# Finite sample approximations of exact and entropic Wasserstein distances between covariance operators and Gaussian processes\*

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Abstract. This work studies finite sample approximations of the exact and entropic regularized Wasserstein distances between centered Gaussian processes and, more generally, covariance operators of functional random processes. We first show that these distances/divergences are fully represented by reproducing kernel Hilbert space (RKHS) covariance and cross-covariance operators associated with the corresponding covariance functions. Using this representation, we show that the Sinkhorn divergence between two centered Gaussian processes can be consistently and efficiently estimated from the divergence between their corresponding normalized finite-dimensional covariance matrices, or alternatively, their sample covariance operators. Consequently, this leads to a consistent and efficient algorithm for estimating the Sinkhorn divergence from finite samples generated by the two processes. For a fixed regularization parameter, the convergence rates are *dimension-independent* and of the same order as those for the Hilbert-Schmidt distance. If at least one of the RKHS is finite-dimensional, we obtain a *dimension-dependent* sample complexity for the exact Wasserstein distance between the Gaussian processes.

Key word. Wasserstein distance, entropic regularization, Gaussian processes, reproducing kernel Hilbert spaces

AMS subject classifications. 60G15, 49Q22

1. Introduction. This work studies exact and entropic regularized Wasserstein distances and divergences between centered Gaussian processes, and more generally, between covariance operators associated with functional random processes. Our main focus is on the finite sample approximations of the entropic divergences, which we show to be *dimension-independent*. Our main results are obtained via the analysis of reproducing kernel Hilbert space (RKHS) covariance and cross-covariance operators associated with the covariance functions of the given random processes. This work builds upon [33, 35], which formulated entropic Wasserstein distances between Gaussian measures on Hilbert spaces and their convergence properties.

The topic of distances/divergences between covariance operators and stochastic processes has attracted increasing interests in statistics and machine learning recently, e.g. [37, 15, 39, 29, 30, 50]. In [30, 50], the Kullback-Leibler divergence between stochastic processes was studied, the latter in the context of functional Bayesian neural networks. In the field of functional data analysis, see e.g. [43, 12, 21], one particular approach for analyzing functional data has been via the analysis of covariance operators. Recent work along this direction includes [37, 15], which utilize the Hilbert-Schmidt distance between covariance operators and [39, 29], which utilize non-Euclidean distances, in particular the Procrustes distance, also known as Bures-Wasserstein distance. The latter distance is precisely the 2-Wasserstein distance between two centered Gaussian measures on Hilbert space in the setting of optimal transport (OT) and can better capture the intrinsic geometry of the set of covariance operators. This

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distance is always well-defined for *singular covariance operators*, which is a distinct advantage over the Kullback-Leibler divergence, which requires equivalent Gaussian measures [34]. OT distances are, however, generally numerically difficult to compute and can have, moreover, poor convergence rates (more below), which motivated the study of entropic regularized OT. This direction has recently attracted much attention in machine learning, statistics, and related fields [7, 13, 18, 31, 38]). This line of research is also closely connected with the *Schrödinger bridge problem* [47], which has been studied extensively [3, 4, 8, 25, 46].

In [28, 22, 9], explicit formulas were obtained for the entropic regularized 2-Wasserstein distance and Sinkhorn divergence between Gaussian measures on Euclidean space. These were generalized to infinite-dimensional Gaussian measures on Hilbert spaces in [33], with the entropic formulation being valid for both settings of *singular* and *nonsingular* covariance operators. The Gaussian setting reveals explicitly several *favorable theoretical properties* of the entropic regularization formulation, including strict convexity, unique solution of barycenter equation in the singular setting, and Fréchet differentiability, in contrast to the 2-Wasserstein distance, which is *not* Fréchet differentiable in the infinite-dimensional setting.

Furthermore, it has been shown that the Sinkhorn divergence has much better convergence behavior and sample complexity compared with the exact Wasserstein distance. It is wellknown that the sample complexity of the Wasserstein distance can grow exponentially in the dimension of the underlying space  $\mathbb{R}^d$ , with the worst case being  $O(n^{-1/d})$  [11, 52, 14, 20]. In [17], it is shown that, as a consequence of entropic regularization, the Sinkhorn divergence between two probability measures with bounded support on  $\mathbb{R}^d$  achieves sample complexity  $O((1+\epsilon^{-\lfloor d/2 \rfloor})n^{-1/2})$ , that is the same as the Maximum Mean Discrepancy (MMD) for a fixed  $\epsilon > 0$ . However, the constant factor in the sample complexity in [17] depends exponentially on the diameter of the support. In [31], the rate of convergence  $O\left(\epsilon\left(1+\frac{\sigma^{\lceil 5d/2 \rceil + 6}}{\epsilon^{\lceil 5d/4 \rceil + 3}}\right)n^{-1/2}\right)$ was obtained for  $\sigma^2$ -subgaussian measures on  $\mathbb{R}^d$ . In [35], it was shown that the Sinkhorn divergence in the RKHS setting achieves the rate of convergence  $O\left((1+\frac{1}{\epsilon})n^{-1/2}\right)$  for all  $\epsilon > 0$ , which is thus dimension-independent. In particular, this applies to Sinkhorn divergence between Gaussian measures on Euclidean space and infinite-dimensional Hilbert spaces.

**Contributions of this work**. In this work, we apply the results in [33, 35] to the setting of centered Gaussian processes, and more generally, covariance operators associated with functional random processes. Specifically,

- 1. We show that the Wasserstein distance/Sinkhorn divergence between centered Gaussian processes are fully represented by RKHS covariance and cross-covariance operators associated with the corresponding covariance functions. From this representation, we show that the Sinkhorn divergence can be consistently and efficiently estimated via the corresponding normalized finite covariance matrices. The convergence rate is dimension-independent and has the form  $O(\frac{1}{\epsilon}n^{-1/2})$  (Section 4). Alternatively, the Sinkhorn divergence can be consistently estimated via the corresponding sample covariance operators with similar convergence rate (Section 7).
- 2. We present an algorithm that consistently and efficiently estimates the Sinkhorn divergence from *finite samples* of the two given random processes. The convergence rate is *dimension-independent*. (Section 5).
- 3. For the exact 2-Wasserstein distance, we obtain the corresponding sample complexity

when the RKHS of at least one of the covariance functions is finite-dimensional. The convergence rate is *dimension-dependent* (Section 6).

