigma})^2,$$

and for $g$ similarly.

Proof. Let $(f_0, g_0)$ be a pair of Schrödinger potentials. Since $(f_0 + C, g_0 - C)$ is also a pair of Schrödinger potentials for any constant $C \in \mathbb{R}$, we assume, w.l.o.g., that $P[f_0] = Q[g_0] = \frac{1}{2} S(P, Q) \geq 0$. Define

$$f(z) := -\log \int e^{g_0(z') - c(z, z')} dQ(z') \quad \text{and} \quad g(z') := -\log \int e^{f(z) - c(z, z')} dP(z).$$

(21)

We claim that the pair $(f, g)$ satisfies the requirements.

Since $(f_0, g_0)$ is a pair of Schrödinger potentials, it holds that

$$g_0(z') \overset{a.s.}{=} -\log \int e^{f_0(z') - c(z, z')} dP(z) \leq -P[f_0] + w_1 E_{P_X} [||X - x'||^2] + w_2 E_{P_Y} [||Y - y'||^2],$$

by Jensen’s inequality. Note that $P[f_0] \geq 0$ and, by Lemma 17, $E_{P_X} [||X||^2] \leq 2d_1 \sigma^2$. It follows that

$$g_0(z') - c(z, z') \leq w_1 \left[ 2d_1 \sigma^2 + 2 ||x'|| (\sqrt{2d_1 \sigma} + ||x||) \right] + w_2 \left[ 2d_2 \sigma^2 + 2 ||y'|| (\sqrt{2d_2 \sigma} + ||y||) \right],$$

and thus

$$\int e^{g_0(z') - c(z, z')} dQ(z') \leq 2^{w_1 d_1 + w_2 d_2} \sigma^{2} \left[ \int e^{4w_1 ||x'|| (\sqrt{2d_1 \sigma} + ||x||)} dQ_X(x') \int e^{4w_2 ||y'|| (\sqrt{2d_2 \sigma} + ||y||)} dQ_Y(y') \right]^{1/2} \leq 2e^{2w_1 d_1 + w_2 d_2} \sigma^{2} \int e^{4d_1 \sigma^2 w_1^2 (\sqrt{2d_1 \sigma} + ||x||)^2 + 4d_2 \sigma^2 w_2^2 (\sqrt{2d_2 \sigma} + ||y||)^2} < \infty,$$

by Lemma 17.

Hence, $f(z)$ is well-defined for all $z \in \mathbb{R}^d$. Moreover, we have the lower bound

$$f(z) \geq -d_1 \sigma^2 \left[ 2w_1 + 4w_2^2 (\sqrt{2d_1 \sigma} + ||x||)^2 \right] - d_2 \sigma^2 \left[ 2w_2 + 4w_2^2 (\sqrt{2d_2 \sigma} + ||y||)^2 \right] - 1$$

$$\geq -d \sigma^2 \left[ 4w_2 + 4w_2^2 (\sqrt{2d_2 \sigma} + ||x||)^2 + 4w_2^2 (\sqrt{2d_2 \sigma} + ||y||)^2 \right] - 1$$

For the upper bound, by Jensen’s inequality, it holds that

$$f(z) \leq -Q[g_0] + w_1 E_{Q_X} [||x - x'||^2] + w_2 E_{Q_Y} [||y - Y'||^2] \leq w_1 (||x|| + \sqrt{2d_1 \sigma})^2 + w_2 (||y|| + \sqrt{2d_2 \sigma})^2.$$

Similar arguments prove the claim for $g$. Now, it remains to show that $(f, g)$ satisfies the optimality conditions (15) for all $z, z' \in \mathbb{R}^d$. By definition, it is clear that

$$\int e^{f(z) + g(z') - c(z, z')} dP(z) = 1 \quad \text{and} \quad \int e^{f(z) + g_0(z') - c(z, z')} dQ(z') = 1, \ \forall z, z' \in \mathbb{R}^d.$$

Since $(f_0, g_0)$ is a pair of Schrödinger potentials, we also have

$$\int e^{f_0(z) + g_0(z') - c(z, z')} dP(z) dQ(z') = 1.$$
Consequently, by Jensen’s inequality
\[
\int (f - f_0) dP + \int (g - g_0) dQ \\
\geq - \log \int e^{f_0 - f} dP - \log \int e^{g_0 - g} dQ \\
= - \log \int e^{f_0(z) + g_0(z') - c(z, z')} dP(z) dQ(z') - \log \int e^{f(z) + g_0(z') - c(z, z')} dP(z) dQ(z') \\
= 0.
\]

Since both \((f_0, g_0)\) and \((f, g)\) are Schrödinger potentials, the above equality holds true. This implies that
\[
\int (g_0 - g) dQ = \log \int e^{g_0 - g} dQ,
\]
and thus \(g = g_0 + C Q\)-almost surely by the strict concavity of \(\log\). Therefore, we have
\[
\int e^{f(z) + g(z') - c(z, z')} dQ(z') = e^C \int e^{f(z) + g(z') - c(z, z')} dQ(z') = e^C, \quad \forall z, z' \in \mathbb{R}^d.
\]

Taking integrals with respect to \(P\) implies that \(C = 0\), which completes the proof.

The next proposition shows that there exist Schrödinger potentials satisfying Hölder-type conditions.

**Definition 4.** For any \(\sigma \in \mathbb{R}_+, d \in \mathbb{N}_+,\) and \(w = (w_1, w_2) \in \mathbb{R}^2_+\), let \(\mathcal{F}_\sigma := \mathcal{F}_{\sigma, d, w}\) be the set of smooth functions such that, for any \(k \in \mathbb{N}_+\) and any multi-index \(\alpha\) with \(|\alpha| = k\),
\[
\left| D^\alpha \left( f(x, y) - w_1 \|x\|^2 - w_2 \|y\|^2 \right) \right| \leq C_{k, d, w} \left\{ \begin{array}{ll}
(1 + \sigma^4) \sigma^k (1 + \sigma)^k & \text{if } k = 0 \\
(1 + \sigma^2) \|x\|^2 \& (\sigma / \|x\|)^k & \text{otherwise},
\end{array} \right.
\]
if \(\|z\| \leq \sqrt{d} \sigma\), and
\[
\left| D^\alpha \left( f(x, y) - w_1 \|x\|^2 - w_2 \|y\|^2 \right) \right| \leq C_{k, d, w} \left\{ \begin{array}{ll}
[1 + (1 + \sigma^2) \|x\|^2] \sigma^k (1 + \sigma)^k & \text{if } k = 0 \\
\|x\|^2 \& (\sigma / \|x\|)^k & \text{otherwise},
\end{array} \right.
\]
if \(\|z\| > \sqrt{d} \sigma\), where \(C_{k, d, w}\) is a constant depending on \(k, d,\) and \(w\).

**Proposition 10.** Under Assumption 3, there exist Schrödinger potentials \((f, g)\) such that the optimality conditions (15) hold for all \(z, z' \in \mathbb{R}^d\) and \(f, g \in \mathcal{F}_\sigma\).

**Proof.** Let \((f, g)\) be a pair of Schrödinger potentials satisfying the requirements in Proposition 9. Denote \(\bar{f}(x, y) := f(x, y) - w_1 \|x\|^2 - w_2 \|y\|^2\). Note that
\[
\bar{f}(z) = - \log e^{-\bar{f}(x, y)} = - \log \int e^{w_1 \|x\|^2 + w_2 \|y\|^2 + g(z') - c(z, z')} dQ(z') \\
= - \log \int e^{g(z') - w_1 \|x\|^2 - w_2 \|y\|^2 + 2w_1 (x, x') + 2w_2 (y, y')} dQ(z')
\]

The desired inequalities for \(k = 0\) follow directly from Proposition 9. We focus on \(k > 0\). According to the multivariate Faá di Bruno formula (Constantine and Savits, 1996), we have
\[
D^\alpha \bar{f}(z) = \sum_{\lambda_1 + \cdots + \lambda_k = \alpha} C_{\lambda_1, \ldots, \lambda_k} \prod_{i=1}^k M_{\lambda_i},
\]
where
\[
M_{\lambda} = \frac{\int (z')^\lambda \exp \left\{ g(z') - w_1 \|x\|^2 - w_2 \|y\|^2 + 2w_1 (x, x') + 2w_2 (y, y') \right\} dQ(z')}{\int \exp \left\{ g(z') - w_1 \|x\|^2 - w_2 \|y\|^2 + 2w_1 (x, x') + 2w_2 (y, y') \right\} dQ(z')}.
\]

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Here \( \tilde{z}' = (2w_1x', 2w_2y') \) and \( z^\lambda = \prod_{i=1}^d z_i^\lambda \). By Lemma 11 below, it holds that
\[
|D^\alpha \tilde{f}(z)| \leq C_{k,d,w} \begin{cases} 
s^k(1 + s^k) & \text{if } \|z\| \leq \sqrt{d}s \\
s^k(s^k(\|z\| + \sqrt{s\|z\|})^k & \text{if } \|z\| > \sqrt{d}s,
\end{cases}
\]

which proves the claim. \( \square \)

