Universal Hypothesis Testing with Kernels: Asymptotically Optimal Tests for Goodness of Fit

Abstract

We characterize the asymptotic performance of nonparametric goodness of fit testing. The exponential decay rate of the type-II error probability is used as the asymptotic performance metric, and a test is optimal if it achieves the maximum rate subject to a constant level constraint on the type-I error probability. We show that two classes of Maximum Mean Discrepancy (MMD) based tests attain this optimality on $\mathbb{R}^d$, while the quadratic-time Kernel Stein Discrepancy (KSD) based tests achieve the maximum exponential decay rate under a relaxed level constraint. Under the same performance metric, we proceed to show that the quadratic-time MMD based two-sample tests are also optimal for general two-sample problems, provided that kernels are bounded continuous and characteristic. Key to our approach are Sanov’s theorem from large deviation theory and the weak metrizable properties of the MMD and KSD.

1 Introduction

Goodness-of-fit tests play an important role in machine learning and statistical analysis. Given a model distribution $P$ and sample $x^n := \{x_i\}_{i=1}^n$ originating from an unknown distribution $Q$, the goal is to decide whether to accept the null hypothesis that $Q$ matches $P$, or the alternative hypothesis that $Q$ and $P$ are different. Traditional (parametric) approaches may require space partitioning or closed-form integrals \[6, 7, 9, 27\]. They become computationally intractable to machine learning applications that involve high dimensional data and complicated models \[30, 39, 46\]. Recently, several efficient tests have been proposed based on Reproducing Kernel Hilbert Space (RKHS) embedding \[36, 43\]. One is to conduct a Maximum Mean Discrepancy (MMD) based two-sample test by drawing samples from the model distribution $P$ \[35\]. A difficulty with this approach is to determine the number of samples drawn from $P$ relative to $n$, the sample number of the test sequence. Other tests are based on classes of Stein transformed RKHS functions \[12, 22, 23, 34, 37\], where the test statistic is the norm of the smoothness-constrained function with the largest expectation under $Q$ and is referred to as the Kernel Stein Discrepancy (KSD). The KSD based tests only require knowing the density function of $P$ up to the normalization constant, and do not need to compute integrals or draw samples. Additionally, constructing explicit features of distributions results in a linear-time goodness-of-fit test that is also more interpretable \[29\].

Motivated by their good performance in practice, this paper investigates the statistical optimality of these kernel based goodness-of-fit tests, a long-standing open problem in information theory and statistics \[15, 17, 28\]. Given distribution $P$, the hypothesis testing between $H_0 : x^n \sim P$ and $H_1 : x^n \sim Q$ can be extremely hard when $Q$ is arbitrary but unknown, as opposed to the simple case when $Q$ is known. With independent sample and a known $Q$, the type-II error probability of an optimal test vanishes exponentially fast w.r.t. the sample size $n$, and the exponential decay rate coincides with the Kullback-Leibler Divergence (KLD) between $P$ and $Q$ (cf. Lemma 1). This motivates the so-called universal hypothesis testing problem, originally proposed by Hoeffding \[28\]: does there exist a nonparametric goodness-of-fit test that achieves the same optimal exponential decay rate as in the simple hypothesis testing problem where $Q$ is known? Over the years, universally optimal tests only exist when the sample space is finite, i.e., when $P$ and $Q$ are
both multinomial \cite{28, 49}. For a more general sample space, attempts have been largely fruitless with the only exception of \cite{53, 51}. Their results, however, were obtained at the cost of a weaker optimality and the proposed tests are rather complicated due to use of Lévy-Prokhorov metric. We remark that even the existence of such a test remains unknown when the sample space is non-finite.

**Contributions.** We first show a simple kernel test, comparing the MMD between the target distribution and the sample empirical distribution with a proper threshold, as an optimal approach to the universal hypothesis testing problem when the sample space is Polish, locally compact Hausdorff, e.g., $\mathbb{R}^d$. To the best of our knowledge, this is the first result on the universal optimality for a general, non-finite sample space. Taking into account the difficulty of obtaining closed-form integrals for non-Gaussian distributions, we then follow \cite{75x-1845} to cast the original problem into a two-sample problem. We establish the same optimality for the quadratic-time kernel two-sample tests proposed in \cite{25}, provided that $\omega(n)$ independent samples are drawn from $P$. For the KSD based tests, the constant level constraint on the type-I error probability is difficult to satisfy for all possible sample sizes. By relaxing the constraint to an asymptotic one and assuming additional conditions, we establish the optimal exponential decay rate of the type-II error probability for the quadratic-time KSD based tests proposed in \cite{12, 34}.

As another contribution, we proceed to investigate the quadratic-time kernel two-sample tests in a more general setting where the sample sizes scale in the same order, e.g., when the two sets of samples have the same size. We show that the type-II error probability also vanishes exponentially fast. The obtained exponential decay rate is further shown to be optimal among all two-sample tests under the same level constraint, and is independent of particular kernels provided that they are bounded continuous and characteristic.

Key to our approach are Sanov’s theorem from large deviation theory \cite{19} and the weak metrizable properties of the MMD \cite{42, 44} and the KSD \cite{25}, which enable us to directly investigate the acceptance region defined by the test, rather than using the test statistic as an intermediate.

**Paper Outline.** Section 2 introduces the asymptotic statistical criterion used in this paper and formally states the problem of universal hypothesis testing. Section 3 reviews related works. In Section 4 we present two classes of MMD based tests that are optimal for universal hypothesis testing and discuss their implications to goodness-of-fit testing. Section 5 considers the KSD based goodness-of-fit tests and Section 6 establishes the universal optimality of the quadratic-time MMD based two-sample tests in a more general setting. We conclude this paper in Section 7.

## 2 Problem

Throughout this paper, let $\mathcal{X}$ be a Polish space (i.e., a separable completely metrizable topological space) and $\mathcal{P}$ the set of Borel probability measures defined on $\mathcal{X}$. Given a distribution $P \in \mathcal{P}$ and sample $x^n$ from an unknown distribution $Q \in \mathcal{P}$, we want to determine whether to accept $H_0 : P = Q$ or $H_1 : P \neq Q$. A test $\Omega(n) = \{\Omega_0(n), \Omega_1(n)\}$ partitions $\mathcal{X}^n$ into two disjoint sets with $\Omega_0(n) \cup \Omega_1(n) = \mathcal{X}^n$. If $x^n \in \Omega_i(n), i = 0, 1$, a decision is made in favor of hypothesis $H_i$. We say that $\Omega_0(n)$ is an acceptance region for the null hypothesis $H_0$ and $\Omega_1(n)$ the rejection region. A type-I error is made when $P = Q$ is rejected while $H_0$ is true, and a type-II error occurs when $P = Q$ is accepted despite $H_1$ being true. The two error probabilities are $P(\Omega_0(n)) := \mathbb{P}_{x^n \sim P}(x^n \in \Omega_0(n))$ and $Q(\Omega_0(n)) := \mathbb{P}_{x^n \sim Q}(x^n \in \Omega_0(n))$ with $Q \neq P$, respectively.

In general, the two error probabilities can not be minimized simultaneously. A commonly used approach, the so-called Neyman-Pearson approach \cite{11}, is to set an upper bound $\alpha$ on the type-I error probability and considers only level $\alpha$ tests, i.e., tests with $P(\Omega_1(n)) \leq \alpha$. However, similar to the two-sample problem \cite{25}, it is not possible to distinguish distributions with high probability at a given, fixed sample, without prior assumptions on the difference between $P$ and $Q$. We therefore consider an asymptotic statistical criterion as the performance metric.

A level $\alpha$ test is said to be consistent if the type-II error probability vanishes in the large sample limit. Such a test is exponentially consistent when the error probability additionally vanishes exponentially fast w.r.t. the sample size, that is, when

$$\liminf_{n \to \infty} \frac{1}{n} \log Q(\Omega_0(n)) > 0.$$  

The above limit is also referred to as the type-II error exponent in information theory. Clearly, the larger the error exponent, the faster the error probability decreases in the sample limit. Under this criterion, an optimal test would achieve the maximum type-II error exponent while satisfying the level constraint. Error exponent is a widely used metric in source coding and channel coding \cite{13}, and is closely related to two other asymptotic statistical criteria \cite{41}. In particular, the Chernoff index equals the minimum of the type-I and type-II error exponents, and the exact Bahadur slope is equivalent to twice of the type-I error exponent with a constant constraint on the type-II error probability.
We present a useful lemma which gives the optimal type-II error exponent of any level \(\alpha\) test for simple hypothesis testing between two known distributions. Let \(D(P\|Q)\) denote the KLD between \(P\) and \(Q\). That is, \(D(P\|Q) = E_P \log(dP/dQ)\) where \(dP/dQ\) stands for the Radon-Nikodym derivative of \(P\) w.r.t. \(Q\) when it exists, and \(D(P\|Q) = \infty\) otherwise [12].

**Lemma 1 (Chernoff-Stein Lemma [13, 19]).** Let \(X^n\) i.i.d. \(\sim R\). Consider simple hypothesis testing between \(H_0 : R = P \in \mathcal{P}\) and \(H_1 : R = Q \in \mathcal{P}\), with \(0 < D(P\|Q) < \infty\). Given \(0 < \alpha < 1\), let \(\Omega^*(n, P, Q) = \{\Omega_0^*(n, P, Q), \Omega_1^*(n, P, Q)\}\) be the optimal level \(\alpha\) test with which the type-II error probability is minimized for each \(n\). It follows that

\[
\lim_{n \to \infty} -\frac{1}{n} \log \Omega^*(n, P, Q)) = D(P\|Q).
\]

**Problem Statement.** Let \(\Omega(n) = \{\Omega_0(n), \Omega_1(n)\}\) be a nonparametric goodness-of-fit test of level \(\alpha\). With \(X^n\) i.i.d. \(\sim Q\) under the alternative hypothesis, the corresponding type-II error probability \(Q(\Omega_0(n))\) can not be lower than \(Q(\Omega_0^*(n, P, Q))\). As such, Chernoff-Stein lemma indicates that its type-II error exponent is bounded by \(D(P\|Q)\). For any given \(P\), the problem is to find a goodness-of-fit test \(\Omega(n)\), if it exists, so that

1. under \(H_0 : P = Q\), \(P_{X^n}(\Omega_1(n)) \leq \alpha\),
2. under \(H_1 : P \neq Q\),

\[
\liminf_{n \to \infty} -\frac{1}{n} \log P_{X^n}(\Omega_0(n)) = D(P\|Q),
\]

for arbitrary \(Q\) with \(0 < D(P\|Q) < \infty\),

giving rise to the name *universal* hypothesis testing.

## 3 Related Work

The decay rate of the type-II error probability has been widely investigated for existing kernel based tests. For the simple kernel tests in [14, 17, 48] and the kernel two-sample tests in [14, 21, 24, 26, 46, 52], analysis is based on the test statistics, through their asymptotic distributions or some probabilistic bounds on their convergence to the population statistics. The resulting characterizations depend on kernels and are loose in general. For the KSD based tests, current statistical characterization is limited to consistency; the asymptotic distributions of the test statistics either have no closed form [12] or are hard to analyze [29, 34].