Notation. Throughout the paper, let  $\mathcal{H}$  be a real, separable Hilbert space, with dim $(\mathcal{H}) = \infty$  unless explicitly stated otherwise. Let  $\mathcal{L}(\mathcal{H})$  denote the set of bounded linear operators on  $\mathcal{H}$ , with norm  $||A|| = \sup_{||x|| \leq 1} ||Ax||$ . Let  $\operatorname{Sym}(\mathcal{H}) \subset \mathcal{L}(\mathcal{H})$  be the set of bounded, self-adjoint linear operators on  $\mathcal{H}$ . Let  $\operatorname{Sym}^+(\mathcal{H}) \subset \operatorname{Sym}(\mathcal{H})$  be the set of self-adjoint, positive operators on  $\mathcal{H}$ , i.e.  $A \in \operatorname{Sym}^+(\mathcal{H}) \iff \langle Ax, x \rangle \geq 0 \forall x \in \mathcal{H}$ . The Banach space  $\operatorname{Tr}(\mathcal{H})$  of trace class operators on  $\mathcal{H}$  is defined by (e.g. [44])  $\operatorname{Tr}(\mathcal{H}) = \{A \in \mathcal{L}(\mathcal{H}) : ||A||_{\operatorname{tr}} = \sum_{k=1}^{\infty} \langle e_k, (A^*A)^{1/2} e_k \rangle < \infty \}$ , for any orthonormal basis  $\{e_k\}_{k \in \mathbb{N}} \in \mathcal{H}$ , where  $|| ||_{\operatorname{tr}}$  is the trace norm. For  $A \in \operatorname{Tr}(\mathcal{H})$ , its trace is then given by  $\operatorname{tr}(A) = \sum_{k=1}^{\infty} \langle e_k, Ae_k \rangle$ . The Hilbert space  $\operatorname{HS}(\mathcal{H}_1, \mathcal{H}_2)$  of Hilbert-Schmidt operators from  $\mathcal{H}_1$  to  $\mathcal{H}_2$  is defined by (e.g.[23])  $\operatorname{HS}(\mathcal{H}_1, \mathcal{H}_2) = \{A \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2) : ||A||_{\operatorname{HS}}^2 = \operatorname{tr}(A^*A) = \sum_{k=1}^{\infty} ||Ae_k||^2 < \infty \}$ , for any orthonormal basis  $\{e_k\}_{k \in \mathbb{N}}$  in  $\mathcal{H}_1$ , with inner product  $\langle A, B \rangle_{\operatorname{HS}} = \operatorname{tr}(A^*B)$ . For  $\mathcal{H}_1 = \mathcal{H}_2 = \mathcal{H}$ , we write  $\operatorname{HS}(\mathcal{H})$ . We give more detail of  $\operatorname{HS}(\mathcal{H}_1, \mathcal{H}_2)$  and the Hilbert-Schmidt norm  $|| ||_{\operatorname{HS}}$  in Section 12.

Proofs for all main results are presented in Section 10.

**2. Background and previous work.** Let (X, d) be a complete separable metric space equipped with a lower semi-continuous cost function  $c : X \times X \to \mathbb{R}_{\geq 0}$ . Let  $\mathcal{P}(X)$  denote the set of all probability measures on X. The optimal transport (OT) problem between two probability measures  $\nu_0, \nu_1 \in \mathcal{P}(X)$  is (see e.g. [51])

(2.1) 
$$\operatorname{OT}(\nu_0, \nu_1) = \min_{\gamma \in \operatorname{Joint}(\nu_0, \nu_1)} \mathbb{E}_{\gamma}[c] = \min_{\gamma \in \operatorname{Joint}(\nu_0, \nu_1)} \int_{X \times X} c(x, y) d\gamma(x, y)$$

where  $\text{Joint}(\nu_0, \nu_1)$  is the set of joint probabilities with marginals  $\nu_0$  and  $\nu_1$ . For  $1 \leq p < \infty$ , let  $\mathcal{P}_p(X)$  denote the set of all probability measures  $\mu$  on X of finite moment of order p, i.e.  $\int_X d^p(x_0, x) d\mu(x) < \infty$  for some (and hence any)  $x_0 \in X$ . The following *p*-Wasserstein distance  $W_p$  between  $\nu_0$  and  $\nu_1$  defines a metric on  $\mathcal{P}_p(X)$  (Theorem 7.3, [51])

(2.2) 
$$W_p(\nu_0, \nu_1) = \mathrm{OT}_{d^p}(\nu_0, \nu_1)^{\frac{1}{p}}.$$

For two Gaussian measures  $\nu_i = \mathcal{N}(m_i, C_i)$ , i = 0, 1 on  $\mathbb{R}^n$  [19, 10, 36, 24] and on a separable Hilbert space  $\mathcal{H}[16, 6]$ ,  $W_2(\nu_0, \nu_1)$  admits the following closed form

(2.3) 
$$W_2^2(\nu_0,\nu_1) = \|m_0 - m_1\|^2 + \operatorname{tr}(C_0) + \operatorname{tr}(C_1) - 2\operatorname{tr}\left(C_0^{1/2}C_1C_0^{1/2}\right)^{1/2}.$$

**Entropic regularization.** The OT problem (2.1) is often computationally challenging and it is more numerically efficient to solve the following regularized optimization problem [7]

(2.4) 
$$\operatorname{OT}_{c}^{\epsilon}(\mu,\nu) = \min_{\gamma \in \operatorname{Joint}(\mu,\nu)} \left\{ \mathbb{E}_{\gamma}[c] + \epsilon \operatorname{KL}(\gamma || \mu \otimes \nu) \right\}, \ \epsilon > 0,$$

where  $\text{KL}(\nu||\mu)$  denotes the Kullback-Leibler divergence between  $\nu$  and  $\mu$ . The KL in (2.4) acts as a bias [13], with the consequence that in general  $\text{OT}_c^{\epsilon}(\mu,\mu) \neq 0$ . The following *p*-Sinkhorn divergence [18, 13] removes this bias

(2.5) 
$$S_p^{\epsilon}(\mu,\nu) = \operatorname{OT}_{d^p}^{\epsilon}(\mu,\nu) - \frac{1}{2}(\operatorname{OT}_{d^p}^{\epsilon}(\mu,\mu) + \operatorname{OT}_{d^p}^{\epsilon}(\nu,\nu)).$$

In the case  $X = \mathcal{H}$  is a separable Hilbert space and  $\mu, \nu$  are Gaussian measures on  $\mathcal{H}$ , both  $OT_{d^2}^{\epsilon}$  and  $S_2^{\epsilon}$  admit closed form expressions, as follows.

Theorem 2.1 (Entropic Wasserstein distance and Sinkhorn divergence between Gaussian measures on Hilbert space, [33], Theorems 3, 4, and 7). Let  $\mu_0 = \mathcal{N}(m_0, C_0)$ ,  $\mu_1 = \mathcal{N}(m_1, C_1)$  be two Gaussian measures on  $\mathcal{H}$ . For each fixed  $\epsilon > 0$ ,

(2.6) 
$$\operatorname{OT}_{d^2}^{\epsilon}(\mu_0, \mu_1) = ||m_0 - m_1||^2 + \operatorname{tr}(C_0) + \operatorname{tr}(C_1) - \frac{\epsilon}{2}\operatorname{tr}(M_{01}^{\epsilon}) + \frac{\epsilon}{2}\log\det\left(I + \frac{1}{2}M_{01}^{\epsilon}\right).$$

(2.7) 
$$S_{2}^{\epsilon}(\mu_{0},\mu_{1}) = ||m_{0} - m_{1}||^{2} + \frac{\epsilon}{4} \operatorname{tr} \left[M_{00}^{\epsilon} - 2M_{01}^{\epsilon} + M_{11}^{\epsilon}\right] \\ + \frac{\epsilon}{4} \log \det \left[\frac{\left(I + \frac{1}{2}M_{01}^{\epsilon}\right)^{2}}{\left(I + \frac{1}{2}M_{00}^{\epsilon}\right)\left(I + \frac{1}{2}M_{11}^{\epsilon}\right)}\right].$$