**Lemma 11.** Recall \( M_\lambda \) in (24). Under Assumption 3, for \( |\lambda| > 0 \), we have
\[
|M_\lambda| \leq C_{|\lambda|,d,w} \begin{cases} 
s^{|\lambda|}(s + s^2)^{|\lambda|} & \text{if } \|z\| \leq \sqrt{d}s \\
s^{|\lambda|}(s^k(\|z\| + \sqrt{s\|z\|})^{|\lambda|} & \text{if } \|z\| > \sqrt{d}s.
\end{cases}
\]

**Proof.** We first bound the denominator. By the optimality conditions (15), it holds that
\[
\begin{aligned}
\left( \int \exp \left\{ g(z') - w_1 \|x'\|^2 - w_2 \|y'\|^2 + 2w_1 \langle x, x' \rangle + 2w_2 \langle y, y' \rangle \right\} dQ(z') \right)^{-1} \\
= e^{f(x,y) - w_1 \|x\|^2 - w_2 \|y\|^2} \leq e^{w_1(2d_1s^2 + 2\sqrt{d}\|z\|) + w_2(2d_2s^2 + 2\sqrt{d}\|z\|)}
\end{aligned}
\]
where the last inequality follows from Proposition 9. To bound the numerator, we use the truncation technique. Let \( A := \{(x', y') : \|2w_1x'\| \leq K, \|2w_2y'\| \leq K \} \) for some constant \( K \) to be determined later. On the set \( A \), it is clear that \( (\tilde{z}')^\lambda \leq \|z\|^{|\lambda|} \leq K^{|\lambda|} \), and thus
\[
\begin{aligned}
\frac{\int_A (\tilde{z}')^{\lambda} \exp \left\{ g(z') - w_1 \|x'\|^2 - w_2 \|y'\|^2 + 2w_1 \langle x, x' \rangle + 2w_2 \langle y, y' \rangle \right\} dQ(z')}{\int \exp \left\{ g(z') - w_1 \|x'\|^2 - w_2 \|y'\|^2 + 2w_1 \langle x, x' \rangle + 2w_2 \langle y, y' \rangle \right\} dQ(z')} \leq K^{|\lambda|}.
\end{aligned}
\]

On the set \( A^c \), we proceed as follows. According to Proposition 9, we have
\[
\begin{aligned}
e^{g(z', y') - w_1 \|x'\|^2 - w_2 \|y'\|^2} & \leq e^{w_1(2d_1s^2 + 2\sqrt{d}\|z\|) + w_2(2d_2s^2 + 2\sqrt{d}\|z\|)}
\end{aligned}
\]

which yields
\[
\begin{aligned}
\int_{A^c} (\tilde{z}')^{2\lambda} dQ(z') & \leq \int_{A^c} e^{2w_1 \|x'\|^2 + 2w_2 \|y'\|^2} dQ(z') \\
& \leq e^{2w_1(d_1 + w_2 d_2)s^2} \left( (\tilde{z}')^{2\lambda} dQ(z') \right)^{1/2}.
\end{aligned}
\]
For any \( z' \in A^c \), we have either \( \|2w_1x'\| > K \) or \( \|2w_2y'\| > K \). If the former is true, then
\[
\begin{aligned}
\int_{A^c} (\tilde{z}')^{2\lambda} dQ(z') & \leq \int_{A^c} e^{-\frac{K^2}{4w_1^2 s^4}} e^{\frac{2w_1 \|x'\|^2}{4w_1^2 s^4}} (\tilde{z}')^{2\lambda} dQ(z') \\
& \leq C_{|\lambda|,d,w} e^{-\frac{K^2}{4w_1^2 d_1 s^4}} e^{4w_1^2(d_1 + w_2 d_2)s^2} dQ(z') \leq e^{4w_1^2(d_1 + w_2 d_2)s^2} dQ(z') \leq e^{4w_1^2 d_1 s^2 (\|x\| + \sqrt{d}\|z\|)^2 + 4w_2^2 d_2 s^2 (\|y\| + \sqrt{d}\|z\|)^2}.
\end{aligned}
\]
Putting all together, we get
\[
\begin{aligned}
\frac{\int_A (\tilde{z}')^{\lambda} \exp \left\{ g(z') - w_1 \|x'\|^2 - w_2 \|y'\|^2 + 2w_1 \langle x, x' \rangle + 2w_2 \langle y, y' \rangle \right\} dQ(z')}{\int \exp \left\{ g(z') - w_1 \|x'\|^2 - w_2 \|y'\|^2 + 2w_1 \langle x, x' \rangle + 2w_2 \langle y, y' \rangle \right\} dQ(z')} & \leq C_{|\lambda|,d,w} \frac{e^{-\frac{K^2}{2w_1^2 d_1 s^4}} e^{2w_1 d_1 s^2 (\|x\| + \sqrt{d}\|z\|)^2 + 2w_2^2 d_2 s^2 (\|y\| + \sqrt{d}\|z\|)^2} |\lambda|}{C_{|\lambda|,d,w} e^{-\frac{K^2}{2w_1^2 d_1 s^4}} e^{2w_1^2 d_1 s^2 (\|x\| + \sqrt{d}\|z\|)^2 + 2w_2^2 d_2 s^2 (\|y\| + \sqrt{d}\|z\|)^2} |\lambda|}.
\end{aligned}
\]
When \( \|z\| \leq \sqrt{d}\sigma \), it holds that \( \|x\| \leq \sqrt{2d}\sigma \) and \( \|y\| \leq \sqrt{2d}\sigma \). Hence, if we choose \( K^2 = C_{|\lambda|,d,w}(\sigma^4 + \sigma^6) \) for some sufficiently large constant \( C_{|\lambda|,d,w} \), then we have
\[
|M_\lambda| \leq C_{|\lambda|,d,w}\sigma^{|\lambda|}(\sigma + \sigma^2)^{|\lambda|}.
\]
When \( \|z\| > \sqrt{d}\sigma \), if we choose \( K^2 = C_{|\lambda|,d,w}(\sigma^4 \|z\|^2 + \sigma^3 \|z\|) \), then we have
\[
|M_\lambda| \leq C_{|\lambda|,d,w}\sigma^{|\lambda|} \left( \sigma \|z\| + \sqrt{\sigma \|z\|} \right)^{|\lambda|}.
\]

When \( P \) and \( Q \) have bounded support, we can further show that the Schrödinger potentials can be chosen to be bounded.

**Proposition 12.** Assume that \( P \) and \( Q \) are supported on a bounded domain of radius \( D \). Then there exist Schrödinger potentials \( (f,g) \) such that 1) the optimality conditions (15) hold for all \( x, y, z \in \mathbb{R}^d \) and 2) \( \|f\|_\infty \leq 8wD^2 \) and \( \|g\|_\infty \leq 8wD^2 \).

**Proof.** Let \( (f,g) \) the Schrödinger potentials defined in (21). By the proof of Proposition 9, they satisfy (15) everywhere. Moreover, we have
\[
f(z) \leq w_1 E_{Q_X} \|x - X'\|^2 + w_2 E_{Q_Y} \|y - Y'\|^2 \leq 8wD^2
\]
and \( g \) similarly. \( \square \)

### B.2 Controlling the Empirical Process and the U-Process

We then upper bound the \( L^1 \) loss \( E|T_n(X,Y) - T(X,Y)| \) by empirical processes and U-processes.

**Proposition 13** (Corollary 2 (Mena and Weed, 2019)). Let \( P, Q, P', Q' \in M_1(\mathbb{R}^d) \) be subG(\( \sigma^2 \)). Then we have
\[
|S(P',Q') - S(P,Q)| \leq \sup_{f \in \mathcal{F}_\sigma} \left| \int f(dP' - dP) \right| + \sup_{g \in \mathcal{F}_\sigma} \left| \int g(dQ' - dQ) \right|
\]
where \( \mathcal{F}_\sigma \) is defined in Definition 4.

To simply the function class \( \mathcal{F}_\sigma \), we show in Lemma 21 in Appendix D that \((1 + \sigma^{3\alpha})^{-1} \mathcal{F}_\sigma \subset \mathcal{F}^s \) for \( \mathcal{F}^s \) defined below. Consequently, we can separate the sub-Gaussian parameter \( \sigma \) from the function class \( \mathcal{F}_\sigma \).