Other asymptotic statistical criteria have also been used for comparing nonparametric goodness-of-fit tests. Jitkrittum et al. [29] used the approximate Bahadur slope and showed that their linear-time test has greater relative efficiency than the linear-time test proposed in [44], assuming a mean-shift alternative. However, it is not clear whether such a result holds for a more general alternative. Balasubramanian et al. [5] investigated the detection boundary and showed that the simple kernel test is suboptimal under this criterion. A minimax optimal test was then proposed for a composite alternative, where the worst-case performance w.r.t. a set of probability measures is optimized. In contrast, our optimality criterion is much stronger in that the optimality must hold for any distribution defining the alternative hypothesis; specifically, the nonparametric test must achieve the maximum type-II error exponent \(D(P\|Q)\) for any \(Q\) satisfying \(0 < D(P\|Q) < \infty\).

## 4 Maximum Mean Discrepancy Based Goodness-of-Fit Tests

This section studies two classes of MMD based tests for universal hypothesis testing, followed by discussions on related aspects. We begin with a brief review of the MMD and of Sanov’s theorem.

Let \(\mathcal{H}_k\) be an RKHS defined on \(\mathcal{X}\) with reproducing kernel \(k\). The mean embedding of \(P \in \mathcal{P}\) in \(\mathcal{H}_k\) is a unique element \(\mu_k(P) \in \mathcal{H}_k\) such that \(E_y \sim P f(y) = \langle f, \mu_k(P) \rangle_{\mathcal{H}_k}\) for all \(f \in \mathcal{H}_k\) [8]. We assume that \(k\) is bounded continuous, hence the existence of \(\mu_k(P)\) is guaranteed by the Riesz representation theorem. The MMD between two probability measures \(P\) and \(Q\) is defined as the RKHS-distance between their mean embeddings, which can be expressed as

\[
d_k(P, Q) = \|\mu_k(P) - \mu_k(Q)\|_{\mathcal{H}_k} = (E_{yy'}k(y, y') + E_{xx'}k(x, x') - 2E_{yx}k(y, x))^{1/2},
\]

where \(y, y'\) i.i.d. \(\sim P\) and \(x, x'\) i.i.d. \(\sim Q\).

If the mean embedding \(\mu_k\) is an injective map, then the kernel \(k\) is said to be characteristic and the MMD \(d_k\) becomes a metric on \(\mathcal{P}\) [45]. A weak metrizable property of \(d_k\) has also been established recently. Consider the weak topology on \(\mathcal{P}\) induced by the weak convergence: a sequence of probability measures \(P_i \to P\) weakly if and only if \(E_{y \sim P_i} f(y) \to E_{y \sim P} f(y)\) for every bounded continuous function \(f : \mathcal{X} \to \mathbb{R}\). The following theorem states when \(d_k\) metrizes this weak convergence [46].

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1. Indeed, Simon-Gabriel and Schölkopf [42] show that \(\mathcal{X}\) only needs to be locally compact Hausdorff. We require \(\mathcal{X}\) be Polish in order to utilize Sanov’s theorem.
Theorem 1 ([42, Theorem 55], [44, Theorem 3.2]). If \( X \) is Polish, locally compact Hausdorff, and \( k \) is continuous and characteristic, then \( d_k \) metrizes the weak convergence on \( \mathcal{P} \).

We note that the weak metrizable property is also favored for training deep generative models [3, 4, 32]. An example of Polish, locally compact Hausdorff space is \( \mathbb{R}^d \), and both Gaussian and Laplacian kernels defined on it are bounded continuous and characteristic [44].

We next introduce Sanov’s theorem from large deviation theory, which, together with the weak metrizable property of the MMD, is critical to establish our main results in this section. Denote by \( Q_n \) the empirical measure of \( x^n \), i.e., \( Q_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i} \), with \( \delta_x \) being the Dirac measure at \( x \).

Theorem 2 (Sanov’s Theorem [40, 19]). Let \( x^n \) i.i.d. \( \sim Q \in \mathcal{P} \). For a set \( \Gamma \subset \mathcal{P} \), it holds that

\[
\lim_{n \to \infty} -\frac{1}{n} \log P_{x^n}(Q_n \in \Gamma) \leq \inf_{R \in \mathcal{F}} D(R||Q),
\]

\[
\lim_{n \to \infty} -\frac{1}{n} \log P_{x^n}(Q_n \in \Gamma') \geq \inf_{R \in \mathcal{F}} D(R||Q),
\]

where \( \mathcal{F} \) is the interior and closure of \( \Gamma \) w.r.t. the weak topology on \( \mathcal{P} \), respectively.

Sanov’s theorem states that if the underlying distribution \( Q \) is not in \( \mathcal{F} \), the closure of a set \( \Gamma \) of distributions, then the probability of its empirical distribution \( Q_n \) lying in \( \mathcal{F} \) goes to 0 at least exponentially fast. This enables us to directly investigate type-II error exponent through the empirical distribution and the acceptance region, rather than through the limiting performance of the test statistics. Moreover, the lower bound on the error exponent would establish the universal optimality if it is no lower than \( D(P||Q) \) for a goodness-of-fit test.

We now state the two classes of MMD based goodness-of-fit tests that are universally optimal.

### 4.1 Simple Kernel Tests

The first test directly computes the MMD between the target distribution \( P \) and the empirical distribution of sample \( x^n \). Though having been investigated in [1, 2, 47, 48], its optimality for the universal hypothesis testing problem remains unknown.

Let also \( Q_n \) be the empirical measure of \( x^n \). We have a simple kernel test with acceptance region

\[
\Omega_0(n) = \left\{ x^n : d_k(P, Q_n) \leq \gamma_n \right\},
\]

where \( \gamma_n \) represents a threshold and \( d_k^2(P, Q_n) \) equals

\[
\frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} k(x_i, x_j) + E_{yy'} k(y, y') - \frac{2}{n} \sum_{i=1}^{n} E_{y} k(x_i, y),
\]

with \( y, y' \) i.i.d. \( \sim P \). On the one hand, we want the threshold \( \gamma_n \) to be small so that the type-II error probability is low; on the other hand, the threshold cannot be too small in order to meet the level constraint on the type-I error probability. The balance between the two error probabilities is attained with a threshold that diminishes at an appropriate rate.

Theorem 3. Let \( X \) be Polish, locally compact Hausdorff. For \( P \in \mathcal{P} \) and \( x^n \) i.i.d. \( \sim Q \in \mathcal{P} \), assume \( 0 < D(P||Q) < \infty \) under the alternative hypothesis \( H_1 \). Further assume that kernel \( k \) is bounded continuous and characteristic, with \( 0 \leq k(\cdot, \cdot) \) and \( K > 0 \). For a given \( \alpha, 0 < \alpha < 1 \), set \( \gamma_n = \sqrt{2K/n} \left( 1 + \sqrt{-\log \alpha} \right) \).

The simple kernel test \( d_k(P, Q_n) \leq \gamma_n \) is an optimal level \( \alpha \) test for the universal hypothesis testing problem, that is,

1. under \( H_0 : P = Q \), \( P_{x^n} \left( d_k(P, Q_n) > \gamma_n \right) \leq \alpha \),
2. under \( H_1 : P \neq Q \), \( \lim_{n \to \infty} -\frac{1}{n} \log P_{x^n} \left( d_k(P, Q_n) \leq \gamma_n \right) = D(P||Q) \).

Proof. That \( d_k(P, Q_n) \leq \gamma_n \) has level \( \alpha \) can be directly verified by [48, Eq. (24)] (see Lemma 2 in Appendix A). Let \( \beta = \lim_{n \to \infty} -\frac{1}{n} \log P_{x^n} \left( d_k(P, Q_n) \leq \gamma_n \right) \) under \( H_1 \). According to Chernoff-Stein lemma, we only need to show \( \beta \geq D(P||Q) \).

To apply Sanov’s theorem, we notice that deciding if \( x^n \in \left\{ x^n : d_k(P, Q_n) \leq \gamma_n \right\} \) is equivalent to deciding if its empirical measure \( Q_n \in \left\{ P' : d_k(P, P') \leq \gamma_n \right\} \). Since \( \gamma_n \to 0 \) as \( n \to \infty \), for any constant \( \gamma > 0 \), there exists an integer \( n \) such that \( \gamma_n < \gamma \) for all \( n > n \). Hence, \( \left\{ P' : d_k(P, P') \leq \gamma_n \right\} \subset \left\{ P' : d_k(P, P') \leq \gamma \right\} \) for large enough \( n \). It follows that for any \( \gamma > 0 \),

\[
\beta \geq \lim_{n \to \infty} -\frac{1}{n} \log P_{x^n} \left( d_k(P, Q_n) \leq \gamma \right) \geq \inf_{\left\{ P' \in \mathcal{P} : d_k(P, P') \leq \gamma \right\}} D(P'||Q),
\]

where the last inequality is from Sanov’s theorem and that \( \left\{ P' \in \mathcal{P} : d_k(P, P') \leq \gamma \right\} \) is closed w.r.t. the weak topology (cf. Theorem 1). Then for any given \( \epsilon > 0 \), there exists some \( \gamma > 0 \) such that \( \inf_{\left\{ P' \in \mathcal{P} : d_k(P, P') \leq \gamma \right\}} D(P'||Q) \geq D(P'||Q) - \epsilon \), using the lower semi-continuity of the KLD [50] (Lemma 3 in Appendix A) and the assumption that \( 0 < D(P||Q) < \infty \) under \( H_1 \). This further implies \( \beta \geq D(P||Q) \).

It is worth noting that we simply select one threshold \( \gamma_n \) in the above theorem. Indeed, any vanishing threshold \( \gamma_n > 0 \) with \( \gamma_n \to 0 \) leads to the same optimality w.r.t. the type-II error exponent, an asymptotic statistical criterion. A larger threshold, however, may
result in a higher type-II error probability in the finite sample regime. A further discussion on the threshold choice will be given in Section 4.3.

The test statistic $d_k^2(P, \hat{Q}_n)$ is a biased estimator of $d_k^2(P, Q)$. By replacing $\frac{1}{m(n-1)} \sum_{i=1}^{n} \sum_{j \neq i} k(x_i, x_j)$ with $\frac{1}{m(m-1)} \sum_{i=1}^{m} \sum_{j \neq i} k(x_i, x_j)$, we obtain an unbiased statistic denoted as $d_k^2(P, \hat{Q}_n)$. We comment that $d_k^2(P, \hat{Q}_n)$ is not a squared quantity and can be negative, due to the unbiasedness. The following result shows that $d_k^2(P, \hat{Q}_n)$ can also be used to construct a universally optimal test.

**Corollary 1.** Under the same conditions of Theorem 3, the test $d_k^2(P, \hat{Q}_n) \leq \gamma^2_n + K/n$ is a level $\alpha$ asymptotically optimal test for universal hypothesis testing.