The optimal joint measure is the unique Gaussian measure  $\gamma^{\epsilon} = \mathcal{N}\left(\begin{pmatrix}m_0\\m_1\end{pmatrix}, \begin{pmatrix}C_0 & C_{XY}\\C_{XY}^* & C_1\end{pmatrix}\right)$ , where  $C_{XY} = \frac{2}{\epsilon}C_0^{1/2}\left(I + \frac{1}{2}M_{01}^{\epsilon}\right)^{-1}C_0^{1/2}C_1$ . Here det is the Fredholm determinant and  $M_{ij}^{\epsilon}$ :  $\mathcal{H} \to \mathcal{H}$  are trace class operators defined by  $M_{ij}^{\epsilon} = -I + \left(I + \frac{16}{\epsilon^2}C_i^{1/2}C_jC_i^{1/2}\right)^{1/2}$ , i, j = 0, 1. In particular,  $\lim_{\epsilon \to 0} \operatorname{OT}_{d^2}^{\epsilon}(\mu_0, \mu_1) = \lim_{\epsilon \to 0} \operatorname{S}_2^{\epsilon}(\mu_0, \mu_1) = W_2^2(\mu_0, \mu_1)$  and  $\lim_{\epsilon \to \infty} \operatorname{S}_2^{\epsilon}(\mu_0, \mu_1) = ||m_0 - m_1||^2$ . When  $\dim(\mathcal{H}) < \infty$ , we recover the finite-dimensional results in [28, 22, 9].

**Convergence property**.  $S_2^{\epsilon}$  is a divergence function on  $Gauss(\mathcal{H})$ , the set of all Gaussian measures on  $\mathcal{H}$  and has the following convergence property.

Theorem 2.2 ([35]-Theorems 2 and 5). Let  $A, B, \{A_n, B_n\}_{n \in \mathbb{N}} \in \text{Sym}^+(\mathcal{H}) \cap \text{Tr}(\mathcal{H}). \forall \epsilon > 0$ ,

(2.8) 
$$S^{\epsilon}[\mathcal{N}(0, A_{n}), \mathcal{N}(0, A)] \leq \frac{3}{\epsilon}[||A_{n}||_{\mathrm{HS}} + ||A||_{\mathrm{HS}}]||A_{n} - A||_{\mathrm{HS}} \\ |S_{2}^{\epsilon}[\mathcal{N}(0, A_{n}), \mathcal{N}(0, B_{n})] - S_{2}^{\epsilon}[\mathcal{N}(0, A), \mathcal{N}(0, B)]| \\ \leq \frac{3}{\epsilon}[||A_{n}||_{\mathrm{HS}} + ||A||_{\mathrm{HS}} + 2||B||_{\mathrm{HS}}]||A_{n} - A||_{\mathrm{HS}} \\ + \frac{3}{\epsilon}[2||A_{n}||_{\mathrm{HS}} + ||A||_{\mathrm{HS}} + ||B||_{\mathrm{HS}}]||B_{n} - B||_{\mathrm{HS}}.$$

In this work, we apply Theorems 2.1 and 2.2 to estimate Sinkhorn divergence between centered Gaussian processes and, more generally, covariance operators of random processes.

**Related work**. The 2-Wasserstein distance was applied to Gaussian processes in [29, 27], however the treatment in [27] is generally only valid in finite dimensions. Sample complexities were obtained in [35] for Sinkhorn divergence between Gaussian measures on Euclidean and Hilbert spaces. In [26], the author obtained results similar to our Theorem 4.5, however the main theoretical analysis carried out in [26] is flawed (see discussion in Section 4).

**3. Kernels, covariance operators, and Gaussian processes.** Throughout the paper, we make the following assumptions

1. Assumption 1 T is a  $\sigma$ -compact metric space, that is  $T = \bigcup_{i=1}^{\infty} T_i$ , where  $T_1 \subset T_2 \subset \cdots$ , with each  $T_i$  being compact.

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- 2. Assumption 2  $\nu$  is a non-degenerate Borel probability measure on T, that is  $\nu(B) > 0$  for each open set  $B \subset T$ .
- 3. Assumption 3  $K, K^1, K^2 : T \times T \to \mathbb{R}$  are continuous, symmetric, positive definite kernels and  $\exists \kappa > 0, \kappa_1 > 0, \kappa_2 > 0$  such that

(3.1) 
$$\int_T K(x,x)d\nu(x) \le \kappa^2, \quad \int_T K^i(x,x)d\nu(x) \le \kappa_i^2.$$

4. Assumption 4  $\xi \sim GP(0, K)$ ,  $\xi^i \sim GP(0, K^i)$ , i = 1, 2, are *centered* Gaussian processes with covariance functions  $K, K^i$ , respectively.

For K satisfying Assumption 3, positivity implies  $K(x,t)^2 \leq K(x,x)K(t,t) \ \forall x,t \in T$ , thus

(3.2) 
$$\int_T K(x,t)^2 d\nu(t) < \infty \ \forall x \in T, \quad \int_{T \times T} K(x,t)^2 d\nu(x) d\nu(t) < \infty$$

The first inequality means  $K_x \in \mathcal{L}^2(T,\nu) \ \forall x \in T$ , where  $K_x : T \to \mathbb{R}$  is defined by  $K_x(t) = K(x,t)$ . Let  $\mathcal{H}_K$  denote the corresponding reproducing kernel Hilbert space (RKHS), then  $\mathcal{H}_K \subset \mathcal{L}^2(T,\nu)$  [49]. Define the following linear operator

(3.3) 
$$R_K = R_{K,\nu} : \mathcal{L}^2(T,\nu) \to \mathcal{H}_K,$$

(3.4) 
$$R_K f = \int_T K_t f(t) d\nu(t), \quad (R_K f)(x) = \int_T K(x, t) f(t) d\nu(t)$$

Since  $||R_K f||_{\mathcal{H}_K} \leq \int_T ||K_t||_{\mathcal{H}_K} |f(t)| d\nu(t) \leq \sqrt{\int_T K(t,t) d\nu(t)} ||f||_{\mathcal{L}^2(T,\nu)}, R_K$  is bounded, with

(3.5) 
$$||R_K : \mathcal{L}^2(T,\nu) \to \mathcal{H}_K|| \le \sqrt{\int_T K(t,t) d\nu(t)} \le \kappa.$$

Its adjoint is  $R_K^* : \mathcal{H}_K \to \mathcal{L}^2(T,\nu) = J : \mathcal{H}_K \hookrightarrow \mathcal{L}^2(T,\nu)$ , the inclusion operator from  $\mathcal{H}_K$  into  $\mathcal{L}^2(T,\nu)$  [45].  $R_K$  then induces the following self-adjoint, positive, compact operator

(3.6) 
$$C_K = C_{K,\nu} = R_K^* R_K : \mathcal{L}^2(T,\nu) \to \mathcal{L}^2(T,\nu),$$