**Definition 5.** For any \( s \geq 2, d \in \mathbb{N}_+ \), and \( w = (w_1, w_2) \in \mathbb{R}^2_+ \), let \( \mathcal{F}^s := \mathcal{F}^{s,d,w} \) be the set of functions satisfying
\[
|f(z)| \leq C_{s,d,w}(1 + \|z\|^2)
\]
\[
|D^\alpha f(z)| \leq C_{s,d,w}(1 + \|z\|^{|\alpha|}), \quad \forall 1 \leq |\alpha| \leq s,
\]
where \( C_{s,d,w} \) is a constant depending on \( s, d, \) and \( w \).

In order to handle the U-process, we also need a variant function class of \( \mathcal{F}^s \) which we also define below.

**Definition 6.** For any \( \sigma \in \mathbb{R}_+, s \geq 2, d \in \mathbb{N}_+ \), and \( w = (w_1, w_2) \in \mathbb{R}^2_+ \), let \( \mathcal{F}_\sigma^s := \mathcal{F}_{\sigma}^{s,d,w} \) be the set of functions satisfying
\[
|f(z)| \leq C_{s,d,w}(1 + \max\{\|z\|^2, \sigma^2\})
\]
\[
|D^\alpha f(z)| \leq C_{s,d,w}(1 + \max\{\|z\|^{|\alpha|}, \sigma^{|\alpha|}\}), \quad \forall 1 \leq |\alpha| \leq s,
\]
where \( C_{s,d,w} \) is a constant depending on \( s, d, \) and \( w \).
Let us control the complexity of $F_s$ and $F_z$, which is achieved by the following covering number bound.

**Proposition 14.** Let $P \in M_1(\mathbb{R}^d)$ be subG($\sigma^4$). Let $\{Z_i\}_{i=1}^n \sim_{i.i.d.} P$ and $\hat{P}_n$ be the empirical measure. There exists a random variable $L \geq 1$ depending on the sample $\{Z_i\}_{i=1}^n$ with $\mathbb{E}[L] \leq 2$ such that

$$
\log N(\tau, F_s, \mathbf{L}^2(\hat{P}_n)) \leq C_{s,d,w} \tau^{-d/s} L^{d/2s} (1 + \sigma^{2d}) \quad \text{and} \quad \max_{f \in F_s} \|f\|^2_{\mathbf{L}^2(\hat{P}_n)} \leq C_{s,d,w} (1 + L\sigma^4).
$$

Moreover, the same bounds hold for $F_z$.

**Proof of Proposition 14.** Define $L := \frac{1}{\tau} \sum_{i=1}^n \mathbb{E}[|Z_i|^2 / 2d\sigma^2] \geq 1$. By the sub-Gaussianity of $P$, we have $\mathbb{E}[L] \leq 2$. In order to apply (van der Vaart and Wellner, 1996, Corollary 2.7.4), we partition $\mathbb{R}^d$ into $\cup_{j \geq 1} B_j$ where $B_1 := [\sigma, \sigma]^d$ and $B_j := [-j\sigma, j\sigma]^d \setminus \{-(j-1)\sigma, (j-1)\sigma\}^d$ for $j \geq 2$. Since $B_j$ is not convex for $j \geq 2$, we further partition it into disjoint hypercubes $\{B_{j,k}\}_{k=1}^{2^d}$, e.g.,

$$B_{j,1} = [(j-1)\sigma, j\sigma] \times [-j\sigma, j\sigma]^{d-1}.$$

Take any $j \geq 2$ and $k \in [2d]$. Firstly, it holds that

$$\lambda(x : d(x, B_{j,k}) \leq 1) \leq (\sigma + 2)(2j\sigma + 2)^{d-1} \leq C_d (1 + j^d \sigma^d),$$

where $\lambda$ is the Lebesgue measure. Secondly, the mass that $\hat{P}_n$ assigns to $B_{j,k}$ can be bounded as follows:

$$\hat{P}_n(Z \in B_{j,k}) \leq \hat{P}_n \left( \|Z\|^2 > d\sigma^2 (j-1)^2 \right) \leq \hat{P}_n \left[ e^{\|Z\|^2 / 2d\sigma^2} \right] e^{-(j-1)^2 / 2} = Le^{-(j-1)^2 / 2}. \quad (25)$$

Finally, we prove that $F_s \subset C_{\lambda}^*(B_{j,k})$ with $M = C_{s,d,w} (1 + j^s \sigma^s)$, where $C_{\lambda}^*(B_{j,k})$ is the set of continuous functions satisfying

$$\|f\| := \max_{|\alpha| \leq s} \sup_{z \in B_{j,k}} |D^\alpha f(z)| + \max_{|\alpha| = s} \sup_{z, w \in B_{j,k}} |D^\alpha f(z) - D^\alpha f(w)| \leq M.$$

In fact, for any $f \in F_s$, we have

$$\max_{|\alpha| \leq s} \sup_{z \in B_{j,k}} |D^\alpha f(z)| \leq C_{s,d,w} \sup_{z \in B_{j,k}} (1 + \|z\|^s) \leq C_{s,d,w} (1 + j^s \sigma^s),$$

and

$$\max_{|\alpha| = s} \sup_{z, w \in B_{j,k}} |D^\alpha f(z) - D^\alpha f(w)| \leq 2 \max_{|\alpha| = s} \sup_{z \in B_{j,k}} |D^\alpha f(z)| \leq C_{s,d,w} (1 + j^s \sigma^s).$$

Note that the same argument holds for any $f \in F_z$ since we can simply replace $1 + \|z\|^s$ by $1 + \max \{\|z\|^s, \sigma^s\}$. Now, applying (van der Vaart and Wellner, 1996, Corollary 2.7.4) with $r = 2$ and $V = d/s$ leads to

$$\log N(\tau, F_s, \mathbf{L}^2(\hat{P}_n)) \leq C_{s,d,w} \tau^{-d/s} L^{d/2s} \left( 1 + \sum_{j=2}^{2d} \sum_{k=1}^{2^d} (1 + j^d \sigma^d)^{\frac{2^d}{d+s}} (1 + j^s \sigma^s)^{\frac{2^d}{d+s}} e^{-\frac{(j-1)^2}{2d\sigma^2}} \right)^\frac{d+2s}{ds} \leq C_{s,d,w} \tau^{-d/s} L^{d/2s} (1 + \sigma^{2d}) \left( 2 \sum_{j=1}^{2d} j^{4d^2} e^{-\frac{(j-1)^2}{2d\sigma^2}} \right)^\frac{d+2s}{ds} = C_{s,d,w} \tau^{-d/s} L^{d/2s} (1 + \sigma^{2d}),$$

by the summability.

To verify the second inequality, we obtain

$$\max_{f \in F_s} \|f\|_{\mathbf{L}^2(\hat{P}_n)}^2 = \max_{f \in F_s} \hat{P}_n[|f(Z)|^2] \leq C_{s,d,w} \hat{P}_n[(1 + \|Z\|^4)]. \quad (26)$$

Note that $\|Z\|^4 \leq C_d \|Z\|^2 / 2d\sigma^2 \sigma^4$. It follows that $\hat{P}_n[\|Z\|^4] \leq C_d L \sigma^4$, and thus

$$\max_{f \in F_s} \|f\|^2_{\mathbf{L}^2(\hat{P}_n)} \leq C_{s,d,w} (1 + L\sigma^4).$$

Again, the same argument hold for $F_z$ by replacing $\|Z\|^4$ with $\max \{\|Z\|^4, \sigma^4\}$. \qed
With this covering number bound at hand, we can control the empirical process by the metric entropy.

**Proposition 15.** Let \( P \in \mathcal{M}_1(\mathbb{R}^d) \) be sub-G(\( \sigma^2 \)). Let \( \{Z_i\}_{i=1}^n \overset{i.i.d.}{\sim} P \) and \( \hat{P}_n \) be the empirical measure. Then,

\[
\mathbb{E}\| \hat{P}_n - P \|_{\mathcal{F}_s}^2 \leq C_{s,d,w}(1 + \sigma^{2d+4}) \frac{1}{n} \quad \text{for all } s > d/2.
\]

Moreover, the same bound holds for \( \mathcal{F}_s^* \).