*Proof (sketch).* As $0 \leq \gamma(\cdot, \cdot) \leq K$, we get $\{x^n : d_k^2(P, \hat{Q}_n) \leq \gamma^2_n \} \subseteq \{x^n : d_k^2(P, \hat{Q}_n) \leq \gamma^2_n + K/n \} \subseteq \{x^n : d_k^2(P, Q) \leq \gamma^2_n + 2K/n \}$. The level constraint and the type-II error exponent can then be verified using the subset and superset, respectively. See Appendix A for details.

The tests in this section still require closed-form integrals, namely, $E_y k(x_i, y)$ and $E_{yy'} k(y, y')$. Our purpose here is to show that the universally optimal type-II error exponent is indeed achievable, giving a meaningful optimality criterion for goodness-of-fit tests. In the next section, we consider another class of MMD based tests without the need of closed-form integrals.

### 4.2 Kernel Two-Sample Tests

In the context of model criticism, Lloyd and Ghaemmaghami cast goodness of fit testing into a two-sample problem, where one draws sample $y^n$ from distribution $P$ and then decide if $y^n$ and $x^n$ are from the same distribution. A question that arises is the choice of number of samples, which is not obvious due to the lack of an explicit criterion. In light of universal hypothesis testing, we could ask how many samples would suffice for a two-sample test to attain the error exponent $D(P||Q)$.

Denote by $\hat{P}_m$ the empirical measure of $y^m$. Notice that the type-I and type-II error probabilities of a two-sample test depend on both $P$ and $Q$. We consider the following two-sample test with acceptance region

$$\Omega_0(m, n) = \{ (y^n, x^n) : d_k(\hat{P}_m, \hat{Q}_n) \leq \gamma_{m,n} \},$$

where $K$ is a finite bound on $k(\cdot, \cdot)$,

$$\gamma_{m,n} = \left( \sqrt{K/m} + \sqrt{K/n} \right) \left( 2 + \sqrt{-2 \log(\alpha/2)} \right),$$

$$d_k^2(\hat{P}_m, \hat{Q}_n) = \sum_{i=1}^{n} \sum_{j=1}^{n} k(x_i, x_j) + \sum_{i=1}^{m} \sum_{j=1}^{m} k(y_i, y_j) - \frac{2mn}{m(m-1)} \sum_{i=1}^{m} \sum_{j \neq i} k(x_i, y_j).$$

The statistic $d_k^2(\hat{P}_m, \hat{Q}_n)$ for estimating the squared MMD was originally proposed in [23]. Although additional randomness is introduced due to the use of $\hat{P}_m$, it does not hurt the type-II error exponent provided that $m$ is large enough, as stated below.

**Theorem 4.** Assume the same conditions as in Theorem 3 and that $y^n$ i.i.d. $\sim P$ and $x^n$ i.i.d. $\sim Q$. Let $\Omega_1(m, n) = \mathcal{X}^{m+n} \setminus \Omega_0(m, n)$ be the rejection region. If $m$ is such that $m/n \to \infty$ as $n \to \infty$, then we have

1. under $H_0 : P = Q$, $P_{y^n \sim x^n}(\Omega_1(m, n)) \leq \alpha$,
2. under $H_1 : P \neq Q$,

$$\lim_{n \to \infty} \frac{1}{n} \log P_{y^n \sim x^n}(\Omega_0(m, n)) = D(P||Q).$$

The level $\alpha$ constraint can be verified by [25, Theorem 7]. We decompose the type-II error probability into two components and show that each decays at least exponentially at a rate of $D(P||Q)$. A complete proof is provided in Appendix B.

We may also replace the first two terms in $d_k^2(\hat{P}_m, \hat{Q}_n)$ with $\frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j \neq i} k(x_i, x_j)$ and $\frac{1}{m(m-1)} \sum_{i=1}^{m} \sum_{j \neq i} k(y_i, y_j)$, which results in an unbiased statistic denoted as $d_k^2(\hat{P}_m, \hat{Q}_n)$ [24]. The following corollary can be shown in a similar manner to Corollary 1 by noting that $|d_k^2(\hat{P}_m, \hat{Q}_n) - d_k^2(\hat{P}_m, \hat{Q}_n)| \leq K/m + K/n$; details are omitted.

**Corollary 2.** Under the same assumptions of Theorem 4, the test $d_k^2(\hat{P}_m, \hat{Q}_n) \leq \gamma_{m,n}^2 + K/m + K/n$ has its type-I error probability below $\alpha$ and type-II error exponent being $D(P||Q)$, when $m/n \to \infty$ as $n \to \infty$.

### 4.3 Remarks

**Threshold Choice.** The distribution-free thresholds used in the MMD based tests are generally too conservative, as the actual distribution $P$ is not taken into account. Alternatively, we may use Monte Carlo or bootstrap methods to empirically estimate the acceptance threshold [12, 25, 29], making the tests asymptotically level $\alpha$. These methods, however, introduce additional randomness on the threshold choice and further on the type-II error probability. As a result, it becomes difficult to characterize the type-II error exponent. A simple fix is to take the minimum of the Monte Carlo or bootstrap threshold and the distribution-free
one, guaranteeing a vanishing threshold and hence the optimal type-II error exponent. In our experiments, the bootstrap threshold is always smaller than the distribution-free threshold.

Finite vs. Asymptotic Regimes. A finitely positive error exponent $D(P\|Q)$ implies that the error probability decays with $O\left(2^{-nD(P\|Q)-\epsilon}\right)$ where $\epsilon \in (0, D(P\|Q))$ can be arbitrarily small. It further implies that kernels affect only the sub-exponential term in the type-II error probability, as long as they are bounded continuous and characteristic. When $n$ is small, the sub-exponential term may dominate and the test performance does depend on the specific kernel. Selecting a proper kernel is an ongoing research topic and we refer the reader to related works such as [20, 26, 46].

Non-i.i.d. Sample. We notice that Chwialkowski et al. [12] considered non-i.i.d. sample by use of wild bootstrap. In general, statistical optimality with non-i.i.d. sample is difficult to establish even for simple hypothesis testing.

General Two-Sample Problem. Studied in Section 6, after studying the KSD based goodness-of-fit, it is not possible for the MMD based two-sample test to decompose the acceptance region $\Omega$ into $\Omega'(n) = \Omega_0(m) \times \Omega_0'(n)$ with $\Omega_0(\alpha)$ and $\Omega_0'(n)$ being respectively decided by $y^n$ and $x^n$, and then apply Sanov’s theorem to each set. Unfortunately, such a decomposition is not possible for the MMD based two-sample tests. We postpone a further investigation until Section 6 after studying the KSD based goodness-of-fit tests in the next section.

5 Kernel Stein Discrepancy Based Goodness-of-Fit Tests

In this section, we investigate the KSD based goodness-of-fit tests recently proposed in [12, 29, 34].

Let $X = \mathbb{R}^d$. Denote by $p$ and $q$ the density functions (w.r.t. Lebesgue measure) of $P$ and $Q$, respectively. In [12, 34], the KSD is defined as

$$d^2_s(P, Q) = \max_{\|f\|_{\mathcal{H}_k} \leq 1} \mathbb{E}_{x \sim P} [s_p(x)f(x) + \nabla_x f(x)],$$

where $\|f\|_{\mathcal{H}_k} \leq 1$ denotes the unit ball in the RKHS $\mathcal{H}_k$, and $s_p(x) = \nabla_x \log p(x)$ is the score function of $p(x)$. An equivalent expression of the KSD is given by

$$d^2_s(P, Q) = \mathbb{E}_{x \sim P} \mathbb{E}_{x' \sim P} h_p(x, x'),$$

where $h_p(x, y) = s^*_p(x)s_p(y)k(x, y) + s^*_p(y)\nabla_x k(x, y) + s^*_p(x)\nabla_y k(x, y) + \text{trace}(\nabla_x k(x, y))$. Given sample $x^n$, we may estimate $d^2_s(P, Q)$ by $d^2_s(P, Q_n) = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n h_p(x_i, x_j)$, which is a degenerate V-statistic under the null hypothesis $H_0: P = Q$ [12].

With $\mathbb{E}_{x \sim P} \| \nabla_x \log p(x) - \nabla_x \log q(x) \|^2 \leq \infty$ and a $C_0$-universal kernel [10], $d_s(P, Q) = 0$ if and only if $P = Q$ [12, Theorem 2.2]. A nice property of the KSD is that this result requires only the knowledge of $p(x)$ up to the normalization constant. The KSD has also been shown to be lower bounded in terms of the MMD or the bounded Lipschitz metric (involving some unknown constants) under suitable conditions [23]. This indicates that $d_s(P, P_t) \to 0$ only if $P_t \to P$ weakly, which is important to applying Sanov’s theorem in our approach.

Unlike the MMD based test statistics, there does not exist a universal or distribution-free probabilistic bound on $d^2_s(P, Q_n)$. As a result, it is difficult to find a test threshold to meet the fixed level constraint for all sample sizes. To proceed, we relax the level constraint to an asymptotic one, and use the result of Proposition 3.2 which shows that $nd^2_s(P, Q_n)$ converges weakly to some distribution under $H_0$. We assume a fixed $\alpha$-quantile $\gamma_\alpha$ of the limiting cumulative distribution function, so that $\lim_{n \to \infty} P(d^2_s(P, Q_n) > \gamma_\alpha/n) = \alpha$. Then if $\gamma_\alpha$ is such that $\gamma_\alpha \to 0$ and $\lim_{n \to \infty} n\gamma_\alpha \to \infty$, e.g., $\gamma_\alpha = 1/\mu_1(1 + \sqrt{-\log \alpha})$, we get $\gamma_\alpha > \gamma_\alpha/n$ in the limit and thus $\lim_{n \to \infty} P(d^2_s(P, Q_n) > \gamma_\alpha) \leq \alpha$. Similarly, this threshold choice may be poor in the finite sample regime and we can take the minimum of this threshold and a bootstrap one [2, 13, 31]. Together with the weak convergence properties of the KSD, we have the following result.

**Theorem 5.** Let $P$ and $Q$ be distributions defined on $\mathbb{R}^d$, with $0 < D(P\|Q) < \infty$ under the alternative hypothesis. Assume $x^n$ i.i.d. ~ $Q$ and set $\gamma_\alpha = 1/\mu_1(1 + \sqrt{-\log \alpha})$. It follows that

1. if $h_p$ is Lipschitz continuous and $\mathbb{E}_{x \sim Q} h_p(x, x) < \infty$, then under $H_0: P = Q$,

$$\lim_{n \to \infty} P_{x^n} \left( d^2_s(P, Q_n) > \gamma_\alpha \right) \leq \alpha.$$

2. if 1) $d = 1$, $k(x, y) = \Phi(x - y)$ for some $\Phi \in C^2$ (twice continuous differentiable) with $\Phi$
non-vanishing generalized Fourier transform; 2) \(k(x,y) = \Phi(x-y)\) for some \(\Phi \in C^2\) with a non-vanishing generalized Fourier transform, and the sequence \(\{\hat{Q}_n\}_{n \geq 1}\) is uniformly tight; 3) \(k(x,y) = (c^2 + \|x-y\|_2^2)^n\) for \(c > 0\) and \(-1 < \eta < 0\), then under \(H_1 : P \neq Q\),

\[
\lim \inf_{n \to \infty} -\frac{1}{n} \log P_{x^n} \left( d_S^2(P, \hat{Q}_n) \leq \gamma_n \right) = D(P\|Q).
\]

**Proof (sketch).** The condition for the asymptotic level constraint is taken from [12, Proposition 3.2]. To establish the type-II error exponent, let \(d_W\) denote the MMD or the bounded Lipschitz metric, which metrize the weak convergence on \(\mathcal{P}\). Under each of the three conditions from [23, Theorems 5, 7, and 8], \(d_W(P, \hat{Q}_n) \leq g(d_W(P, Q_n))\) where \(g(d_W) \to 0\) as \(d_W \to 0\). Then there exists \(\gamma_n'\) such that \(\{x^n : d_S^2(P, \hat{Q}_n) \leq \gamma_n'\} \subset \{x^n : d_W(P, \hat{Q}_n) \leq \gamma_n\}\) and \(\gamma_n' \to 0\) as \(n \to \infty\). Thus, the type-II error exponent is lower bounded by \(D(P\|Q)\), following the same argument of Theorem 3.