(3.7) 
$$(C_K f)(x) = \int_T K(x,t) f(t) d\nu(t), \quad \forall f \in \mathcal{L}^2(T,\nu),$$

(3.8) 
$$||C_K||^2_{\mathrm{HS}(\mathcal{L}^2(T,\nu))} = \int_{T \times T} K(x,t)^2 d\nu(x) d\nu(t) \le \kappa^4.$$

The operator  $C_K$  has been studied extensively, e.g. [5, 49, 45]. Let  $\{\lambda_k\}_{k\in\mathbb{N}}$  be its eigenvalues with normalized eigenfunctions  $\{\phi_k\}_{k\in\mathbb{N}}$  forming an orthonormal basis in  $\mathcal{L}^2(T,\nu)$ . A fundamental result for positive definite kernels is Mercer's Theorem, which states that

(3.9) 
$$K(x,y) = \sum_{k=1}^{\infty} \lambda_k \phi_k(x) \phi_k(y) \quad \forall (x,y) \in T \times T,$$

(see version in [49]), where the series converges absolutely for each pair  $(x, y) \in T \times T$  and uniformly on any compact subset of T. By Mercer's Theorem, K is completely determined by  $C_K$  and vice versa. The RKHS  $\mathcal{H}_K$  is explicitly described by

(3.10) 
$$\mathcal{H}_{K} = \left\{ f \in \mathcal{L}^{2}(T,\nu), f = \sum_{k=1}^{\infty} a_{k} \phi_{k} : ||f||_{\mathcal{H}_{K}}^{2} = \sum_{k=1,\lambda_{k}>0}^{\infty} \frac{a_{k}^{2}}{\lambda_{k}} < \infty \right\} \subset \mathcal{L}^{2}(T,\nu).$$

Furthermore,  $C_K \in \text{Sym}^+(\mathcal{H}) \cap \text{Tr}(\mathcal{H}), \ \mathcal{H} = \mathcal{L}^2(T, \nu)$ , with

(3.11) 
$$\operatorname{tr}(C_K) = \sum_{k=1}^{\infty} \lambda_k = \int_T K(t,t) d\nu(t) \le \kappa^2.$$

**Gaussian processes.** Consider the correspondence between Gaussian measures, covariance operators  $C_K$  as defined in Eq.(3.6), and Gaussian processes with paths in  $\mathcal{L}^2(T,\nu)$  [42]. Let  $(\Omega, \mathcal{F}, P)$  be a probability space,  $\xi = (\xi(t))_{t \in T} = (\xi(\omega, t))_{t \in T}$  be a real Gaussian process on  $(\Omega, \mathcal{F}, P)$ , with mean *m* and covariance function *K*, denoted by  $\xi \sim GP(m, K)$ , where

(3.12) 
$$m(t) = \mathbb{E}\xi(t), \quad K(s,t) = \mathbb{E}[(\xi(s) - m(s))(\xi(t) - m(t))], \quad s,t \in T.$$

The sample paths  $\xi(\omega, \cdot) \in \mathcal{H} = \mathcal{L}^2(T, \nu)$  almost *P*-surely, i.e.  $\int_T \xi^2(\omega, t) d\nu(t) < \infty$  almost *P*-surely, if and only if ([42], Theorem 2 and Corollary 1)

(3.13) 
$$\int_T m^2(t)d\nu(t) < \infty, \quad \int_T K(t,t)d\nu(t) < \infty.$$

In this case,  $\xi$  induces the following *Gaussian measure*  $P_{\xi}$  on  $(\mathcal{H}, \mathscr{B}(\mathcal{H}))$ :  $P_{\xi}(B) = P\{\omega \in \Omega :$  $\xi(\omega, \cdot) \in B\}, B \in \mathscr{B}(\mathcal{H}),$  with mean  $m \in \mathcal{H}$  and covariance operator  $C_K : \mathcal{H} \to \mathcal{H},$  defined by Eq.(3.6). Conversely, let  $\mu$  be a Gaussian measure on  $(\mathcal{H}, \mathscr{B}(\mathcal{H})),$  then there is a Gaussian process  $\xi = (\xi(t))_{t \in T}$  with sample paths in  $\mathcal{H},$  with induced probability measure  $P_{\xi} = \mu$ .

Since Gaussian processes are fully determined by their means and covariance functions, the latter being fully determined by their covariance operators, we can define distance/divergence functions between two Gaussian processes as follows, see also e.g. [37, 15, 39, 29].

Definition 3.1 (Divergence between Gaussian processes). Assume Assumptions 1-4. Let  $\mathcal{H} = \mathcal{L}^2(T, \nu)$ . Let  $\xi^i \sim \operatorname{GP}(m_i, K_i)$ , i = 1, 2, be two Gaussian processes with mean  $m_i \in \mathcal{H}$  and covariance function  $K^i$ . Let D be a divergence function on  $\operatorname{Gauss}(\mathcal{H}) \times \operatorname{Gauss}(\mathcal{H})$ . The corresponding divergence  $D_{\operatorname{GP}}$  between  $\xi^1$  and  $\xi^2$  is defined to be

(3.14) 
$$D_{\rm GP}(\xi^1 || \xi^2) = D(\mathcal{N}(m_1, C_{K^1}) || \mathcal{N}(m_2, C_{K^2})).$$

It is clear then that  $D_{\text{GP}}(\xi^1 || \xi^2) \ge 0$  and  $D_{\text{GP}}(\xi^1 || \xi^2) = 0 \iff m_1 = m_2, K^1 = K^2$ . Subsequently, we assume  $m_1 = m_2 = 0$  and compute  $S_2^{\epsilon}[\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})]$ .

**RKHS covariance operators.** To empirically estimate  $S_2^{\epsilon}[\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})]$ , we employ *RKHS covariance operators and cross-covariance operators*. The operator  $R_K$  defined in Eq.(3.4) induces the following self-adjoint, positive, compact *RKHS covariance operator* 

(3.15) 
$$L_K = R_K R_K^* : \mathcal{H}_K \to \mathcal{H}_K, \ L_K = \int_T (K_t \otimes K_t) d\nu(t),$$

(3.16) 
$$L_K f(x) = \int_T K_t(x) \langle f, K_t \rangle_{\mathcal{H}_K} d\nu(t) = \int_T K(x, t) f(t) d\nu(t), \quad f \in \mathcal{H}_K.$$

 $L_K$  has the same nonzero eigenvalues as  $C_K$  and thus  $L_K \in \text{Sym}^+(\mathcal{H}_K) \cap \text{Tr}(\mathcal{H}_K)$ , with

(3.17) 
$$\operatorname{tr}(L_K) = \operatorname{tr}(C_K) \le \kappa^2, \quad ||L_K||_{\operatorname{HS}(\mathcal{H}_K)} = ||C_K||_{\operatorname{HS}(\mathcal{L}^2(T,\nu))} \le \kappa^2.$$

We note also that for  $f \in \mathcal{H}_K$ ,  $C_K f = L_K f$ . However, as we see below, despite their many common properties,  $C_K$  and  $L_K$  are generally **not** interchangeable.