**Proof.** Define the symmetrized version of \( \hat{P}_n - P \) by

\[
\| \hat{S}_n \|_{\mathcal{F}_s} := \sup_{f \in \mathcal{F}} \left\| \frac{1}{n} \sum_{i=1}^n \xi_i f(Z_i) \right\|,
\]

where \( \{\xi_i\}_{i=1}^n \) are i.i.d. Rademacher random variables that are independent with \( \{Z_i\}_{i=1}^n \). According to (Wainwright, 2019, Proposition 4.11), it holds that

\[
\mathbb{E}\| \hat{P}_n - P \|_{\mathcal{F}_s}^2 \leq 4 \mathbb{E}\| \hat{S}_n \|_{\mathcal{F}_s}^2.
\]

Conditioning on \( \{Z_i\}_{i=1}^n \), the random variable \( Z(f) := \frac{1}{\sqrt{n}} \sum_{i=1}^n \xi_i f(Z_i) \) is a linear combination of independent Rademacher random variables. Hence, \( Z(f) \) is a sub-Gaussian process (see Definition 7) with respect to

\[
\|f - g\|_{\mathbb{L}^2(\hat{P}_n)} = \sqrt{\frac{1}{n} \sum_{i=1}^n [f(Z_i) - g(Z_i)]^2}.
\]

It then follows from (Giné and Nickl, 2015, Exercise 2.3.1) that

\[
\mathbb{E}_z \sup_{f \in \mathcal{F}} |Z(f)|^2 \leq C \left( \int_0^{\max \tau \mathcal{F}_s} \|f\|_{\mathbb{L}^2(\hat{P}_n)}^2 \sqrt{\log N(\tau, \mathcal{F}_s, \mathbb{L}^2(\hat{P}_n))} d\tau \right)^2
\]

\[
\leq C_{s,d,w} \left( \int_0^{C\sqrt{1 + L^2}} \tau^{-d/2s} L^{d/4s} \sqrt{1 + \sigma^{2d}} d\tau \right)^2, \quad \text{by Proposition 14}
\]

\[
= C_{s,d,w}(1 + \sigma^{2d}) L^{d/2s} (1 + L\sigma^2)^{1-d/2s}, \quad \text{by } s > d/2
\]

\[
\leq C_{s,d,w}(1 + \sigma^{2d+4}) L, \quad \text{by } L \geq 1.
\]

Note that \( \mathbb{E}\| \hat{S}_n \|_{\mathcal{F}_s}^2 = \frac{1}{n} \mathbb{E}\sup_{f \in \mathcal{F}_s} |Z(f)|^2 \). Consequently, we have

\[
\mathbb{E}\| \hat{P}_n - P \|_{\mathcal{F}_s}^2 \leq C_{s,d,w}(1 + \sigma^{2d+4}) \frac{1}{n}.
\]

The same argument holds for \( \mathcal{F}_s^* \) since Proposition 14 holds true for \( \mathcal{F}_s^* \). ∎

**B.3 Proofs of Main Results**

We now prove the main consistency results in Section 3. For simplicity of the notation, we focus on the quadratic cost function, i.e., \( w_1 = w_2 = 1 \), and drop the dependency on \( w \) (e.g., we write \( C_{s,d} = C_{s,d,w} \)). The proofs can be adapted to weighted quadratic costs with minor modifications. Let \( P_X \in \mathcal{M}_1(\mathbb{R}^{d_1}) \) and \( P_Y \in \mathcal{M}_1(\mathbb{R}^{d_2}) \) with \( d := d_1 + d_2 \). Suppose that \( \{(X_i, Y_i)\}_{i=1}^n \) is an i.i.d. sample from some joint distribution \( P_{XY} \) with marginals \( P_X \) and \( P_Y \), where \( P_{XY} \) may or may not equal \( P_X \otimes P_Y \). Let \( P_n \) and \( Q_n \) be the empirical measures of \( \{X_i\}_{i=1}^n \) and \( \{Y_i\}_{i=1}^n \), respectively.
Proof of Proposition 3. The proof is similar to Proposition 14. Define $L_1 := \hat{P}_X [e^{\|X\|^2/(2\sigma^2)}] \geq 1$ and $L_2 := \hat{P}_Y [e^{\|Y\|^2/(2\sigma^2)}] \geq 1$. By the sub-Gaussian assumption, it is clear that $\mathbb{E}[L_1] \leq 2$ and $\mathbb{E}[L_2] \leq 2$. There are two places in the proof of Proposition 14 where the measure is involved. The first place is (25), where we replace it by
\[
(\hat{P}_X \otimes \hat{P}_Y) \{ (X,Y) \in B_{j,k} \} \leq (\hat{P}_X \otimes \hat{P}_Y) \left\{ \|X\|^2 + \|Y\|^2 > d\sigma^2(j-1)^2 \right\}
\]
\[
\leq (\hat{P}_X \otimes \hat{P}_Y) \left\{ \exp \left[ \frac{\|X\|^2 + \|Y\|^2}{4d\sigma^2} \right] \right\} e^{-(j-1)^2/4}, \text{ by Chernoff bound}
\]
\[
= L_1 L_2 e^{-(j-1)^2/4}.
\]
The second place is (26), where we replace it by
\[
\max_{f \in \mathcal{F}} \|f\|_{L^2(\hat{P}_X \otimes \hat{P}_Y)}^2 = \max_{f \in \mathcal{F}} (\hat{P}_X \otimes \hat{P}_Y) \{ |f(X,Y)|^2 \} \leq C_{d_\mathcal{F},d}(\hat{P}_X \otimes \hat{P}_Y) [1 + \|X\|^4 + \|Y\|^4].
\]
Note that $\|Z\|^4 \leq C_d e^{\|Z\|^2/(2\sigma^2)} \sigma^4$. It follows that $(\hat{P}_X \otimes \hat{P}_Y) \{ |X|^4 + |Y|^4 \} \leq C_d (L_1 + L_2) \sigma^4$. Hence, the claim holds true for $L := (L_1 + L_2)/2$. \hfill \Box

Proof of Proposition 4. Step 1. Degeneration and Decoupling. We first consider the case when $P_{XY} = P_X \otimes P_Y$. Let $(X,Y) \sim P_X \otimes P_Y$. For $f \in \mathcal{F}$, we define $\theta_f := \mathbb{E}[f(X,Y)]$,
\[
f_{1,0}(X) := \mathbb{E}[f(X,Y) \mid X] \quad \text{and} \quad f_{0,1}(Y) := \mathbb{E}[f(X,Y) \mid Y].
\]
As a result, $\hat{f}(x,y) := f(x,y) - f_{1,0}(x) - f_{0,1}(y) + \theta_f$ satisfies
\[
\mathbb{E}[\hat{f}(X,Y) \mid X] \overset{a.s.}{=} 0 \quad \Rightarrow \quad \mathbb{E}[\hat{f}(X,Y) \mid Y].
\]
Note that
\[
\mathbb{E} \left[ \left\| \hat{P}_X \otimes \hat{P}_Y - P_X \otimes P_Y \right\|_{\mathcal{F},\mathcal{F}}^2 \right]
\]
\[
= \mathbb{E} \left[ \sup_{f \in \mathcal{F}} \frac{1}{n^2} \sum_{i,j=1}^n (f(X_i,Y_j) - \theta_f) \right]^2
\]
\[
\leq C \mathbb{E} \left[ \sup_{f \in \mathcal{F}} \left( \frac{1}{n^2} \sum_{i,j=1}^n \hat{f}(X_i,Y_j) \right)^2 + \sup_{f \in \mathcal{F}} \left( \frac{1}{n} \sum_{i=1}^n f_{1,0}(X_i) - \theta_f \right)^2 + \sup_{f \in \mathcal{F}} \left( \frac{1}{n} \sum_{i=1}^n f_{0,1}(Y_i) - \theta_f \right)^2 \right]
\]
\[
\leq C \mathbb{E} \left[ \sup_{f \in \mathcal{F}} \left( \frac{1}{n^2} \sum_{i,j=1}^n \hat{f}(X_i,Y_j) \right)^2 + \left\| \hat{P}_X - P_X \right\|_{\mathcal{F},\mathcal{F}}^2 + \left\| \hat{P}_Y - P_Y \right\|_{\mathcal{F},\mathcal{F}}^2 \right], \text{ by Lemma 22.} \tag{31}
\]
Since the last two terms above can be controlled by Proposition 15, it remains to consider the first term.