The upper bound is from Chernoff-Stein lemma which also holds for an asymptotic level constraint. \(\square\)

Liu et al. [34] proposed an unbiased U-statistic \(d_{S(u)}^2(P, \hat{Q}_n) = \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} h_P(x_i, x_j)\) for estimating \(d_S^2(P, Q)\). A similar result holds under an additional assumption on the boundedness of \(h_P(\cdot, \cdot)\), using the same argument of Corollary 1.

**Corollary 3.** Assume the same conditions as in Theorem 2 and further that \(h_P(\cdot, \cdot) \leq H_P\) for some \(H_P \in \mathbb{R}^+\). Then the test \(d_{S(u)}^2(P, \hat{Q}_n) \leq \gamma_n + H_P/\sqrt{n}\) is asymptotically level \(\alpha\) and achieves the optimal type-II error exponent \(D(P\|Q)\).

**The Weak Convergence Property.** To use Sanov’s theorem, we find a superset of probability measures for the equivalent acceptance region, which is required to be closed and to converge in terms of weak convergence to \(P\) in the large sample limit. Without the weak convergence property, the equivalent acceptance region may contain probability measures that are not close to \(P\), and the minimum KLD over the superset would be hard to obtain. An example can be found in [29, Theorem 6] where the KSDs are driven to zero by sequences of probability measures not converging to \(P\). Consequently, our approach does not establish the optimal type-II error exponent for the linear-time KSD based tests in [29, 34], the linear-time kernel two-sample test in [23], the B-test in [52], and a pseudo-metric based two-sample test in [43], due to lack of the weak convergence property.

## 6 General Two-Sample Problem

In this section, we investigate the kernel two-sample tests in a more general setting. As discussed in Section 2.3, the key is to establish an extended Sanov’s theorem that is able to handle two sample sequences.

### 6.1 Extended Sanov’s Theorem

We define pairwise weak convergence for probability measures: we say \((P, Q_1) \rightarrow (P, Q)\) weakly if and only if both \(P_1 \rightarrow P\) and \(Q_1 \rightarrow Q\) weakly. We consider \(\mathcal{P} \times \mathcal{P}\) endowed with the topology induced by this pairwise weak convergence. It can be verified that this topology is equivalent to the product topology on \(\mathcal{P} \times \mathcal{P}\) where each \(\mathcal{P}\) is endowed with the topology of weak convergence. An extended version of Sanov’s theorem is stated below.

**Theorem 6 (Extended Sanov’s Theorem).** Let \(\mathcal{X}\) be a Polish space, \(y^n\) i.i.d. ~ \(P\), and \(x^n\) i.i.d. ~ \(Q\). Assume \(0 < \lim_{m,n \to \infty} \frac{m}{m+n} = c < 1\). Then for a set \(\Gamma \subset \mathcal{P} \times \mathcal{P}\), it holds that

\[
\inf_{(R,S) \in \Gamma} cD(R\|P) + (1-c)D(S\|Q)
\geq \lim \sup_{m,n \to \infty} -\frac{1}{m+n} \log P_{y^m x^n}((\hat{P}_m, \hat{Q}_n) \in \Gamma)
\geq \lim \inf_{m,n \to \infty} -\frac{1}{m+n} \log P_{y^m x^n}((\hat{P}_m, \hat{Q}_n) \in \Gamma)
\geq \inf_{(R,S) \in \Gamma} cD(R\|P) + (1-c)D(S\|Q),
\]

where \(\inf\Gamma\) and \(c\Gamma\) denote the interior and closure of \(\Gamma\) w.r.t. the pairwise weak convergence, respectively.

We comment that this extension is not apparent as existing tools, e.g., Cramér theorem [19], used for proving Sanov’s theorem can only deal with a single distribution. In Appendix C, we first prove the above result in finite sample space and then extend it to general Polish space, with two simple combinatorial lemmas as prerequisites.

### 6.2 Exact and Optimal Error Exponent

With the extended Sanov’s theorem and a vanishing threshold \(\gamma_{m,n}\), we are ready to establish the exponential decay of the type-II error probability. A proof is provided in Appendix D.

**Theorem 7.** Assume the same conditions as in Theorem 4 and \(\lim_{m,n \to \infty} \frac{m}{m+n} = c \in (0,1)\). Under the alternative hypothesis \(H_1 : P \neq Q\), further assume that

\[
0 < D^* := \inf_{R \in \mathcal{P}} cD(R\|P) + (1-c)D(R\|Q) < \infty.
\]

Given \(0 < \alpha < 1\), the test \(d_k(\hat{P}_m, \hat{Q}_n) \leq \gamma_{m,n}\) with
Theorem 7. For a nonparametric two-sample test bounded by $D_\text{cally})$ level $\alpha$, partially consistent with the type-II error exponent being $\gamma_{m,n}$ defined in Section 4.2 is level $\alpha$ and also exponentially consistent with the type-II error exponent being

$$\liminf_{m,n \to \infty} -\frac{1}{m+n} \log P_{y=x^*}(\Omega_0(m, n)) = D^*. $$

Here we consider the error exponent w.r.t. $m + n$, the total number of observations for testing. Therefore, when $0 < c < 1$, the type-II error probability vanishes as $O(2^{-\gamma_{m,n}}D^{-c})$, where $c \in (0, D^*)$ is fixed and can be arbitrarily small. Similarly, this result only requires kernels be bounded continuous and characteristic.

Our next theorem provides an upper bound on the type-II error exponent of any (asymptotically) level $\alpha$ two-sample test. This further shows that the kernel test $d_k(\hat{P}_m, \hat{Q}_n) \leq \gamma_{m,n}$ is asymptotically optimal, by choosing the type-II error exponent as the performance metric. See Appendix B for a proof.

**Theorem 8.** Assume the same conditions as in Theorem 7. For a nonparametric two-sample test $\Omega'(m, n) = \{\Omega'_0(m, n), \Omega'_1(m, n)\}$ which is (asymptotically) level $\alpha, 0 < \alpha < 1$, its type-II error exponent is bounded by $D^*$, that is,

$$\liminf_{m,n \to \infty} -\frac{1}{m+n} \log P_{y=x^*}(\Omega'_0(m, n)) \leq D^*. $$

We can use Theorems 7 and 8 to identify more asymptotically optimal two-sample tests:

- Assuming $n = m$, the unbiased test $d^2_u(\hat{P}_m, \hat{Q}_n) \leq (4K\sqrt{\alpha} \log \alpha^{-1})$, with a tighter threshold, is also level $\alpha$ [22]. As $k(\cdot, \cdot)$ is finitely bounded by $K$, its type-II error probability vanishes exponentially at a rate of $\inf_{R \in \mathcal{P}} \frac{1}{2} \mathcal{D}(R|P) + \frac{1}{2} \mathcal{D}(R|Q)$, which can be shown by the same argument of Corollary 1.

- It is also possible to consider a family of kernels for the test statistic [21, 44]. For a given family $\kappa$, the test statistic is $\sup_{k \in \kappa} d_k(\hat{P}_m, \hat{Q}_n)$ which also metrizes weak convergence under suitable conditions, e.g., when $\kappa$ consists of finitely many Gaussian kernels [44, Theorem 3.2]. If $K$ remains to be an upper bound for all $k \in \kappa$, then comparing $\sup_{k \in \kappa} d_k(\hat{P}_m, \hat{Q}_n)$ with $\gamma_{m,n}$ in Section 4.2 results in an asymptotically optimal level $\alpha$ test.

**Fair Alternative.** In [22], a notion of fair alternative is proposed when investigating how a two-sample test performs as dimension increases. The idea is to fix $D(P\|Q)$ under the alternative hypothesis for all dimensions, guided by the fact that the KLD is a fundamental information-theoretic quantity determining the hardness of hypothesis testing problems. This approach, however, does not take into account the impact of sample sizes. In light of our results, perhaps a better choice is to fix $D^*$ defined in Theorem 7 when the sample sizes grow in the same order. In practice, $D^*$ may be hard to compute, so fixing its upper bound $(1 - c)D(P\|Q)$ and hence $D(P\|Q)$ is reasonable.

**Other Discrepancy Measures.** Other discrepancy measures between distributions may also metrize the weak convergence on $\mathcal{P}$, including Lévy-Prokhorov metric, the bounded Lipschitz metric, and Wasserstein distance. We may directly compute such a discrepancy between the empirical measures and then compare it with a decreasing threshold. However, there also does not exist a uniform or distribution-free threshold such that the level constraint is satisfied for all sample sizes. A possible remedy, as in Section 5, is to relax the level constraint to an asymptotic one. We will not expand into this direction, as computing such discrepancy measures from samples is generally more costly than the MMD and KSD based statistics.

7 Concluding Remarks

In this paper, we established the statistical optimality of the MMD and KSD based goodness-of-fit tests in the spirit of universal hypothesis testing. The KSD based tests are more computationally efficient, as there is no need to draw samples or compute integrals. In comparison, the MMD based tests are statistically favorable, as they require weaker assumptions and can meet the level constraint for any sample size. The quadratic-time MMD based two-sample tests are also shown to be optimal when sample sizes scale in the same order. Our findings not only solve a long-standing open problem in statistics, but also provide meaningful optimality criteria for nonparametric goodness-of-fit and two-sample testing.

While the optimality criterion is defined in the asymptotic sense, we also conduct experiments of these kernel based goodness-of-fit tests in the finite sample regime, with results given in Appendix C due to space limit. Whereas we cannot tell much statistical difference in our experiments, some experiments in the literature showed that the MMD based tests performed better than the KSD based tests and others showed the opposite [12, 22, 34, 29]. The finite sample performance depends on kernel choice as well as specific distributions. Under the universal setting, no test is known to be optimal in terms of the type-II error probability subject to a given level constraint. Statistical optimality can only be established in the large sample limit, as the one considered in the present work.
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A Proof of Corollary 1

We first present the two lemmas used in the proof of Theorem 3: one establishes the convergence of \( d_k(P, \hat{P}_m) \) and the other describes the lower semi-continuity of the KLD.