**Empirical RKHS covariance operator**. Let  $\mathbf{X} = (x_i)_{i=1}^m$  be independently sampled from T according to  $\nu$ . This defines the following empirical version of  $L_K$ 

(3.18) 
$$L_{K,\mathbf{X}} = \frac{1}{m} \sum_{i=1}^{m} (K_{x_i} \otimes K_{x_i}) : \mathcal{H}_K \to \mathcal{H}_K$$

(3.19) 
$$L_{K,\mathbf{X}}f = \frac{1}{m}\sum_{i=1}^{m} K_{x_i}\langle f, K_{x_i}\rangle_{\mathcal{H}_K} = \frac{1}{m}\sum_{i=1}^{m} f(x_i)K_{x_i}, \ f \in \mathcal{H}_K.$$

Let  $\mathcal{H}_{K,\mathbf{X}} = \operatorname{span}\{K_{x_i}\}_{i=1}^m \subset \mathcal{H}_K$ , then  $L_{K,\mathbf{X}} : \mathcal{H}_K \to \mathcal{H}_{K,\mathbf{X}}$ . In particular,  $L_{K,\mathbf{X}} : \mathcal{H}_{K,\mathbf{X}} \to \mathcal{H}_{K,\mathbf{X}}$  and  $\forall j, 1 \leq j \leq m, L_{K,\mathbf{X}}K_{x_j} = \frac{1}{m}\sum_{i=1}^m K(x_j, x_i)K_{x_i}$ . Let  $K[\mathbf{X}]$  denote the  $m \times m$  Gram matrix, with  $(K[\mathbf{X}])_{ij} = K(x_i, x_j)$ , then the matrix representation of  $L_{K,\mathbf{X}} : \mathcal{H}_{K,\mathbf{X}} \to \mathcal{H}_{K,\mathbf{X}}$  in  $\operatorname{span}\{K_{x_i}\}_{i=1}^m$  is  $\frac{1}{m}K[\mathbf{X}]$ . In particular, the nonzero eigenvalues of  $L_{K,\mathbf{X}}$  are precisely those of  $\frac{1}{m}K[\mathbf{X}]$ , corresponding to eigenvectors that must lie in  $\mathcal{H}_{K,\mathbf{X}}$ . Thus, the nonzero eigenvalues of  $C_K : \mathcal{L}^2(T,\nu) \to \mathcal{L}^2(T,\nu)$ ,  $\operatorname{tr}(C_K)$ ,  $||C_K||_{\mathrm{HS}}$ , which are the same as those of  $L_K : \mathcal{H}_K \to \mathcal{H}_K$ , can be empirically estimated from those of the  $m \times m$  matrix  $\frac{1}{m}K[\mathbf{X}]$  (see [45]).

**RKHS cross-covariance operators**. Let  $K^1, K^2$  be two kernels satisfying Assumptions 1-4, and  $\mathcal{H}_{K^1}, \mathcal{H}_{K^2}$  the corresponding RKHS. Let  $R_{K^i} : \mathcal{L}^2(T, \nu) \to \mathcal{H}_{K^i}, i = 1, 2$  be as defined in Eq.(3.4). They give rise to the following *RKHS cross-covariance operators* 

(3.20) 
$$R_{12} = R_{K^1} R_{K^2}^* : \mathcal{H}_{K^2} \to \mathcal{H}_{K^1}, \quad R_{21} = R_{K^2} R_{K^1}^* : \mathcal{H}_{K^1} \to \mathcal{H}_{K^2} = R_{12}^*.$$

Both  $L_K$  and  $R_{12}$ ,  $R_{21}$  are encompassed in the following, which is straightforward to verify.

Lemma 3.2. The operators  $R_{ij} = R_{K^i}R_{K^j}^* : \mathcal{H}_{K^j} \to \mathcal{H}_{K^i}, i, j = 1, 2, are given by$ 

(3.21) 
$$R_{ij} = \int_T (K_t^i \otimes K_t^j) d\nu(t), \quad R_{ij}f = \int_T K_t^i \langle f, K_t^j \rangle_{\mathcal{H}_{K^j}} d\nu(t), \quad i, j = 1, 2,$$

(3.22) 
$$R_{ij}f(x) = \int_T K_t^i(x)f(t)d\nu(t) = \int_T K^i(x,t)f(t)d\nu(t), \ f \in \mathcal{H}_{K^j}$$

Then  $R_{ii} = L_{K^i}$ ,  $R_{12}^* = R_{21}$ , and the operator  $R_{12}^*R_{12} : \mathcal{H}_{K^2} \to \mathcal{H}_{K^2}$  is given by

(3.23) 
$$R_{12}^*R_{12}f = \int_T K_t^2 \int_T K^1(t,u)f(u)d\nu(u)d\nu(t), \quad f \in \mathcal{H}_{K^2},$$
$$(R_{12}^*R_{12}f)(x) = \int_{T \times T} K^2(x,t)K^1(t,u)f(u)d\nu(u)d\nu(t), \quad \forall x \in T.$$

We remark that with  $f\in \mathcal{L}^2(T,\nu),$   $C_{K^1}f(t)=\int_T K^1(t,u)f(u)d\nu(u)$  and

$$(3.24) \quad (C_{K^2}C_{K^1}f)(x) = \int_T K^2(x,t)(C_{K^1}f)(t)d\nu(t) = \int_{T\times T} K^2(x,t)K^1(t,u)f(u)d\nu(u)d\nu(t).$$

Thus for  $f \in \mathcal{H}_{K^2}$ ,  $C_{K^2}C_{K^1}f = R_{12}^*R_{12}f \in \mathcal{H}_{K^2}$ , however  $C_{K^2}C_{K^1} : \mathcal{L}^2(T,\nu) \to \mathcal{L}^2(T,\nu)$  is generally not self-adjoint, whereas  $R_{12}^*R_{12} \in \text{Sym}^+(\mathcal{H}_{K^2})$ .

Lemma 3.3 (Hilbert-Schmidt norm). Under Assumptions 1-3,  $R_{ij} \in \mathrm{HS}(\mathcal{H}_{K^j}, \mathcal{H}_{K^i})$ , with  $||R_{ij}||_{\mathrm{HS}(\mathcal{H}_{K^j}, \mathcal{H}_{K^i})} \leq \kappa_i \kappa_j$ , i, j = 1, 2.