We then consider the case when $P_{XY} \neq P_X \otimes P_Y$. We use the so-called decoupling technique (Peña and Giné, 1999) to reduce the first term to the case when $P_{XY} = P_X \otimes P_Y$. Note that, by the Cauchy-Schwarz inequality,
\[
\mathbb{E} \left[ \sup_{f \in \mathcal{F}} \left( \frac{1}{n^2} \sum_{i,j=1}^n \hat{f}(X_i,Y_j) \right)^2 \right] \leq C \mathbb{E} \left[ \sup_{f \in \mathcal{F}} \left( \frac{1}{n^2} \sum_{i \neq j} \hat{f}(X_i,Y_j) \right)^2 \right].
\]
Note that the second term on the RHS is a lower order term and can be taken care of by Proposition 15. Hence, it suffices to control the first term. Let $\{\xi_i\}_{i=1}^n$ be i.i.d. Rademacher random variables and $\{(X_{i}',Y_{i}')\}_{i=1}^n$ be an independent copy of $\{(X_i,Y_i)\}_{i=1}^n$. Define
\[
A_i := \begin{cases} X_i & \text{if } \xi_i = 1 \\ X_i' & \text{if } \xi_i = -1 \end{cases} \quad \text{and} \quad B_i := \begin{cases} Y_i' & \text{if } \xi_i = 1 \\ Y_i & \text{if } \xi_i = -1 \end{cases}.
\]
For any functional \( F : \mathcal{F}^* \to \mathbb{R}_+ \), let \( \Phi(F) := \sup_{f \in \mathcal{F}^*} F(f)^2 \). For instance, we define \( U_{X,Y}(f) := \frac{1}{n^2} \sum_{i \neq j} \hat{f}(X_i, Y_j) \). It is clear that \( \Phi \) is convex and increasing, and the target reads

\[
\mathbb{E}[\Phi(U_{X,Y})] = \mathbb{E} \left[ \Phi \left( \frac{1}{n^2} \sum_{i \neq j} \mathbb{E} \left[ \hat{f}(X_i, Y_j) + \hat{f}(X_i', Y_j) + \hat{f}(X_i, Y_j') + \hat{f}(X_i', Y_j') \mid Z \right] \right) \right],
\]

where \( Z := \{(X_i, Y_j)\}_{i=1}^n \). Since, for any \( i \neq j \),
\[
\hat{f}(X_i, Y_j) + \hat{f}(X_i', Y_j) + \hat{f}(X_i, Y_j') + \hat{f}(X_i', Y_j') = 4 \mathbb{E} \left[ \hat{f}(A_i, B_j) \mid Z, Z' \right],
\]

it follows from the convexity and the monotonicity of \( \Phi \) that
\[
\mathbb{E}[\Phi(U_{X,Y})] \leq \mathbb{E}[\Phi(4U_{A,B})].
\]

Finally, the joint distribution of \((X_1, \ldots, X_n, Y_1', \ldots, Y_n')\) is the same as \((A_1, \ldots, A_n, B_1, \ldots, B_n)\), so we have
\[
\mathbb{E}[\Phi(U_{X,Y})] \leq \mathbb{E}[\Phi(4U_{X,Y'})].
\]

Adding back the diagonal terms proves the claim since \((X_i, Y_i') \sim P_X \otimes P_Y \).

**Step 2. Randomization.** We work under the measure \( P_{XY} = P_X \otimes P_Y \). Note that

\[
\mathbb{E} \left[ \sup_{f \in \mathcal{F}^*} \left( \frac{1}{n^2} \sum_{i,j=1}^n \hat{f}(X_i, Y_j) \right)^2 \right] = \mathbb{E}_Y \mathbb{E}_X \left[ \sup_{f \in \mathcal{F}^*} \left( \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n \hat{f}(X_i, Y_j) - \mathbb{E}_{X'} \left[ \sum_{j=1}^n \hat{f}(X_i', Y_j) \right] \right)^2 \right], \text{ by (30)}
\]

\[
\leq \mathbb{E}_Y \mathbb{E}_{X,X',\varepsilon} \left[ \sup_{f \in \mathcal{F}^*} \left( \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n \varepsilon_i \left[ \sum_{j=1}^n \hat{f}(X_i, Y_j) - \sum_{j=1}^n \hat{f}(X_i', Y_j) \right] \right)^2 \right], \text{ by Jensen’s inequality}
\]

\[
= \mathbb{E}_Y \mathbb{E}_{X,X',\varepsilon} \left[ \sup_{f \in \mathcal{F}^*} \left( \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n \varepsilon_i \hat{f}(X_i, Y_j) \right)^2 \right], \text{ by the Cauchy-Schwarz inequality.}
\]

Repeating above arguments gives
\[
\mathbb{E} \left[ \sup_{f \in \mathcal{F}^*} \left( \frac{1}{n^2} \sum_{i,j=1}^n \hat{f}(X_i, Y_j) \right)^2 \right] \leq C \mathbb{E} \left[ \sup_{f \in \mathcal{F}^*} \left( \frac{1}{n^2} \sum_{i,j=1}^n \varepsilon_i \varepsilon_j' \hat{f}(X_i, Y_j) \right)^2 \right] \leq C \mathbb{E} \left[ \sup_{f \in \mathcal{F}^*} \left( \frac{1}{n^2} \sum_{i,j=1}^n \varepsilon_i \varepsilon_j' \hat{f}(X_i, Y_j) \right)^2 \right],
\]

where the last inequality follows from the Cauchy-Schwarz inequality and Jensen’s inequality. Hence, it suffices to bound
\[
A := \mathbb{E} \sup_{f \in \mathcal{F}^*} \left( \frac{1}{n^2} \sum_{i,j=1}^n \varepsilon_i \varepsilon_j' \hat{f}(X_i, Y_j) \right)^2.
\]
Step 3. Metric entropy. Define the process $Z(f) := \frac{1}{n^{3/2}} \sum_{i,j=1}^{n} \varepsilon_i \varepsilon_j f(X_i, Y_j)$ for any $f \in \mathcal{F}_s$. We claim that it is a sub-Gaussian process with respect to

$$\|f - g\|_{L^2(p_n \otimes q_n)} = \sqrt{\frac{1}{n^2} \sum_{i,j=1}^{n} \|f(X_i, Y_j) - g(X_i, Y_j)\|^2}. \quad (32)$$

To prove it, let us control the moment generating function of the increment $Z(f) - Z(g)$. Denote $a_i := \sum_{j=1}^{n} \varepsilon_j f(X_i, Y_j) - g(X_i, Y_j))$. Conditioning on $\{X_i, Y_i, \varepsilon_i\}_{i=1}^{n}$,

$$Z(f) - Z(g) = \frac{1}{n^{3/2}} \sum_{i=1}^{n} a_i \varepsilon_i$$

is a linear combination of independent Rademacher random variables. Consequently,

$$\mathbb{E}_\varepsilon \exp \{\lambda |Z(f) - Z(g)|\} \leq \exp \left\{ \frac{\lambda^2 \sum_{i=1}^{n} a_i^2}{2n^3} \right\}. \quad (33)$$

Note that, by the Cauchy-Schwarz inequality,

$$a_i^2 \leq \left[ \sum_{j=1}^{n} (\varepsilon_j')^2 \right] \left[ \sum_{j=1}^{n} |f(X_i, Y_j) - g(X_i, Y_j)|^2 \right] = n \left[ \sum_{j=1}^{n} |f(X_i, Y_j) - g(X_i, Y_j)|^2 \right].$$

This yields that

$$\mathbb{E}_\varepsilon \exp \{\lambda |Z(f) - Z(g)|\} \leq \exp \left\{ \frac{\lambda^2 \sum_{i,j=1}^{n} |f(X_i, Y_j) - g(X_i, Y_j)|^2}{2n^2} \right\} = \exp \left\{ \frac{\lambda^2 \|f - g\|_{L^2(p_n \otimes q_n)}^2}{2} \right\}, \quad (34)$$

and thus the claim follows. Analogous to the proof of Proposition 15, we obtain, by Proposition 3, that

$$A = \frac{1}{n} \mathbb{E} \sup_{f \in \mathcal{F}_s} |Z(f)|^2 \leq C_{s,d}(1 + \sigma^{2d+4}) \frac{1}{n}.$$ 

Therefore, by (31), we have

$$\mathbb{E} \bigg\| \hat{P}_n \otimes \hat{Q}_n - P \otimes Q \bigg\|_{\mathcal{F}_s}^2 \leq C_{s,d}(1 + \sigma^{2d+4}) \frac{1}{n}. \quad \square$$

Remark 6. Note that, when $\mathcal{F}$ is a singleton, the quantity $\mathbb{E} \bigg\| \hat{P}_n \otimes \hat{Q}_n - P \otimes Q \bigg\|_{\mathcal{F}_s}^2$ reduces to the variance of a two-sample U-statistic, which can be shown to be of order $O(n^{-1})$. This implies that the bound in Proposition 4 is tight in terms of the dependency on $n$.

Now we are ready to prove Theorem 2.