**Lemma 2.** [24, 25] Assume \( 0 \leq k(\cdot, \cdot) \leq K \). Given \( y^n \) i.i.d. \( \sim P \), denote by \( \hat{P}_m \) the empirical measure of \( y^n \). It follows that

\[
P_{y^n} \left( d_k(P, \hat{P}_m) > (2K/m)^{1/2} + \epsilon \right) \leq \exp \left( -\frac{e^2m}{2K} \right).
\]

**Proof of Corollary 1** Since \( 0 \leq k(\cdot, \cdot) \leq K \), we have

\[
\left| d^2_k(P, \hat{Q}_n) - d^2_k(P, \hat{Q}_n) \right| = \frac{1}{n^2(n-1)} \sum_{i=1}^{n} \sum_{j=1, j \neq i}^{n} k(x_i, x_j) - \frac{1}{n^2} \sum_{i=1}^{n} k(x_i, x_i) \leq K/n.
\]

It then holds that

\[
\left\{ x^n : d^2_k(P, \hat{Q}_n) \leq \gamma^2_n \right\} \subseteq \left\{ x^n : d^2_k(P, \hat{Q}_n) \leq \gamma^2_n + K/n \right\} \subseteq \left\{ x^n : d^2_k(P, \hat{Q}_n) \leq \gamma^2_n + 2K/n \right\}.
\]

Thus, under \( H_0 : P = Q \), we have

\[
P \left( d^2_k(P, \hat{Q}_n) > \gamma^2_n + K/n \right) \leq P \left( d^2_k(P, \hat{Q}_n) > \gamma^2_n \right) \leq \alpha,
\]

where the last inequality is from Lemma 2 and the fact that \( d_k(P, \hat{Q}_n) \geq 0 \). The type-II error exponent follows from

\[
\liminf_{n \to \infty} \frac{1}{n} \log \mathbb{Q} \left( d^2_k(P, \hat{Q}_n) \leq \gamma^2_n + K/n \right) \\
\geq \liminf_{n \to \infty} \frac{1}{n} \log \mathbb{Q} \left( d^2_k(P, \hat{Q}_n) \leq \gamma^2_n + 2K/n \right) \\
\geq D(P||Q).
\]

The last inequality can be shown by similar argument of Eq. (1) because \( \gamma^2_n + 2K/n \to 0 \) as \( n \to \infty \). Applying Chernoff-Stein lemma completes the proof.

B Proof of Theorem 4

We use a result from [25] to verify the two-sample test to be level \( \alpha \).

**Lemma 4** [25, Theorem 7]. Let \( P, Q, y^n, x^n, \hat{P}_m, \hat{Q}_n \) be defined in Theorem 4. Assume \( 0 \leq k(\cdot, \cdot) \leq K \). Then under the null hypothesis \( H_0 : P = Q \),

\[
P_{y^n,x^n} \left( d_k(\hat{P}_m, \hat{Q}_n) > 2(K/m)^{1/2} + (2K/m)^{1/2} + \epsilon \right) \leq 2 \exp \left( -\frac{e^2mn}{2K(m+n)} \right).
\]

**Proof of Theorem 4** That the two-sample test is level \( \alpha \) can be verified by the above lemma. The rest is to show the type-II error exponent being \( D(P||Q) \).

We can write the type-II error probability as

\[
P_{y^n,x^n} \left( d_k(\hat{P}_m, \hat{Q}_n) \leq \gamma_{m,n} \right) = \beta_{m,n} + \beta_{m,n}.
\]
where
\[
\gamma'_{m,n} = \sqrt{2K/m} + \sqrt{2K/nD(P\|Q)/m}
\]
\[
\beta_{m,n} = P_{y^m x^n} \left( d_k(\hat{P}_m, \hat{Q}_n) \leq \gamma_{m,n}, d_k(P, \hat{P}_m) > \gamma'_{m,n} \right),
\]
\[
\beta'_{m,n} = P_{y^m x^n} \left( d_k(\hat{P}_m, \hat{Q}_n) \leq \gamma_{m,n}, d_k(P, \hat{P}_m) \leq \gamma'_{m,n} \right).
\]

It suffices to show that \(\max\{\beta_{m,n}, \beta'_{m,n}\}\) decreases exponentially as \(n\) scales. We first have
\[
\beta_{m,n} \leq P_y = \left( d_k(P, \hat{P}_m) > \gamma'_{m,n} \right) \leq e^{-nD(P\|Q)},
\]
where the last inequality is due to Lemma 2. Thus, \(\beta_{m,n}\) vanishes at least exponentially fast with the error exponent being \(D(P\|Q)\).

For \(\beta'_{m,n}\), we have
\[
\beta'_{m,n} = \sum_{\{\hat{P}_m : d_k(P, \hat{P}_m) \leq \gamma'_{m,n}\}} P\left( \hat{P}_m \right) Q\left( d_k(\hat{P}_m, \hat{Q}_n) < \gamma_{m,n} \right)
\]
\[
= \left( \sum_{\{\hat{P}_m : d_k(P, \hat{P}_m) \leq \gamma'_{m,n}\}} P(\hat{P}_m) \right) \sup_{\{P_n : d_k(P, P_n) \leq \gamma'_{m,n}\}} Q\left( d_k(\hat{P}_m, \hat{Q}_n) < \gamma_{m,n} \right)
\]
\[
\leq \sup_{\{P_n : d_k(P, P_n) \leq \gamma'_{m,n}\}} Q\left( d_k(\hat{P}_m, \hat{Q}_n) < \gamma_{m,n} \right)
\]
\[
\leq Q\left( d_k(P, \hat{Q}_n) \leq \gamma_{m,n} + \gamma'_{m,n} \right),
\]
where the last inequality is from the triangle inequality for metric \(d_k\). Similar to Eq. (1), we get
\[
\liminf_{n \to \infty} \frac{-1}{n} \log \beta'_{m,n} \geq D(P\|Q),
\]
because \(\gamma_{m,n} + \gamma'_{m,n} \to 0\) as \(n \to \infty\). Together with Eq. (3), we have under \(H_1 : P \neq Q\),
\[
\liminf_{n \to \infty} \frac{-1}{n} \log P_{y^m x^n} \left( d_k(\hat{P}_m, \hat{Q}_n) \leq \gamma_{m,n} \right) \geq D(P\|Q).
\]

We next show the other direction under \(H_1\). We can write
\[
P_{y^m x^n} \left( d_k(\hat{P}_m, \hat{Q}_n) \leq \gamma_{m,n} \right) \overset{(a)}{=} P_{y^m x^n} \left( d_k(\hat{P}_m, P) \leq \gamma'_{m,n}, d_k(P, \hat{Q}_n) \leq \gamma'_{n} \right)
\]
\[
= P\left( d_k(\hat{P}_m, P) \leq \gamma'_{m} \right) Q\left( d_k(P, \hat{Q}_n) \leq \gamma'_{n} \right).
\]

where (a) is because \(d_k\) is a metric, and we choose \(\gamma'_{m} = \sqrt{2K/m(1 + \sqrt{-\log \alpha})}\) and \(\gamma'_{n} = \sqrt{2K/n(1 + \sqrt{-\log \alpha})}\) so that \(\gamma_{m,n} > \gamma'_{m,n} + \gamma'_{n}\). Then Lemma 2 gives \(P(d_k(P, \hat{P}_m) \leq \gamma'_{m,n}) > 1 - \alpha\) and \(P(d_k(P, \hat{Q}_n) \leq \gamma'_{n}) > 1 - \alpha\), where the latter implies that \(d_k(P, \hat{Q}_n) \leq \gamma'_{n}\) is a level \(\alpha\) test for testing \(H_0 : x^n \sim P\) and \(H_1 : x^n \sim Q\) with \(P \neq Q\). Together with Chernoff-Stein Lemma, we get
\[
\liminf_{n \to \infty} \frac{-1}{n} \log P_{y^m x^n} \left( d_k(\hat{P}_m, \hat{Q}_n) \leq \gamma_{m,n} \right)
\]
\[
\leq \liminf_{n \to \infty} \frac{-1}{n} \log \left( P\left( d_k(\hat{P}_m, P) \leq \gamma'_{m} \right) Q\left( d_k(P, \hat{Q}_n) \leq \gamma'_{n} \right) \right)
\]
\[
\leq \liminf_{n \to \infty} \frac{-1}{n} \log (1 - \alpha) + \liminf_{n \to \infty} \frac{-1}{n} \log Q\left( d_k(P, \hat{Q}_n) \leq \gamma'_{n} \right)
\]
\[
\leq D(P\|Q).
\]

The proof is complete.
C Proof of the Extended Sanov’s Theorem

Our proof is inspired by [16] which proved the original Sanov’s theorem w.r.t. the τ-topology. We first prove the result with a finite sample space and then extend it to the case with general Polish space. The prerequisites are two combinatorial lemmas that are standard tools in information theory.

For a positive integer t, let \( \mathcal{P}_m(t) \) denote the set of probability distributions defined on \( \{1, \ldots, t\} \) of form \( P = (\frac{m_1}{m}, \ldots, \frac{m_t}{m}) \), with integers \( m_1, \ldots, m_t \). Stated below are the two lemmas.

**Lemma 5** ([15, Theorem 11.1.1]). \(|\mathcal{P}_m(t)| \leq (m + 1)^t\).

**Lemma 6** ([15, Theorem 11.1.4]). Assume \( y^m \) i.i.d. \( \sim R \) where \( R \) is a distribution defined on \( \{1, \ldots, t\} \). For any \( P \in \mathcal{P}_m(t) \), the probability of the empirical distribution \( \hat{P}_m \) of \( y^m \) equal to \( P \) satisfies

\[
(m + 1)^t e^{-mD(P||R)} \leq \mathbb{P}_{y^m}(\hat{P}_m = P) \leq e^{-mD(P||R)}.
\]

C.1 Finite Sample Space

**Upper bound** Let \( t \) denote the cardinality of \( X \). Without loss of generality, assume that \( \inf_{(R,S) \in \text{int } \Gamma} cD(R||P) + (1 - c)D(S||Q) < \infty \). Hence, the open set \( \text{int } \Gamma \) is non-empty. As \( 0 < c = \lim_{m,n \to \infty} \frac{m}{m+n} < 1 \), we can find \( m_0 \) and \( n_0 \) such that there exists \( (P'_m, Q'_n) \in \text{int } \Gamma \cap \mathcal{P}_m(t) \times \mathcal{P}_n(t) \) for all \( m > m_0 \) and \( n > n_0 \), and that \( cD(P'_m||P) + (1 - c)D(Q'_n||Q) \to \inf_{(R,S) \in \text{int } \Gamma} cD(R||P) + (1 - c)D(S||Q) \) as \( m, n \to \infty \). Then we have, with \( m > m_0 \) and \( n > n_0 \),

\[
\mathbb{P}_{y^m}(\hat{P}_m = R, \hat{Q}_n = S) = \sum_{(R,S) \in \text{int } \Gamma} \mathbb{P}_{y^m}(\hat{P}_m = R, \hat{Q}_n = S) \geq \sum_{(R,S) \in \text{int } \Gamma} \mathbb{P}_{y^m}(\hat{P}_m = R, \hat{Q}_n = S) = \mathbb{P}_{y^m}(\hat{P}_m = R') \mathbb{P}_{x^n}(\hat{Q}_n = Q') \geq (m + 1)^t(n + 1)^t e^{-mD(P'||P)} e^{-nD(Q'||Q)},
\]

where the last inequality is from Lemma 6. It follows that

\[
\lim_{m,n \to \infty} \frac{1}{m+n} \log \mathbb{P}_{y^m}(\hat{P}_m, \hat{Q}_n) \leq \lim_{m,n \to \infty} \frac{1}{m+n} (-t \log((m + 1)(n + 1)) + mD(P'||P) + nD(Q'||Q)) = \lim_{m,n \to \infty} \frac{1}{m+n} (mD(P'||P) + nD(Q'||Q)) = \inf_{(R,S) \in \text{int } \Gamma} cD(R||P) + (1 - c)D(S||Q).
\]