Lemma 3.4 (Empirical RKHS covariance and cross-covariance operators). Let  $\mathbf{X} = \{x_1, \ldots, x_m\}$  in  $T^m$ . Define the empirical integral operators  $R_{ij,\mathbf{X}} : \mathcal{H}_{K^j} \to \mathcal{H}_{K^i} \ i, j = 1, 2, by$ 

(3.25) 
$$R_{ij,\mathbf{X}} = \frac{1}{m} \sum_{k=1}^{m} (K_{x_k}^i \otimes K_{x_k}^j) : \mathcal{H}_{K^j} \to \mathcal{H}_{K^i},$$

(3.26) 
$$R_{ij,\mathbf{X}}f = \frac{1}{m}\sum_{k=1}^{m}K_{x_k}^i \langle f, K_{x_k}^j \rangle_{\mathcal{H}_{K^j}} = \frac{1}{m}\sum_{k=1}^{m}f(x_k)K_{x_k}^i, \ f \in \mathcal{H}_{K^j},$$

Then  $R_{ii,\mathbf{X}} = L_{K^i,\mathbf{X}}$ ,  $R^*_{12,\mathbf{X}} = R_{21,\mathbf{X}}$ , and the operator  $R^*_{12,\mathbf{X}}R_{12,\mathbf{X}} : \mathcal{H}_{K^2} \to \mathcal{H}_{K^2}$  is given by

(3.27) 
$$R_{12,\mathbf{X}}^* R_{12,\mathbf{X}} f = \frac{1}{m^2} \sum_{i,j=1}^m f(x_i) K^1(x_i, x_j) K_{x_j}^2 \in \mathcal{H}_{K^2,\mathbf{X}}$$

Thus  $R_{12,\mathbf{X}}^* R_{12,\mathbf{X}} : \mathcal{H}_{K^2} \to \mathcal{H}_{K^2,\mathbf{X}}$  and on the subspace  $\mathcal{H}_{K^2,\mathbf{X}}$ , in span $\{K_{x_j}^2\}_{j=1}^m$ ,  $R_{12,\mathbf{X}}^* R_{12,\mathbf{X}} : \mathcal{H}_{K^2,\mathbf{X}} \to \mathcal{H}_{K^2,\mathbf{X}}$  has matrix representation  $\frac{1}{m^2}K^1[\mathbf{X}]K^2[\mathbf{X}]$ .

4. Estimation of Sinkhorn divergence from finite covariance matrices. Main goal. Assume Assumptions 1-4. Our main goal in this work is to estimate  $W_2[\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})]$ and  $S_2^{\epsilon}[\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})]$  given finite samples  $\{\{\xi_i^1(x_j)\}_{i=1}^{N_1}, \{\xi_i^2(x_j)\}_{i=1}^{N_2}\}_{j=1}^m$  from the two processes  $\xi^1, \xi^2$  on the set of points  $\mathbf{X} = (x_j)_{j=1}^m$  in T. These correspond to  $N_i$  realizations of process  $\xi^i, i = 1, 2$ , sampled at the m points in T given by  $\mathbf{X}$ .

Let  $\mathbf{X} = (x_i)_{i=1}^m$  be independently sampled from  $(T, \nu)$ . The Gaussian process assumption  $\xi^i \sim \operatorname{GP}(0, K^i)$  means that  $(\xi^i(., x_j))_{j=1}^m$  are *m*-dimensional Gaussian random variables, with  $(\xi^i(., x_j))_{j=1}^m \sim \mathcal{N}(0, K^i[\mathbf{X}])$ , where  $(K^i[\mathbf{X}])_{jk} = K^i(x_j, x_k), 1 \leq j, k \leq m$ . We first assume that the covariance matrices  $K^i[\mathbf{X}]$  are *known*. In this section, we show that

$$\mathbf{S}_{2}^{\epsilon}\left[\mathcal{N}\left(0,\frac{1}{m}K^{1}[\mathbf{X}]\right), \mathcal{N}\left(0,\frac{1}{m}K^{2}[\mathbf{X}]\right)\right] \text{ consistently estimates } \mathbf{S}_{2}^{\epsilon}[\mathcal{N}(0,C_{K^{1}}),\mathcal{N}(0,C_{K^{2}})].$$

Let  $\mathcal{H}$  be any separable Hilbert space. Let  $c \in \mathbb{R}, c \neq 0$  be fixed. Consider the following function  $G: \operatorname{Sym}^+(\mathcal{H}) \cap \operatorname{Tr}(\mathcal{H}) \to \mathbb{R}$  defined by

(4.1) 
$$G(A) = \operatorname{tr}[M(A)] - \log \det \left(I + \frac{1}{2}M(A)\right)$$
, where  $M(A) = -I + (I + c^2 A)^{1/2}$ .

With this definition, with  $c = \frac{4}{\epsilon}$ ,  $S_2^{\epsilon}[\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})]$  can be expressed as

(4.2) 
$$S_{2}^{\epsilon}[\mathcal{N}(0, C_{K^{1}}), \mathcal{N}(0, C_{K^{2}})] = \frac{1}{c} \left[ G(C_{K^{1}}^{2}) + G(C_{K^{2}}^{2}) - 2G(C_{K^{1}}^{1/2}C_{K^{2}}C_{K^{1}}^{1/2}) \right].$$

We now represent this via the RKHS covariance and cross-covariance operators in Section 3.

**RKHS covariance operator terms.** Since  $C_{K^i} \in \text{Tr}(\mathcal{L}^2(T,\nu))$  and  $L_{K^i} \in \text{Tr}(\mathcal{H}_{K^i})$ , i = 1, 2, have the same nonzero eigenvalues, we have  $G(C_{K^i}^2) = G(L_{K^i}^2)$ , which can be approximated by their empirical versions  $G(L_{K^i,\mathbf{X}}^2)$ , i = 1, 2, which are the same as  $G(\frac{1}{m^2}(K^i[\mathbf{X}])^2)$ .

**RKHS cross-covariance operator term**. Consider the term  $G(C_{K^1}^{1/2}C_{K^2}C_{K^1}^{1/2})$  in Eq. (4.2). Recall that  $R_{K^i} : \mathcal{L}^2(T,\nu) \to \mathcal{H}_{K^i}, R_{K^i}^* : \mathcal{H}_{K^i} \to \mathcal{L}^2(T,\nu)$ , with  $C_{K^i} = R_{K^i}^*R_{K^i} : \mathcal{L}^2(T,\nu) \to \mathcal{L}^2(T,\nu)$ . The nonzero eigenvalues of  $C_{K^1}^{1/2}C_{K^2}C_{K^1}^{1/2}$  are the same as those of

(4.3) 
$$C_{K^1}C_{K^2} = (R_{K^1}^*R_{K^1})(R_{K^2}^*R_{K^2}) : \mathcal{L}^2(T,\nu) \to \mathcal{L}^2(T,\nu),$$

which, in turns, are the same as the nonzero eigenvalues of the operator

(4.4) 
$$R_{12}^* R_{12} = R_{K^2} (R_{K^1}^* R_{K^1}) R_{K^2}^* : \mathcal{H}_{K^2} \to \mathcal{H}_{K^2},$$

or equivalently, of  $R_{21}^*R_{21} = R_{K^1}(R_{K^2}^*R_{K^2})R_{K^1}^* : \mathcal{H}_{K^1} \to \mathcal{H}_{K^1}$ . Thus  $G(C_{K^1}^{1/2}C_{K_2}C_{K_1}^{1/2}) = G(R_{12}^*R_{12})$ , with the empirical version being  $G(R_{12,\mathbf{X}}^*R_{12,\mathbf{X}})$ . By Lemma 3.4, the nonzero eigenvalues of  $R_{12,\mathbf{X}}^*R_{12,\mathbf{X}}$  are those of  $\frac{1}{m^2}K^1[\mathbf{X}]K^2[\mathbf{X}]$ , or equivalently, of  $\frac{1}{m^2}(K^1[\mathbf{X}])^{1/2} \times K^2[\mathbf{X}](K^1[\mathbf{X}])^{1/2}$ . Thus  $G(R_{12,\mathbf{X}}^*R_{12,\mathbf{X}}) = G(\frac{1}{m^2}(K^1[\mathbf{X}])^{1/2}K^2[\mathbf{X}]K^1([\mathbf{X}])^{1/2})$ . We thus have