Proof of Theorem 2. We prove the statement for $\varepsilon = 1$ and write $S := S_1$. The result for general $\varepsilon > 0$ follows immediately from Lemma 23. By the triangle inequality, it holds that

$$|T_n(X, Y) - T(X, Y)| \leq \left| S(\hat{P}_{XY}, \hat{P}_X \otimes \hat{P}_Y) - S(P_{XY}, P_X \otimes P_Y) \right| + \frac{1}{2} \left| S(\hat{P}_{XY}, \hat{P}_{XY}) - S(P_{XY}, P_{XY}) \right| + \frac{1}{2} \left| S(\hat{P}_X \otimes \hat{P}_Y, \hat{P}_X \otimes \hat{P}_Y) - S(P_X \otimes P_Y, P_X \otimes P_Y) \right|. \quad (35)$$

We begin with deriving the bound for the first term

$$A := \left| S(\hat{P}_{XY}, \hat{P}_X \otimes \hat{P}_Y) - S(P_{XY}, P_X \otimes P_Y) \right|. \quad (36)$$
Step 1. Upper bound via empirical processes. According to Lemma 18 and Lemma 19, the joint distribution $P_{XY}$ is subG($2\sigma^2$), and thus there exist a zero-measure set $S_{P_{XY}} \subset \Omega$ and a random variable $\sigma_{P_{XY}}^r$ such that $\hat{P}_{XY}(\omega)$ and $P_{XY}$ are subG($\sigma_{P_{XY}}^r(\omega)$) for every $\omega \in S_{P_{XY}}$. Similarly, by Lemma 20, there exist a zero-measure set $S_{P_X, P_Y} \subset \Omega$ and a random variable $\sigma_{P_X, P_Y}^r$ such that $\hat{P}_X(\omega) \otimes \hat{P}_Y(\omega)$ and $P_X \otimes P_Y$ are subG($\sigma_{P_X, P_Y}^r(\omega)$) for every $\omega \in S_{P_X, P_Y}$. Take $S := S_{P_{XY}} \cap S_{P_X, P_Y}$ and $\sigma^2 := \max\{\sigma^2_{P_{XY}}, \sigma^2_{P_X, P_Y}\}$. It follows that $\hat{P}_{XY}(\omega), \hat{P}_X(\omega) \otimes \hat{P}_Y(\omega), P_{XY}$, and $P_X \otimes P_Y$ are subG($\sigma^2(\omega)$) for every $\omega \in S$. Now, by Proposition 13,

$$\sup_{f \in F_{\sigma(\omega)}} \left| \int f(d\hat{P}_{XY}(\omega) - dP_{XY}) + \sup_{g \in F_{\sigma(\omega)}} \left| \int g(d\hat{P}_X(\omega) \otimes \hat{P}_Y(\omega) - dP_X \otimes P_Y) \right|, \ \forall \omega \in S. \right.$$ 

Note that $P(S) = P(S_{P_{XY}} \cap S_{P_X, P_Y}) = 1$. This implies, almost surely,

$$A \leq \sup_{f \in F_{\sigma}} \left| \int f(d\hat{P}_{XY} - dP_{XY}) + \sup_{g \in F_{\sigma}} \left| \int g(d\hat{P}_X \otimes \hat{P}_Y - dP_X \otimes P_Y) \right| \right. \tag{37}$$

According to Lemma 21, we have

$$E[A] \leq E \left[ (1 + \sigma^3) \left\| \hat{P}_{XY} - P_{XY} \right\|_{F_{\sigma}} \right] + E \left[ (1 + \sigma^3) \left\| \hat{P}_X \otimes \hat{P}_Y - P_X \otimes P_Y \right\|_{F_{\sigma}} \right] \leq \sqrt{E[(1 + \sigma^3)^2] \left( E \left\| \hat{P}_{XY} - P_{XY} \right\|^2_{F_{\sigma}} + E \left\| \hat{P}_X \otimes \hat{P}_Y - P_X \otimes P_Y \right\|^2_{F_{\sigma}} \right).}$$

Step 2. Control empirical processes via metric entropy. Let $s = [d/2] + 1$. Since the joint probability $P_{XY}$ is subG($2\sigma^2$), it follows from Proposition 15 that

$$\sqrt{E \left\| \hat{P}_{XY} - P_{XY} \right\|^2_{F_{\sigma}}} \leq C_d(1 + \sigma^{d+2}) \frac{1}{\sqrt{n}}. \tag{38}$$

The same bound holds for $\sqrt{E \left\| \hat{P}_X \otimes \hat{P}_Y - P_X \otimes P_Y \right\|^2_{F_{\sigma}}}$ by Proposition 4. Note that

$$E[(1 + \sigma^3)^2] \leq C(1 + \sigma^{6s}) \leq C_s(1 + E \sigma_{P_{XY}}^{6s} + E \sigma_{P_X, P_Y}^{6s}) \leq C_s(1 + \sigma^{6s}),$$

where the last inequality follows from Lemma 18 and Lemma 20. Recall that we have chosen $s = [d/2] + 1$. As a result, $E[A] \leq C_d(1 + \sigma^{[5d/2]+6})n^{-1/2}$. A similar argument shows that the same bound hold for the second and third term in (35). Hence,

$$E[T_n(X, Y)] \leq C_d(1 + \sigma^{[5d/2]+6}) \frac{1}{\sqrt{n}}. \tag{39}$$

C Exponential Tail Bounds

We now prove the exponential tail bound in Section 3. For simplicity of the notation, we focus on the quadratic cost function, i.e., $w_1 = w_2 = 1$, and drop the dependency on $w$ (e.g., we write $C_{s,d} = C_{s,d,w}$. The proofs can be adapted to weighted quadratic costs with minor modifications. Let $P_X \in \mathcal{M}_1(\mathbb{R}^d)$ and $P_Y \in \mathcal{M}_1(\mathbb{R}^d)$ with $d := d_1 + d_2$. Suppose that $\{(X_i, Y_i)\}_{i=1}^n$ is an i.i.d. sample from some joint distribution $P_{XY}$ with marginals $P_X$ and $P_Y$, where $P_{XY}$ may or may not equal $P_X \otimes P_Y$. Let $P_n$ and $\hat{Q}_n$ be the empirical measures of $\{X_i\}_{i=1}^n$ and $\{Y_i\}_{i=1}^n$, respectively.

**Proposition 16.** For any $b$-uniformly bounded class of functions $\mathcal{F}$, we have

$$\mathbb{P} \left\{ \left\| \hat{P}_X \otimes \hat{P}_Y - P_X \otimes P_Y \right\|_{\mathcal{F}} - E \left\| \hat{P}_X \otimes \hat{P}_Y - P_X \otimes P_Y \right\|_{\mathcal{F}} > t \right\} \leq \exp \left( -\frac{nt^2}{8b^2} \right), \ \text{for any } t \geq 0.$$
Proof. For any function $f$ defined on $\mathbb{R}^d$, we define $\tilde{f}(x, y) = f(x, y) - (P_X \otimes P_Y)[f]$. As a results, we have $\|\tilde{P}_X \otimes \tilde{P}_Y - P_X \otimes P_Y \|_F = \sup_{f \in F} \left| \frac{1}{n^2} \sum_{i,j=1}^n \tilde{f}(X_i, Y_j) \right|$. Consider the function

$$F(z_1, \ldots, z_n) := \sup_{f \in F} \left| \frac{1}{n^2} \sum_{i,j=1}^n \tilde{f}(x_i, y_j) \right|,$$

where $z_i = (x_i, y_i) \in \mathbb{R}^d$. We claim that $F$ satisfies the bounded difference property required in the McDiarmid inequality. Since $F$ is permutation invariant, it suffices to verify the property for the first coordinate. Let $z'_i \neq z_i$ for all $i \neq 1$. It holds that

$$\left| \frac{1}{n^2} \sum_{i,j=1}^n \tilde{f}(x_i, y_j) - F(z'_1, \ldots, z'_n) \right| \leq \frac{1}{n^2} \sum_{i,j=1}^n \left| \tilde{f}(x_i, y_j) - \tilde{f}(x'_i, y'_j) \right| \leq \frac{4b}{n},$$

where the last inequality uses the boundedness of $f$. Taking the supremum over $F$ yields that $F(z_1, \ldots, z_n) - F(z'_1, \ldots, z'_n) \leq 4b/n$. By symmetry, it follows that $|F(z_1, \ldots, z_n) - F(z'_1, \ldots, z'_n)| \leq 4b/n$. Note that $\{Z_i := (X_i, Y_i)\}_{i=1}^n$ is an i.i.d. sample. According to the McDiarmid inequality, it holds that

$$\mathbb{P} \left\{ \left\| \tilde{P}_X \otimes \tilde{P}_Y - P_X \otimes P_Y \right\|_F - \mathbb{E} \left\| \tilde{P}_X \otimes \tilde{P}_Y - P_X \otimes P_Y \right\|_F > t \right\} \leq \exp \left( -\frac{nt^2}{8b^2} \right), \text{ for any } t \geq 0.$$ 



Proof of Theorem 5. We prove the statement for $\varepsilon = 1$ and write $S := S_1$. The result for general $\varepsilon > 0$ follows immediately from Lemma 23. By the bounded support assumption, it holds that $P_X$ and $P_Y$ are both subG($D^2/d$). According to the proof of Lemma 18, we have $\{\tilde{P}_X\}_{n \geq 1}, \{\tilde{P}_Y\}_{n \geq 1}, P_X,$ and $P_Y$ are uniformly subG($\tau^2$) for $\tau^2 := D^2e^{1/2}/d \leq 2D^2/d$. Moreover, it follows from Lemma 19 that $\{\tilde{P}_{XY}\}_{n \geq 1}$ and $P_{XY}$ are uniformly subG($2\tau^2$). As a result, we obtain, by Proposition 13,

$$A := \left| S(\tilde{P}_{XY}, \tilde{P}_X \otimes \tilde{P}_Y) - S(P_{XY}, P_X \otimes P_Y) \right| \leq \sup_{f \in F_2^r} \left| \int f(d\tilde{P}_{XY} - dP_{XY}) \right| + \sup_{g \in F_1} \left| \int g(d\tilde{P}_X \otimes \tilde{P}_Y - dP_X \otimes P_Y) \right|.$$ 