**Lower bound**

\[
\mathbb{P}_{y^m}(\hat{P}_m = R) \mathbb{P}_{x^n}(\hat{Q}_n = S) = \sum_{(R,S) \in \text{int } \Gamma} \mathbb{P}_{y^m}(\hat{P}_m = R) \mathbb{P}_{x^n}(\hat{Q}_n = S) \leq \sum_{(R,S) \in \text{int } \Gamma} e^{-mD(R||P)} e^{-nD(S||Q)} \leq (m + 1)^t(n + 1)^t \sup_{(R,S) \in \Gamma} e^{-mD(R||P)} e^{-nD(S||Q)},
\]

where (a) and (b) are due to Lemma 5 and Lemma 6 respectively. This gives

\[
\lim_{m,n \to \infty} \frac{1}{m+n} \log \mathbb{P}_{y^m}(\hat{P}_m, \hat{Q}_n) \geq \inf_{(R,S) \in \Gamma} cD(R||P) + (1 - c)D(S||Q),
\]

and hence the lower bound by noting that \( \Gamma \in \text{cl } \Gamma \). Indeed, when the right hand side is finite, the infimum over \( \Gamma \) equals the infimum over \( \text{cl } \Gamma \) as a result of the continuity of KLD for finite alphabets.
C.2 Polish Sample Space

We consider the general case with \(\mathcal{X}\) being a Polish space. Now \(\mathcal{P}\) is the space of probability measures on \(\mathcal{X}\) endowed with the topology of weak convergence. To proceed, we introduce another topology on \(\mathcal{P}\) and an equivalent definition of the KLD.

\(\tau\)-topology: denote by \(\Pi\) the set of all partitions \(A = \{A_1, \ldots, A_t\}\) of \(\mathcal{X}\) into a finite number of measurable sets \(A_i\). For \(P \in \mathcal{P}\), \(A \in \Pi\), and \(\zeta > 0\), denote

\[
U(P, A, \zeta) = \{P' \in \mathcal{P} : |P'(A_i) - P(A_i)| < \zeta, i = 1, \ldots, t\}.
\]

The \(\tau\)-topology on \(\mathcal{P}\) is the coarsest topology in which the mapping \(P \rightarrow P(F)\) are continuous for every measurable set \(F \subset \mathcal{X}\). A base for this topology is the collection of the sets \((5)\). We will use \(\mathcal{P}_\tau\) when we refer to \(\mathcal{P}\) endowed with this \(\tau\)-topology, and write the interior and closure of a set \(\Gamma \in \mathcal{P}_\tau\) as \(\text{int}_\tau \Gamma\) and \(\text{cl}_\tau \Gamma\), respectively.

We remark that the \(\tau\)-topology is stronger than the weak topology: any open set in \(\mathcal{P}\) w.r.t. weak topology is also open in \(\mathcal{P}_\tau\) (see more details in \([10, 19]\)). The product topology on \(\mathcal{P}_\tau \times \mathcal{P}_\tau\) is determined by the base of the form of

\[
U(P, A_1, \zeta_1) \times U(Q, A_2, \zeta_2),
\]

for \((P, Q) \in \mathcal{P}_\tau \times \mathcal{P}_\tau\), \(A_1, A_2 \in \Pi\), and \(\zeta_1, \zeta_2 > 0\). We still use \(\text{int}_\tau \Gamma\) and \(\text{cl}_\tau \Gamma\) to denote the interior and closure of a set \(\Gamma \subset \mathcal{P}_\tau \times \mathcal{P}_\tau\). As there always exists \(A \in \Pi\) that refines both \(A_1\) and \(A_2\), any element from the base has an open subset

\[
\hat{U}(P, Q, A, \zeta) := U(P, A, \zeta) \times U(Q, A, \zeta) \subset \mathcal{P}_\tau \times \mathcal{P}_\tau,
\]

for some \(\zeta > 0\).

Another definition of the KLD: an equivalent definition of the KLD will also be used:

\[
D(P||Q) = \sup_{A \in \Pi} \sum_{i=1}^{t} P(A_i) \log \frac{P(A_i)}{Q(A_i)} = \sup_{A \in \Pi} D(P^A||Q^A),
\]

with the conventions \(0 \log 0 = 0 \log 0^0 = 0\) and \(a \log \frac{a}{0} = +\infty\) if \(a > 0\). Here \(P^A\) denotes the discrete probability measure \((P(A_1), \ldots, P(A_t))\) obtained from probability measure \(P\) and partition \(A\). It is not hard to verify that for \(0 < c < 1\),

\[
cD(R||P) + (1 - c)D(S||Q) = c \sup_{A_1 \in \Pi} D(R^A_1||P^A_1) + (1 - c) \sup_{A_2 \in \Pi} D(S^A_2||Q^A_2)
\]

\[
= \sup_{A \in \Pi} \left(cD(R^A||P^A) + (1 - c)D(S^A||Q^A)\right),
\]

due to the existence of \(A\) that refines both \(A_1\) and \(A_2\) and the log-sum inequality \([15]\).

We are ready to show the extended Sanov’s theorem with Polish space.

Upper bound It suffices to consider only non-empty open \(\Gamma\). If \(\Gamma\) is open in \(\mathcal{P} \times \mathcal{P}\), then \(\Gamma\) is also open in \(\mathcal{P}_\tau \times \mathcal{P}_\tau\). Therefore, for any \((R, S) \in \Gamma\), there exists a finite (measurable) partition \(A = \{A_1, \ldots, A_t\}\) of \(\mathcal{X}\) and \(\zeta > 0\) such that

\[
\hat{U}(R, S, A, \zeta) = \{(R', S') : |R(A_i) - R'(A_i)| < \zeta, |S(A_i) - S'(A_i)| < \zeta, i = 1, \ldots, t\} \subset \Gamma.
\]

Define the function \(T : \mathcal{X} \rightarrow \{1, \ldots, t\}\) with \(T(x) = i\) for \(x \in A_i\). Then \((\tilde{P}_m, \tilde{Q}_m) \in \hat{U}(R, S, A, \zeta)\) with \(R, S \in \Gamma\) if and only if the empirical measures \(\tilde{P}_m\) of \(\{T(y_1), \ldots, T(y_m)\}\) and \(\tilde{Q}_m\) of \(\{T(x_1), \ldots, T(x_n)\}\) lie in \(U^\circ(R, S, A, \zeta) = \{(R^\circ, S^\circ) : |R^\circ(i) - R(A_i)| < \zeta, |S^\circ(i) - S(A_i)| < \zeta, i = 1, \ldots, t\} \subset \mathbb{R}^t \times \mathbb{R}^t\).

Thus, we have

\[
P_{y=x^\circ}(\{\tilde{P}_m, \tilde{Q}_n\} \in \Gamma) \geq P_{y=x^\circ}(\{\tilde{P}_m, \tilde{Q}_n\} \in \hat{U}(R, S, A, \zeta)) = P_{T(y^m)T(x^n)}(\{\tilde{P}_m^\circ, \tilde{Q}_n^\circ\} \in U^\circ(R, S, A, \zeta)).
\]
As \( T(x) \) and \( T(y) \) takes values from a finite alphabet and \( \mathcal{U}(R, S, \zeta) \) is open, we obtain that

\[
\lim_{m,n \to \infty} \frac{1}{m+n} \log \mathbb{P}_{y=x^n}(\hat{P}_m, \hat{Q}_n) \leq \lim_{m,n \to \infty} \frac{1}{m+n} \log \mathbb{P}_{T(y^n)T(x^n)}(\hat{P}_m^\circ, \hat{Q}_n^\circ) \leq \inf_{(R^\circ, S^\circ) \in \mathcal{U}(R, S, \mathcal{A}, \zeta)} cD(R^\circ || P^A) + (1-c)D(S^\circ || Q^A)
\]

where we have used definition of KLD in Eq. (3) and \((R, S) \in \hat{\mathcal{U}}(R, S, \mathcal{A}, \zeta)\) in the last inequality. As \((R, S)\) is arbitrary in \( \Gamma \), the lower bound is established by taking infimum over \( \Gamma \).

**Lower bound** With notations

\[
\Gamma^A = \{(R^A, S^A) : (R, S) \in \Gamma\}, \quad \Gamma(A) = \{(R, S) : (R^A, S^A) \in \Gamma^A\},
\]

where \( \mathcal{A} = \{A_1, \ldots, A_t\} \) is a finite partition, it holds that

\[
\mathbb{P}_{y=x^n}(\hat{P}_m, \hat{Q}_n) \leq \mathbb{P}_{y=x^n}(\hat{P}_m^A, \hat{Q}_n^A) \leq (n+1)^t (m+1)^t \max_{(R^\circ, S^\circ) \in \Gamma^A \cap \mathcal{P}_n(t) \times \mathcal{P}_m(t)} \mathbb{P}_{y=x^n}(\hat{P}_n = R^\circ, \hat{Q}_n = S^\circ) \leq (n+1)^t (m+1)^t \exp \left( -\inf_{(R, S) \in \Gamma} \left( nD(R^A || P^A) + mD(S^A || Q^A) \right) \right),
\]

where the last two inequalities are from Lemmas 5 and 6. As the above holds for any \( \mathcal{A} \in \Pi \), Eq. (6) indicates

\[
\lim_{m,n \to \infty} \frac{1}{m+n} \log \mathbb{P}_{y=x^n}(\hat{P}_m, \hat{Q}_n) \leq \inf_{\mathcal{A}} \left( -\inf_{(R, S) \in \Gamma} \left( cD(R^A || P^A) + (1-c)D(S^A || Q^A) \right) \right) = -\sup_{\mathcal{A}} \inf_{(R, S) \in \Gamma} cD(R^A || P^A) + (1-c)D(S^A || Q^A).
\]

Then the remaining of obtaining the lower bound is to show

\[
\sup_{\mathcal{A}} \inf_{(R, S) \in \Gamma} cD(R^A || P^A) + (1-c)D(S^A || Q^A) \geq \inf_{(R, S) \in \text{cl} \Gamma} cD(R || P) + (1-c)D(S || Q).
\]