Proposition 4.1 (RKHS covariance and cross-covariance operator representation for Sinkhorn divergence). Under Assumptions 1-4, let  $\mathbf{X} = (x_i)_{i=1}^m \in T^m$ . Then

(4.5) 
$$S_{2}^{\epsilon}[\mathcal{N}(0, C_{K^{1}}), \mathcal{N}(0, C_{K^{2}})] = \frac{1}{c} \left[ G(L_{K^{1}}^{2}) + G(L_{K^{2}}^{2}) - 2G(R_{12}^{*}R_{12}) \right]$$
$$S_{2}^{\epsilon} \left[ \mathcal{N} \left( 0, \frac{1}{m}K^{1}[\mathbf{X}] \right), \mathcal{N} \left( 0, \frac{1}{m}K^{2}[\mathbf{X}] \right) \right]$$
$$(4.6) \qquad \qquad = \frac{1}{c} \left[ G(L_{K^{1}, \mathbf{X}}^{2}) + G(L_{K^{2}, \mathbf{X}}^{2}) - 2G(R_{12, \mathbf{X}}^{*}R_{12, \mathbf{X}}) \right].$$

The representations in Proposition 4.1 suggest that, given a random sample  $\mathbf{X} = (x_i)_{i=1}^m$ ,  $S_2^{\epsilon} \left[ \mathcal{N} \left( 0, \frac{1}{m} K^1[\mathbf{X}] \right), \mathcal{N} \left( 0, \frac{1}{m} K^2[\mathbf{X}] \right) \right] \to S_2^{\epsilon} [\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})]$  as  $m \to \infty$ . We now analyze the rate of this convergence. The function G as defined in Eq.(4.1) satisfies the following

Proposition 4.2. Let  $\mathcal{H}, \mathcal{H}_1, \mathcal{H}_2$  be separable Hilbert spaces. Then

(4.7) 
$$|G(A) - G(B)| \le \frac{3c^2}{4} ||A - B||_{\mathrm{tr}} \quad \forall A, B \in \mathrm{Sym}^+(\mathcal{H}) \cap \mathrm{Tr}(\mathcal{H}).$$

$$(4.8) \quad |G(A^2) - G(B^2)| \le \frac{3c^2}{4} [||A||_{\mathrm{HS}} + ||B||_{\mathrm{HS}}] ||A - B||_{\mathrm{HS}}, \quad \forall A, B \in \mathrm{Sym}(\mathcal{H}) \cap \mathrm{HS}(\mathcal{H}).$$

Let  $A, B \in \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ , then  $A^*A, B^*B \in \mathrm{Sym}^+(\mathcal{H}_1) \cap \mathrm{Tr}(\mathcal{H}_1)$  and

(4.9) 
$$|G(A^*A) - G(B^*B)| \le \frac{3c^2}{4} [||A||_{\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)} + ||B||_{\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)}]||A - B||_{\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)}.$$

By Proposition 4.2, we thus need to estimate  $||L_{K^i,\mathbf{X}} - L_{K^i}||_{\mathrm{HS}(\mathcal{H}^i)}$ , i = 1, 2 and  $||R_{12,\mathbf{X}} - R_{12}||_{\mathrm{HS}(\mathcal{H}_{K^2},\mathcal{H}_{K^1})}$ . We apply the following law of large numbers for Hilbert space-valued random variables, which is a consequence of a general result by Pinelis ([40], Theorem 3.4).

Proposition 4.3 ([48]). Let  $(Z, \mathcal{A}, \rho)$  be a probability space and  $\xi : (Z, \rho) \to \mathcal{H}$  be a random variable. Assume that  $\exists M > 0$  such that  $||\xi|| \leq M < \infty$  almost surely. Let  $\sigma^2(\xi) = \mathbb{E}||\xi||^2$ . Let  $(z_i)_{i=1}^m$  be independently sampled from  $(Z, \rho)$ .  $\forall 0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

(4.10) 
$$\left\|\frac{1}{m}\sum_{i=1}^{m}\xi(z_i) - \mathbb{E}\xi\right\| \le \frac{2M\log\frac{2}{\delta}}{m} + \sqrt{\frac{2\sigma^2(\xi)\log\frac{2}{\delta}}{m}}.$$

**4.1. Estimation with bounded kernels.** We first consider the following setting **Assumption 5.**  $K, K^1, K^2$  are *bounded*, i.e.  $\exists \kappa, \kappa_1, \kappa_2 > 0$  such that

(4.11) 
$$\sup_{x \in T} K(x, x) \le \kappa^2, \quad \sup_{x \in T} K^i(x, x) \le \kappa_i^2, i = 1, 2.$$

This is satisfied for exponential kernels  $\exp(-a||x-y||^p)$ ,  $a > 0, 0 , on <math>T = \mathbb{R}^d$  and for all continuous kernels if T is compact. Applying Proposition 4.3, we obtain the following.

Proposition 4.4 (Convergence of RKHS empirical covariance and cross-covariance operators). Under Assumptions 1-5,  $||R_{ij,\mathbf{X}}||_{\mathrm{HS}(\mathcal{H}_{K^j},\mathcal{H}_{K^i})} \leq \kappa_i \kappa_j$ ,  $i, j = 1, 2, \forall \mathbf{X} \in T^m$ . Let  $\mathbf{X} = (x_i)_{i=1}^m$  be independently sampled from  $(T, \nu)$ .  $\forall 0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

(4.12) 
$$||R_{ij,\mathbf{X}} - R_{ij}||_{\mathrm{HS}(\mathcal{H}_{K^{j}},\mathcal{H}_{K^{i}})} \leq \kappa_{i}\kappa_{j} \left[\frac{2\log\frac{2}{\delta}}{m} + \sqrt{\frac{2\log\frac{2}{\delta}}{m}}\right],$$

(4.13) 
$$||R_{ij,\mathbf{X}}^*R_{ij,\mathbf{X}} - R_{ij}^*R_{ij}||_{\operatorname{tr}(\mathcal{H}_{K^j})} \le 2\kappa_i^2\kappa_j^2 \left[\frac{2\log\frac{2}{\delta}}{m} + \sqrt{\frac{2\log\frac{2}{\delta}}{m}}\right]$$

In particular,  $||L_{K^i,\mathbf{X}}||_{\mathrm{HS}(\mathcal{H}_{K^i})} \leq \kappa_i^2$ , and  $\forall 0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

(4.14) 
$$\left\|L_{K^{i},\mathbf{X}} - L_{K^{i}}\right\|_{\mathrm{HS}(\mathcal{H}_{K^{i}})} \leq \kappa_{i}^{2} \left(\frac{2\log\frac{2}{\delta}}{m} + \sqrt{\frac{2\log\frac{2}{\delta}}{m}}\right)$$

Proposition 4.4 generalizes Proposition 4 in [35], which states the bound in Eq.(4.14). Combining Propositions 4.1, 4.2, and 4.4, we are led to our first main result.