Fix $s = [d/2] + 1$. According to Lemma 21, we have

$$A \leq C_d(1 + D^{3d+12}) \left[ \left\| \tilde{P}_{XY} - P_{XY} \right\|_{F^s} + \left\| \tilde{P}_X \otimes \tilde{P}_Y - P_X \otimes P_Y \right\|_{F^s} \right],$$

where we have used $\tau^{3s} \leq C_d D^{3d+12}$. Proposition 12 shows that we can further constraint the function class $F^s$ to $F^s_\delta := \{f \in F^s : \|f\|_{\infty} \leq \delta \}$ for $b = 2D^2$. Hence, by (Wainwright, 2019, Theorem 4.10), it holds that

$$\mathbb{P} \left\{ \left\| \tilde{P}_{XY} - P_{XY} \right\|_{F^s_\delta} - \mathbb{E} \left\| \tilde{P}_{XY} - P_{XY} \right\|_{F^s_\delta} > t \right\} \leq \exp \left( -\frac{nt^2}{2b^2} \right), \text{ for any } t \geq 0.$$ 

It is clear from Proposition 15 that

$$\mathbb{E} \left\| \tilde{P}_{XY} - P_{XY} \right\|_{F^s_\delta} \leq \mathbb{E} \left\| \tilde{P}_{XY} - P_{XY} \right\|_{F^s} \leq C_d(1 + D^{2d+4}) \frac{1}{\sqrt{n}}.$$ 

Consequently, we get

$$\mathbb{P} \left\{ \left\| \tilde{P}_{XY} - P_{XY} \right\|_{F^s_\delta} > t + C_d(1 + D^{2d+4}) \frac{1}{\sqrt{n}} \right\} \leq \exp \left( -\frac{nt^2}{2b^2} \right), \text{ for any } t \geq 0.$$ 

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Similarly, using Proposition 4 and Proposition 16, we obtain
\[
P\left\{ \left\| \hat{P}_{XY} - P_{XY} \right\|_{F^2} > t + C_d(1 + D^{2d+4}) \frac{1}{\sqrt{n}} \right\} \leq \exp\left(-\frac{nt^2}{8b^2}\right), \quad \text{for any } t \geq 0.
\]
Now it follows from (41) that
\[
P\left\{ A \geq C_d(1 + D^{3d+12}) \left[ t + (1 + D^{2d+4}) \frac{1}{\sqrt{n}} \right] \right\} \leq 2 \exp\left(-\frac{nt^2}{8b^2}\right), \quad \text{for any } t \geq 0.
\]
Analogously, we have, for any \( t \geq 0 \)
\[
P\left\{ B \geq C_d(1 + D^{3d+12}) \left[ t + (1 + D^{2d+4}) \frac{1}{\sqrt{n}} \right] \right\} \leq 2 \exp\left(-\frac{nt^2}{8b^2}\right)
\]
and
\[
P\left\{ B' \geq C_d(1 + D^{3d+12}) \left[ t + (1 + D^{2d+4}) \frac{1}{\sqrt{n}} \right] \right\} \leq 2 \exp\left(-\frac{nt^2}{8b^2}\right),
\]
where \( B := |S(\hat{P}_{XY}, \hat{P}_{XY}) - S(P_{XY}, P_{XY})| \) and \( B' := |S(\hat{P}_X \otimes \hat{P}_Y, \hat{P}_X \otimes \hat{P}_Y) - S(P_X \otimes P_Y, P_X \otimes P_Y)|. \)
Since \( |T_n(X, Y) - T(X, Y)| \leq A + \frac{B}{2} + \frac{B'}{2} \), it holds that
\[
P\left\{ |T_n(X, Y) - T(X, Y)| \geq C_d(1 + D^{3d+12}) \left[ t + (1 + D^{2d+4}) \frac{1}{\sqrt{n}} \right] \right\} \leq 6 \exp\left(-\frac{nt^2}{8b^2}\right).
\]
Therefore, we have, with probability at least \( 1 - \delta \),
\[
|T_n(X, Y) - T(X, Y)| \leq C_d \left( 1 + D^{2d+2} \sqrt{\log \frac{6}{\delta}} \right) \frac{D^{3d+14}}{\sqrt{n}}.
\]
\[\square\]

D Technical Lemmas

In this section, we give several technical lemmas used to prove the main results. We use \( C \) to denote a constant whose value may change from line to line.

**Lemma 17.** If \( P \in \mathcal{M}_1(\mathbb{R}^d) \) is subG(\( \sigma^2 \)), then, for any \( k \in \mathbb{N}_+ \),
\[
\mathbb{E}_P \|Z\|^{2k} \leq (2d\sigma^2)^k k!.
\]
Moreover, for any \( v \in \mathbb{R}^d \), it holds that
\[
\mathbb{E}_P e^{(v, Z)} \leq \mathbb{E}_P e^{\|v\|Z} \leq 2e^{d\sigma^2\|v\|^2} / 2.
\]
**Proof.** By Taylor’s expansion, we have
\[
e^{\|Z\|^2/2\sigma^2} - 1 \geq \frac{\|Z\|^{2k}}{(2\sigma^2)^k k!}.
\]
Taking the expectation on both sides gives
\[
\mathbb{E}_P \|Z\|^{2k} \leq (2d\sigma^2)^k k!.
\]
The inequalities (43) follows from the Cauchy-Schwarz inequality and the sub-gaussianity of \( P \). \[\square\]

**Lemma 18.** Let \( P \in \mathcal{M}_1(\mathbb{R}^d) \) be subG(\( \sigma^2 \)) and \( \hat{P}_n \) be the empirical measure. There exist a zero-measure set \( S_P \subset \Omega \) and a random variable \( \sigma^2_P \) depending on the sample \( \{Z_i\}_{i=1}^n \) such that \( \hat{P}_n(\omega) \) and \( P \) are subG(\( \sigma^2_P(\omega) \)) for any \( \omega \in S_P \), and, for any \( k \in \mathbb{N}_+ \),
\[
\mathbb{E}\sigma^{2k}_P \leq 2k^k \sigma^{2k}.
\]

We call it a sub-Gaussian process with respect to a metric \( \sigma \).

Lemma 21. \( 2019 \) without proof.

Take any \( P \).

Definition 7 (Sub-Gaussian process) Similar to Lemma 18.

Lemma 20. If \( P \).

Proof. By the strong law of large numbers, there exists a zero-measure set \( S_P \subset \Omega \) such that, for all \( \omega \in S_P \),

\[
\hat{P}_n(\omega) \left[ e^{\|Z\|^2/2d\sigma^2} \right] \to P \left[ e^{\|Z\|^2/2d\sigma^2} \right] \leq 2, \quad \text{as} \quad n \to \infty. \tag{44}
\]

Let \( \tau^2 := \sup_n \hat{P}_n \left[ e^{\|Z\|^2/2d\sigma^2} \right] \). It follows from (44) that \( \tau^2(\omega) \) is finite for all \( \omega \in S_P \). Since \( \tau^2(\omega) \geq 1 \), by Jensen’s inequality, we obtain, for all \( \omega \in S_P \)

\[
\hat{P}_n(\omega) \left[ e^{\|Z\|^2/2d\sigma^2} \right] \leq \left( \hat{P}_n(\omega) \left[ e^{\|Z\|^2/2d\sigma^2} \right] \right)^{1/\tau^2(\omega)} \leq (\tau^2(\omega))^{1/\tau^2(\omega)} < 2.
\]

As a result, \( \hat{P}_n(\omega) \) is \( subG(\sigma^2\tau^2(\omega)) \). Moreover, \( P \) is also \( subG(\sigma^2\tau^2(\omega)) \) since \( \tau^2(\omega) \geq 1 \). Applying the same argument to \( \frac{\sigma^2}{\tau_k} := \sup_n \hat{P}_n \left[ e^{\|Z\|^2/2k\sigma^2d\sigma^2} \right] \) implies that \( \hat{P}_n(\omega) \) and \( P \) are both \( subG(k\sigma^2\tau^2_k(\omega)) \). Define \( \sigma^2_P := \min_{k \geq 1} k\sigma^2\tau^2_k \). Then we have, for each \( k \geq 1 \),

\[
E_P[\sigma^2_P^2] \leq E_P \left[ \hat{P}_n \left[ k^2\sigma^2_k e^{\|Z\|^2/2d\sigma^2} \right] \right] = k^2 \sigma^2 e^{\|Z\|^2/2d\sigma^2} \leq 2k^2 \sigma^2.
\]

The sub-Gaussianity of two marginals implies the sub-Gaussianity of the joint.