Assuming, without loss of generality, that the left hand side is finite, we only need to show

\[
\text{cl} \Gamma \cap B(P, Q, \eta) \neq \emptyset,
\]

whenever

\[
\eta > \sup_{\mathcal{A}} \inf_{(R, S) \in \Gamma} cD(R^A || P^A) + (1-c)D(S^A || Q^A).
\]

Here \( B(P, Q, \eta) \) is the divergence ball defined as follows

\[
B(P, Q, \eta) = \{(R, S) : cD(R || P) + (1-c)D(S || Q) \leq \eta\},
\]

which is compact in \( \mathcal{P} \times \mathcal{P} \) w.r.t. the weak topology, due to the lower semi-continuity of \( D(\cdot || P) \) and \( D(\cdot || Q) \) as well as the fact that \( 0 < c < 1 \).
To this end, we first show the following:

$$\text{cl}\Gamma = \bigcap_{\mathcal{A}} \text{cl}\Gamma(\mathcal{A}).$$

The inclusion is obvious since $\Gamma \in \text{cl}\Gamma(\mathcal{A})$. The reverse means that if $(R, S) \in \text{cl}\Gamma(\mathcal{A})$ for each $\mathcal{A}$, then any neighborhood of $(R, S)$ w.r.t. the weak convergence intersects $\Gamma$. To verify this, let $O(R, S)$ be a neighborhood of $(R, S)$ w.r.t. the weak convergence, then there exists $\tilde{U}(R, S, B, \zeta) \in O(R, S)$ over a finite partition $\mathcal{B}$ as $O(R, S)$ is also open in $\mathcal{P}_\tau \times \mathcal{P}_\tau$. Furthermore, the partition $\mathcal{B}$ can be chosen to refine $\mathcal{A}$ so that $\text{cl}\Gamma(\mathcal{B}) \subset \text{cl}\Gamma(\mathcal{A})$. As $\tau$-topology is stronger than the weak topology, a closed set in the $\mathcal{P}_\tau \times \mathcal{P}_\tau$ is closed in $\mathcal{P} \times \mathcal{P}$, and hence $\text{cl}\Gamma(\mathcal{B}) \subset \text{cl}\Gamma(\mathcal{B})$. That $(R, S) \in \text{cl}\Gamma(\mathcal{B})$ implies that there exists $(R', S') \in \tilde{U}(R, S, B, \zeta) \cap \text{cl}\Gamma(\mathcal{B})$. By the definition of $\text{cl}\Gamma(\mathcal{B})$, we can also find $(\tilde{R}, \tilde{S}) \in \Gamma$ such that $\tilde{R}(B_i) = R'(B_i)$ and $\tilde{S}(B_i) = S'(B_i)$ for each $B_i \in \mathcal{B}$, and hence $(\tilde{R}, \tilde{S}) \in \tilde{U}(\tilde{R}, \tilde{S}, B, \zeta) \subset O(R, S)$ and $(\tilde{R}, \tilde{S}) \in \Gamma$. Therefore, $\Gamma \cap O(R, S) \neq \emptyset$ and the claim follows.

Next we show that, for each partition $\mathcal{A}$,

$$\Gamma(\mathcal{A}) \cap B(P, Q, \eta) \neq \emptyset. \quad \text{(10)}$$

By Eq. (10), there exists $(\tilde{P}, \tilde{Q})$ such that $cD(\tilde{P}^A || P^A) + (1-c)D(\tilde{Q}^A || Q^A) \leq \eta$. For such $(\tilde{P}, \tilde{Q})$, we can construct $(P', Q') \in \Gamma(\mathcal{A})$ as

$$P'(F) = \sum_{i=1}^t \frac{\tilde{P}(A_i)}{P(A_i)} P(F \cap A_i),$$

$$Q'(F) = \sum_{i=1}^t \frac{\tilde{Q}(A_i)}{Q(A_i)} Q(F \cap A_i),$$

for any measurable subset $F \subset \mathcal{X}$. If $P(A_i) = 0$ ($Q(A_i) = 0$) and hence $\tilde{P}(A_i) = 0$ ($\tilde{Q}(A_i) = 0$), as $D(\tilde{P}^A || P^A) < \infty$ ($D(\tilde{Q}^A || Q^A) < \infty$), for some $i$, the corresponding term in the above equation is set equal to 0. Then $(P', Q')$ belongs to $\Gamma(\mathcal{A})$ and also lies in $B(P, Q, \eta)$. The latter is because $D(P' || P) = D(\tilde{P}^A || Q^A)$ and $D(Q' || Q) = D(\tilde{Q}^A || Q^A)$: one can verify that any $B$ that refines $\mathcal{A}$ satisfies

$$D(P^B || P^B) = D(\tilde{P}^A || P^A), D(Q^B || Q^B) = D(\tilde{Q}^A || Q^A).$$

For any finite collection of partitions $\mathcal{A}_i \in \Pi$ and $\mathcal{A} \in \Pi$ refining each $\mathcal{A}_i$, each $\Gamma(A_i)$ contains $\Gamma(\mathcal{A})$. This implies that

$$\bigcap_{i=1}^r (\Gamma(A_i) \cap B(p, q, \eta)) \neq \emptyset,$$

for any finite $r$. Finally, the set $\text{cl}\Gamma(\mathcal{A}) \cap B(P, Q, \eta)$ for any $\mathcal{A}$ is compact due to the compactness of $B(P, Q, \eta)$, and any finite collection of them has non-empty intersection. It follows that all these sets is also non-empty.

This completes the proof.

D Proof of Theorem [7]

Proof. According to Theorem 1, $d_k$ metrizes the weak convergence over $\mathcal{P}$. For convenience, we will write the type-I and type-II error probabilities as $\alpha_{m,n}$ and $\beta_{m,n}$, respectively; we will also use $\beta$ to denote the type-II error exponent. That $\alpha_{m,n} \leq \alpha$ is clear from Lemma [1] and we only need to show that $\beta_{m,n}$ vanishes exponentially as $m$ and $n$ scale.

We first show $\beta \geq D^*$. With a fixed $\gamma > 0$, we have $\gamma_{m,n} \leq \gamma$ for sufficiently large $n$ and $m$. Therefore,

$$\beta = \liminf_{m,n \to \infty} - \frac{1}{m+n} \log \mathbf{P}_{y \sim x^m}(d_k(\hat{P}_m, \hat{Q}_n) \leq \gamma_{m,n})$$

$$\geq \liminf_{m,n \to \infty} - \frac{1}{m+n} \log \mathbf{P}_{y \sim x^m}(d_k(\hat{P}_m, \hat{Q}_n) \leq \gamma)$$

$$\geq \inf_{(R, S): d_k(R, S) \leq \gamma} cD(R || P) + (1-c)D(S || Q)$$

$$:= D^* \gamma,$$
where the last inequality is from the extended Sanov’s theorem and that $d_k$ metrizes weak convergence of $P$ so that $\{(R, S) : d_k(R, S) \leq \gamma\}$ is closed in the product topology on $\mathcal{P} \times \mathcal{P}$. Since $\gamma > 0$ can be arbitrarily small, we have

$$\beta \geq \lim_{\gamma \to 0^+} D^*_{\gamma},$$

where the limit on the right hand side must exist as $D^*_{\gamma}$ is positive, non-decreasing when $\gamma$ decreases, and bounded by $D^*$ that is assumed to be finite. Then it suffices to show

$$\lim_{\gamma \to 0^+} D^*_{\gamma} = D^*.$$

To this end, let $(R_\gamma, S_\gamma)$ be such that $d_k(R_\gamma, S_\gamma) \leq \gamma$ and $cD(R_\gamma\|P) + (1 - c)D(S_\gamma\|Q) = D^*_{\gamma}$. Notice that $R_\gamma$ and $S_\gamma$ must lie in

$$\left\{ W : D(W\|P) \leq \frac{D^*}{c}, D(W\|Q) \leq \frac{D^*}{1 - c} \right\} =: \mathcal{W},$$

for otherwise $D^*_{\gamma} > D^*$. We remark that $\mathcal{W}$ is a compact set in $\mathcal{P}$ as a result of the lower semi-continuity of KLD w.r.t. the weak topology on $\mathcal{P}$. Existence of such a pair can be seen from the facts that $\{(R, S) : d_k(R, S) \leq \gamma\}$ is closed and convex, and that both $D(\cdot\|P)$ and $D(\cdot\|Q)$ are convex functions.

Assume that $D^*$ cannot be achieved. We can write

$$\lim_{\gamma \to 0^+} D^*_{\gamma} = D^* - \epsilon,$$

for some $\epsilon > 0$. By the definition of lower semi-continuity, there exists a $\kappa_\mathcal{W} > 0$ for each $W \in \mathcal{W}$ such that

$$cD(R\|P) + (1 - c)D(S\|Q) \geq cD(W\|P) + (1 - c)D(W\|Q) - \frac{\epsilon}{2} \geq D^* - \frac{\epsilon}{2},$$

whenever $R$ and $S$ are both from

$$\mathcal{S}_\mathcal{W} = \{ R : d_k(R, W) < \kappa_\mathcal{W} \}.$$

Here the last inequality comes from the definition of $D^*$ given in Theorem. To find a contradiction, define

$$\mathcal{S}'_\mathcal{W} = \{ R : d_k(R, W) < \frac{\kappa_\mathcal{W}}{2} \}.$$

Since $\mathcal{S}'_\mathcal{W}$ is open and $\bigcup_i \mathcal{S}'_{W_i}$ covers $\mathcal{W}$, the compactness of $\mathcal{W}$ implies that there exists finite $\mathcal{S}'_{W_i}$’s, denoted by $\mathcal{S}'_{W_1}, \ldots, \mathcal{S}'_{W_N}$, covering $\mathcal{W}$. Define $\kappa^* = \min_{i=1}^N \kappa_{W_i} > 0$. Now let $\gamma < \kappa^*/2$ as $\gamma$ can be made arbitrarily small. Since $\bigcup_i^N \mathcal{S}'_{W_i}$ covers $\mathcal{W}$, we can find a $W_i$ with $R_\gamma \in \mathcal{S}'_{W_i}$, $S_\gamma \in \mathcal{S}'_{W_i}$. Thus, it holds that

$$d_k(S_\gamma, W_i) \leq d_k(S_\gamma, R_\gamma) + d_k(R_\gamma, W_i) < \kappa_{W_i}.$$

That is, $S_\gamma$ also lies in $\mathcal{S}'_{W_i}$. By Eq. (13) we get

$$cD(R_\gamma\|P) + (1 - c)D(S_\gamma\|Q) \geq D^* - \epsilon/2.$$

However, by our assumption in Eq. (12), it should hold that

$$cD(R_\gamma\|P) + (1 - c)D(S_\gamma\|Q) \leq D^* - \epsilon.$$

Therefore, $\beta \geq D^*$.

The other direction can be simply seen from the optimal type-II error exponent in Theorem. Alternatively, we can use Chernoff-Stein lemma in a similar manner to the proof of Theorem. Let $P'$ be such that $cD(P'\|P) + (1 - c)D(P'\|Q) = D^*$. Such $P'$ exists because $0 < D^* < \infty$ and $D(\cdot\|P)$ and $D(\cdot\|Q)$ are convex w.r.t. $\mathcal{P}$. That $D^*$ is bounded implies that both $D(P'\|P)$ and $D(P'\|Q)$ are finite. We have

$$\beta_{m, n} = \mathbf{P}_{y^{n \times m}}(d_k(\hat{P}_m, \hat{Q}_n) \leq \gamma_{m, n})$$

$$(a) \geq \mathbf{P}_{y^{n \times m}}(d_k(P', \hat{P}_m) + d_k(P', \hat{Q}_n) \leq \gamma_{m, n})$$

$$(b) \geq \mathbf{P}_{y^{n \times m}}(d_k(P', \hat{P}_m) \leq \gamma_m, d_k(P', \hat{Q}_n) \leq \gamma_n)$$

$$= \mathbf{P}(d_k(P', \hat{P}_m) \leq \gamma_m) \mathbf{Q}(d_k(P', \hat{Q}_n) \leq \gamma_n),$$

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where \((a)\) and \((b)\) are from the triangle inequality of the metric \(d_k\), and we pick \(\gamma_n = \sqrt{2K/m(1 + \sqrt{-\log \alpha})}\), and \(\gamma_m = \sqrt{2K/m(1 + \sqrt{-\log \alpha})}\) so that \(\gamma_{m,n} > \gamma_n + \gamma_m\). Then Lemma 2 implies \(P' \vert (P', \hat{P}_m) \leq \gamma_m > 1 - \alpha\).

For now assume that \(D(P'\|P) > 0\) and \(D(P'\|Q) > 0\). We can regard \(\{y^m : d_k(P', \hat{P}_m) \leq \gamma_m\}\) as an acceptance region for testing \(H_0 : y^m \sim P'\) and \(H_1 : y^m \sim P\). Clearly, this test performs no better than the optimal level \(\alpha\) test for this simple hypothesis testing in terms of the type-II error probability. Therefore, Chernoff-Stein lemma implies

\[
\lim \inf_{m \to \infty} \frac{1}{m} \log P(d_k(P', \hat{P}_m) \leq \gamma_m) \leq D(P'\|P). \tag{14}
\]

Analogously, we have

\[
\lim \inf_{n \to \infty} \frac{1}{n} \log Q(d_k(P', \hat{Q}_n) \leq \gamma_n) \leq D(P'\|Q). \tag{15}
\]

Now assume without loss of generality that \(D(P'\|P) = 0\), i.e., \(P' = P\). Then \(D(P'\|Q) > 0\) under the alternative hypothesis \(H_1 : P \neq Q\), and Eq. (15) still holds. Using Lemma 2 we have \(P'(d_k(P', \hat{P}_m) \leq \gamma_m) > 1 - \alpha\), which gives zero exponent. Therefore, Eq. (14) holds with \(P' = P\).

As \(\lim_{m,n \to \infty} m = c\), we conclude that

\[
\beta = \lim \inf_{m,n \to \infty} \frac{1}{m+n} \log \beta_{m,n} \leq D^*.
\]

The proof is complete.

\[\square\]

E Proof of Theorem 8

Proof. Let \(P'\) be such that \(cD(P'\|P) + (1 - c)D(P'\|Q) = D^*\). Consider first \(D(P'\|P) \neq 0\) and \(D(P'\|Q) \neq 0\). Since \(D^*\) is assumed to be finite, we have both \(D(P'\|P)\) and \(D(P'\|Q)\) being finite. This implies that \(P'\) is absolutely continuous w.r.t. both \(P\) and \(Q\), so the Radon-Nikodym derivatives \(dP'/dP\) and \(dP'/dQ\) exist.

Define two sets

\[
A_m = \left\{ y^m : D(P'\|P) - \epsilon \leq \frac{1}{m} \log \frac{dP'(y^m)}{dP(y^m)} \leq D(P'\|P) + \epsilon \right\},
\]

\[
B_n = \left\{ x^n : D(P'\|Q) - \epsilon \leq \frac{1}{n} \log \frac{dP'(x^n)}{dQ(x^n)} \leq D(P'\|Q) + \epsilon \right\}.
\]

Recall the definition of the KLD: \(D(P'\|P) = E_{x \sim P'} \log (dP'(x)/dP(x))\) and \(D(P'\|Q) = E_{x \sim P'} \log (dP'(x)/dQ(x))\). By law of large numbers, we have for any given \(\epsilon > 0\),

\[
P_{y^m x^n}(A_m \times B_n) \geq 1 - \epsilon, \text{ for large enough } m \text{ and } n,
\]

with \(y^m\) and \(x^n\) i.i.d. \(\sim P'\).

Now consider the type-II error probability of level \(\alpha\) tests. First, for a level \(\alpha\) test, we have its acceptance region satisfies

\[
P_{y^m x^n}(\Omega^*_0(m,n)) > 1 - \alpha,
\]

when \(y^m\) and \(x^n\) i.i.d. \(\sim P'\), i.e., when the null hypothesis \(H_0 : P = Q\) holds. Then under the alternative
hypothesis $H_1: P \neq Q$, we have

$$P_{g^{m,x}}(\Omega'_0(m,n)) \geq P_{g^{m,x}}(A_m \times B_n \cap \Omega'_0(m,n))$$

$$= \int_{A_m \times B_n \cap \Omega'_0(m,n)} dP(y^{m}) dQ(x^{n})$$

$$\geq \left( a \right) \int_{A_m \times B_n \cap \Omega'_0(m,n)} 2^{-m(D(P'^{\|P})+\epsilon)} 2^{-n(D(P'^{\|Q})+\epsilon)} dP'(y^{m}) dP'(x^{n})$$

$$= 2^{-mD(P'^{\|P})-n(D(P'^{\|Q})-(m+n)\epsilon)} \int_{A_m \times B_n \cap \Omega'_0(m,n)} dP'(y^{m}) dP'(x^{n})$$

$$\geq \left( b \right) 2^{-mD(P'^{\|P})-nD(P'^{\|Q})-(m+n)\epsilon}(1-\alpha-\epsilon),$$

where $(a)$ is from Eq. (16) and $(b)$ is due to Eqs. (17) and (18). Thus, when $\epsilon$ is small enough so that $1-\alpha-\epsilon > 0$, we get

$$\liminf_{m,n \to \infty} -\frac{1}{m+n} \log P_{g^{m,x}}(\Omega'_0(m,n)) \leq \liminf_{m,n \to \infty} -\frac{1}{m+n} (mD(P'^{\|P})+n(D(P'^{\|Q})+(m+n)\epsilon)$$

$$= D^* + \epsilon. \quad (19)$$

If a test is an asymptotic level $\alpha$ test, we can replace $\alpha$ by $\alpha + \epsilon'$ where $\epsilon'$ can be made arbitrarily small provided that $m$ and $n$ are large enough. Thus, Eq. (16) holds too. Finally, since $\epsilon$ can also be arbitrarily small, we conclude that

$$\liminf_{m,n \to \infty} -\frac{1}{m+n} \log P_{g^{m,x}}(\Omega'_0(m,n)) \leq D^*.$$

If $P' = P$, then $A_m$ contains all $g^{m} \in X^{m}$ and the above procedure gives the same result. \hfill $\square$

F Experiments

This section presents empirical results of the MMD and KSD based goodness-of-fit tests in the finite sample regime. We note that there have been extensive experiments in [12, 23, 34, 29] and the sample size $m$ drawn from $P$ is usually fixed for the kernel two-sample test. As such, we only consider two toy experiments and let $m$ scale as required in Theorem 1.

We evaluate the following tests with a fixed level $\alpha = 0.1$, all using Gaussian kernel $k(x,y) = e^{-\|x-y\|^2/(2w)}$.

1) Simple: the simple kernel test $d_k(P,\hat{Q}_n)$. The acceptance threshold is estimated by drawing i.i.d. samples from $P$, i.e., the Monte Carlo method. The number of trials is 500.

2) Two-sample: the two-sample test $d_k(\hat{P}_m,\hat{Q}_n)$ with $m = n^{1.5}$. Threshold is obtained from the bootstrap method in [25] with 500 bootstrap replicates.

3) KSD: the KSD based test $d^2_{KSD}(P,\hat{Q}_n)$. We use wild bootstrap method from [12] with 500 replicates to estimate the $\alpha$-quantile.

Gaussian vs. Laplace. We use a similar experiment setting in [29]. Consider $P : \mathcal{N}(0,2\sqrt{2})$ and $Q : \text{Laplace}(0,2)$, a zero-mean Laplace distribution with scale parameter 2. The parameters are chosen so that $P$ and $Q$ have the same mean and variance. We pick a fixed bandwidth $w = 1$ for all the kernel based tests and repeat 500 trials of each sample size $n$ for both hypotheses. We also evaluate the likelihood ratio test LR, an oracle approach assuming both $P$ and $Q$ are known. In Figure 1a, LR has the lowest type-II error probabilities as expected, while Simple and Two-sample perform slightly better than KSD. As shown in Figure 1b, all the kernel based tests have the type-I error probabilities around the given level $\alpha = 0.1$, except for KSD with $n = 5$ samples.

Gaussian Mixture. The next experiment is taken from [34]. The i.i.d. observations $x^n$ are drawn from $Q : \sum_{i=1}^5 a_i \mathcal{N}(x; \mu_i, \sigma^2)$ with $a_i = 1/5$, $\sigma^2 = 1$, and $\mu_i$ randomly drawn from Uniform[0,10]. We then generate $P$ by adding standard Gaussian noise (perturbation) to $\mu_i$. In [34], the sample number $m$ drawn from $P$ is fixed while the observed sample number $n$ varies. We report the type-II error probabilities in Figure 2, averaged over 500 random trials.
Universal Hypothesis Testing with Kernels

With the median heuristic for bandwidth choice, KSD and Two-sample perform similarly whereas Simple has its type-II error probability decreasing slowly, as shown in Figure 2a. Picking a fixed bandwidth \( w = 1 \) for Simple again results in a better performance. In light of the role of kernels, we then search over the kernel bandwidths in \([0, 8]\) for a fixed sample size \( n = 50 \). In Figure 2b Simple and Two-sample tend to achieve lower type-II error probabilities when \( w \) is small, while KSD has a lower error probability around \( w = 5 \). The optimal type-II error probabilities of Simple and KSD are close and slightly lower than that of Two-sample. While computational issue is not the focus of this paper, we do observe that KSD is more efficient in this experiment, as it does not need to draw samples.

Whereas we cannot tell much statistical difference in our experiments, some experiments in the literature showed that the MMD based tests performed better than the KSD based tests and others showed the opposite \[12, 23, 34, 29\]. The finite sample performance depends on kernel choice as well as specific distributions. Under the universal setting, no test is known to be optimal in terms of the type-II error probability subject to a given level constraint. Statistical optimality can only be established in the large sample limit, as the one considered in the present work.