Lemma 19. If \( P_X \) and \( P_Y \) are \( subG(\sigma^2) \), then \( P_{XY} \) is \( subG(2\sigma^2) \) for any \( P_{XY} \in \Pi(P_X, P_Y) \).

Proof. By the Cauchy-Schwarz inequality,

\[
E_{P_{XY}} e^{\|Z\|^2/4d\sigma^2} = E_{P_{XY}} \left[ e^{\|X\|^2/4d\sigma^2} e^{\|Y\|^2/4d\sigma^2} \right] \leq \sqrt{E_{P_X} [e^{\|X\|^2/2d\sigma^2}] E_{P_Y} [e^{\|Y\|^2/2d\sigma^2}]}.
\]

Since \( P_X \) and \( P_Y \) are \( subG(\sigma^2) \), it follows that \( E_{P_{XY}} e^{\|Z\|^2/4d\sigma^2} \leq 2 \) and thus \( P_{XY} \) is \( subG(2\sigma^2) \).

The next result is for the uniform sub-Gaussianity of the product of two empirical measures.

Lemma 20. If \( P_X \) and \( P_Y \) are \( subG(\sigma^2) \), then there exist a zero-measure set \( S_{P_X, P_Y} \subset \Omega \) and a random variable \( \sigma^2_{P_{X, P_Y}} \), depending on the sample \( \{(X_i, Y_i)\}_{i=1}^n \) such that \( \hat{P}_n(\omega) \otimes \hat{P}_n(\omega) \) and \( P_X \otimes P_Y \) are \( subG(\sigma^2_{P_{X, P_Y}}(\omega)) \) for any \( \omega \in S_{P_X, P_Y} \), and, for any \( k \in \mathbb{N}_+ \),

\[
E_{P_X, P_Y} \sigma^2_{P_{X, P_Y}} \leq 2^{k+1} k \sigma^2.
\]

Proof. Similar to Lemma 18.

The sub-Gaussian processes play an central role in our analysis. We give its definition here; see, e.g., (Wainwright, 2019, Section 5.3).

Definition 7 (Sub-Gaussian process). Let \( \{Z(\theta) : \theta \in \Theta\} \) be a collection of mean-zero random variables. We call it a sub-Gaussian process with respect to a metric \( \rho \) in \( \Theta \) if

\[
E[e^{\lambda (Z(\theta) - Z(\theta'))}] \leq \exp \left[ \lambda^2 \rho^2(\theta, \theta')/2 \right].
\]

To facilitate the analysis of \( F_\sigma \) defined in Proposition 10, it is convenient to separate the sub-Gaussian parameter from the function class by the following lemma. Note that this result is used in (Mena and Weed, 2019) without proof.

Lemma 21. For any \( \sigma > 0 \) and \( s \geq 2 \), we have \( \frac{1}{1+s^{\sigma^2}} F_\sigma \subset F^s \), where \( F^s := F^{s, d, w} \) is defined in Definition 5.

Proof. Take any \( f \in F_\sigma \), it suffices to show \( f/(1+\sigma^2) \in F^s \). According to Proposition 10, it holds that

\[
|f(z)| - w_1 \|z\|^2 - w_2 \|y\|^2 \leq f(z) - w_1 \|z\|^2 - w_2 \|y\|^2 \leq C_{k, d, w} \left\{ \frac{(1+\sigma^4)}{[1+(1+\sigma^2)\|z\|^2]} \right\} \text{ if } \|z\| \leq \sqrt{d}\sigma.
\]

\[
\left\{ \frac{(1+\sigma^4)}{[1+(1+\sigma^2)\|z\|^2]} \right\} \text{ if } \|z\| > \sqrt{d}\sigma.
\]

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Consequently,
\[ \left| \frac{f(z)}{1 + \sigma^{3s}} \right| \leq C_{k,d,w} \left\{ \begin{array}{ll}
\frac{1 + \sigma^4}{1 + (1 + \sigma^2)\|z\|^2} & \text{if } \|z\| \leq \sqrt{d}\sigma \\
1 + \sigma^{3s} & \text{if } \|z\| > \sqrt{d}\sigma.
\end{array} \right. \]

Since \( s \geq 2 \), it is clear that \( \frac{1 + \sigma^4}{1 + \sigma^2} \leq C \) and \( 1 + \sigma^{3s} \leq C \), and thus
\[ \left| \frac{f(z)}{1 + \sigma^{3s}} \right| \leq C_{k,d,w}(1 + \|z\|^2). \]

The other inequality can be proved analogously.

**Lemma 22.** Let \( P \in \mathcal{M}_1(\mathbb{R}^{d_1}) \) and \( Q \in \mathcal{M}_1(\mathbb{R}^{d_2}) \) be sub\( G(\sigma^2) \). Denote \( d := d_1 + d_2 \). For any \( s \geq 1 \) and \( f \in \mathcal{F}_s^* \), there exist constants \( C_{s,d,w} \) such that \( f_{1,0} \in \mathcal{F}_s^* \) and \( f_{0,1} \in \mathcal{F}_s^* \), where \( \mathcal{F}_s^* \) is defined in Definition 6,
\[ f_{1,0}(x) := \int f(x,y)dQ(y) \quad \text{and} \quad f_{0,1}(y) := \int f(x,y)dP(x). \]

**Proof.** We only prove it for \( f_{1,0} \). By Jensen’s inequality, it holds that
\[ |f_{1,0}(x)| \leq \int |f(x,y)|dQ(y) \leq C_{s,d,w} \left( \|x\|^2 + \int \|y\|^2dQ(y) \right) \leq C_{s,d,w}(1 + \max\{\|x\|^2, \sigma^2\}), \]
where the last inequality follows from Lemma 17. The inequality for \( |D^\alpha f_{1,0}(x)| \) can be verified similarly.

The next lemma suggests that it is enough to consider the case \( \varepsilon = 1 \) for \( S_\varepsilon \).

**Lemma 23.** Let \( \varepsilon > 0 \). For any \( P,Q \in \mathcal{M}_1(\mathbb{R}^d) \), it holds that
\[ S_\varepsilon(P,Q) = \varepsilon S(P^\varepsilon, Q^\varepsilon), \]
where \( P^\varepsilon \) and \( Q^\varepsilon \) are the pushforwards of \( P \) and \( Q \) under the map \( x \mapsto \varepsilon^{-1/2}x \), respectively.

**Proof.** By a change of variable argument.

### E Additional Experimental Results

#### E.1 Adaptive ETIC Test

Recall from (8) that the adaptive ETIC test is defined as
\[ \psi_a(\alpha) := 1 \left\{ \max_{\varepsilon \in \varepsilon^*} \mathcal{T}_{n,\alpha}^\varepsilon(X,Y) > H_{n,\varepsilon}(\alpha) \right\}. \]
Figure 8: Power curves in the linear dependency model (left) and subspaces dependency model (right).

In order to compute $\hat{T}_{n,\varepsilon}(X,Y)$, we use resampling (20 permutations) to estimate the mean and standard deviation of $T_{n,\varepsilon}(X,Y)$.

Following the trick in Section 4, we select the cost function to be the weighted quadratic cost with weights given by the median heuristic. We set $E = \{0.25, 1, 4\}$ and perform the adaptive ETIC test on the linear dependency model and the subspace dependency model. As shown in Figure 7, it is slightly worse than the best ETIC test in both models. We also run it on the bilingual text data. The power and type I error rate of adaptive ETIC are 1 and 0.07 on the dependent sample and the independent sample, respectively. The power achieved is 0.535 on the partially dependent sample; whereas the worst and best power of ETIC are 0.38 and 0.635, respectively.

Finally, we consider a Bonferroni-type ETIC test which is adaptive to both the regularization parameter and the weights in the cost function. Following the formulation in Section 4, we let $\psi_{r_1,r_2}(\alpha)$ be the decision rule of ETIC with hyper-parameters $r_1$ and $r_2$. Consider the following Bonferroni-type ETIC test

$$\psi(\alpha) := \max_{r_1,r_2 \in \mathcal{R}} \psi_{r_1,r_2}(\alpha/|\mathcal{R}|).$$

We perform this Bonferroni-type ETIC test on the linear dependency model and the subspace dependency model for $\mathcal{R} = \{0.25, 4\}$. As shown in Figure 8, it is slightly worse than the best ETIC test in both models. Compared to the adaptive ETIC test, it performs similar in the linear dependency model and slightly better in the subspace dependency model. We also run it on the bilingual text data. The power and type I error rate of adaptive ETIC are 1 and 0.045 on the dependent sample and the independent sample, respectively. The power achieved is 0.5 on the partially dependent sample, which is smaller than the power of the adaptive ETIC.