Theorem 4.5 (Estimation of Sinkhorn divergence between Gaussian processes from finite covariance matrices - bounded kernels). Assume Assumptions 1-5. Let  $\mathbf{X} = (x_i)_{i=1}^m$  be independently sampled from  $(T, \nu)$ . For any  $0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

(4.15) 
$$\left| S_{2}^{\epsilon} \left[ \mathcal{N}\left(0, \frac{1}{m} K^{1}[\mathbf{X}]\right), \mathcal{N}\left(0, \frac{1}{m} K^{2}[\mathbf{X}]\right) - S_{2}^{\epsilon} \left[\mathcal{N}(0, C_{K^{1}}), \mathcal{N}(0, C_{K^{2}})\right] \right] \right| \\ \leq \frac{6}{\epsilon} (\kappa_{1}^{2} + \kappa_{2}^{2})^{2} \left[ \frac{2\log\frac{6}{\delta}}{m} + \sqrt{\frac{2\log\frac{6}{\delta}}{m}} \right].$$

**Discussion**. Similar results to Theorem 4.5 were reported in ([26], Theorem 8). However, the main theoretical analysis in [26] is flawed, in particular Proposition 2 there. We note that in the last term of Eq.(4.2),  $C_{K^i} \in \text{Tr}(\mathcal{L}^2(T,\nu))$  cannot be replaced by  $L_{K^i} \in \text{Tr}(\mathcal{H}_{K^i})$ . This is because in general  $\mathcal{H}_{K^1}$  and  $\mathcal{H}_{K^2}$  are different. For example, let  $T \subset \mathbb{R}^n$  be compact with nonempty interior,  $K^1$  be the Gaussian kernel  $K(x,y) = \exp(-\sigma ||x - y||^2), \sigma > 0$ , and  $K^2$  be any polynomial kernel. Then  $\mathcal{H}_{K^1}$  does not contain any polynomial [32], that is  $\mathcal{H}_{K^1} \cap \mathcal{H}_{K^2} = \{0\}$ . Thus, while  $C_{K^1}C_{K^2}$  and  $(C_{K^1})^{1/2}C_{K^2}(C_{K^1})^{1/2}$  are well-defined on  $\mathcal{L}^2(T,\nu)$ , the products  $L_{K^1}^{1/2}L_{K^2}L_{K^1}^{1/2}$  and  $L_{K^1}L_{K^2}$  are generally not defined. Furthermore, for any compact operators  $A_i \in \mathcal{L}(\mathcal{H})$ , i = 1, 2, the operators  $A_i^*A$  and  $A_iA_i^*$  have the same nonzero eigenvalues, but this is generally *not* true for the products  $A_1^*A_1A_2^*A_2$  and  $A_1A_1^*A_2A_2^*$ , which generally have different nonzero eigenvalues. This can be readily verified numerically when  $\mathcal{H} = \mathbb{R}^n$ .

Thus ([26], Proposition 2) and the most crucial step in its proof, which substitutes  $C_{K^i}$  by  $L_{K^i}$ , is *not* valid. We note also that Kato's Theorem ([26], Theorem 1) does not apply to operators of the form AB,  $A, B \in \text{Sym}^+(\mathcal{H})$  compact, since AB is generally not self-adjoint.

**4.2. Estimation with general kernels.** Consider the following more general setting, where the kernels are *not* necessarily bounded, e.g. polynomial kernels on  $T = \mathbb{R}^d$ ,  $d \in \mathbb{N}$ . In this case, the sample bounds are less tight compared to those in Section 4.1.

Assumption 6  $\exists \kappa, \kappa_1, \kappa_2 > 0$  such that

(4.16) 
$$\int_{T} [K(x,x)]^2 d\nu(x) \le \kappa^4, \quad \int_{T} [K^i(x,x)]^2 d\nu(x) \le \kappa_i^4, \ i = 1, 2.$$

This is related to the fourth moments of the processes (Assumption 6(\*) in Section 8) and implies (3.1) in Assumption 3. The following is the corresponding version of Proposition 4.4.

Proposition 4.6. Under Assumptions 1-4 and 6, let  $\mathbf{X} = (x_i)_{i=1}^m$  be independently sampled from  $(T, \nu)$ . For any  $0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

$$(4.17) \qquad ||R_{ij,\mathbf{X}}||_{\mathrm{HS}(\mathcal{H}_{K^{j}},\mathcal{H}_{K^{i}})} \leq \frac{2\kappa_{i}\kappa_{j}}{\delta}, \quad ||R_{ij,\mathbf{X}}-R_{ij}||_{\mathrm{HS}(\mathcal{H}_{K^{j}},\mathcal{H}_{K^{i}})} \leq \frac{2\kappa_{i}\kappa_{j}}{\sqrt{m\delta}}.$$

In particular, for  $K^i = K^j = K$ ,  $\forall 0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

(4.18) 
$$||L_{K,\mathbf{X}}||_{\mathrm{HS}(\mathcal{H}_K)} \leq \frac{2\kappa^2}{\delta}, \quad ||L_{K,\mathbf{X}} - L_K||_{\mathrm{HS}(H_K)} \leq \frac{2\kappa^2}{\sqrt{m\delta}}.$$

Combining Propositions 4.2 and 4.6, we obtain the corresponding version of Theorem 4.5.

Theorem 4.7 (Estimation of Sinkhorn divergence between Gaussian processes from finite covariance matrices - general kernels). Under Assumptions 1-4 and 6, let  $\mathbf{X} = (x_i)_{i=1}^m$ be independently sampled from  $(T, \nu)$ . For any  $0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

(4.19) 
$$\begin{aligned} \left| \mathbf{S}_{2}^{\epsilon} \left[ \mathcal{N}\left(0, \frac{1}{m} K^{1}[\mathbf{X}]\right), \mathcal{N}\left(0, \frac{1}{m} K^{2}[\mathbf{X}]\right) \right] - \mathbf{S}_{2}^{\epsilon} [\mathcal{N}(0, C_{K^{1}}), \mathcal{N}(0, C_{K^{2}})] \right| \\ &\leq \frac{18}{\epsilon} (\kappa_{1}^{2} + \kappa_{2}^{2})^{2} \left(1 + \frac{6}{\delta}\right) \frac{1}{\sqrt{m\delta}}. \end{aligned}$$

5. Estimation of Sinkhorn divergence from finite samples. We now return to our main goal stated in Section 4, where we are only given finite samples of the Gaussian processes  $\xi^1, \xi^2$ . It is then necessary to estimate the covariance matrices  $K^1[\mathbf{X}], K^2[\mathbf{X}]$  and the Sinkhorn divergence between them. For simplicity and without loss of generality, in the theoretical analysis we let  $N_1 = N_2 = N$ . We recall that the Gaussian process  $\xi = (\xi(\omega, t))$  is defined on the probability space  $(\Omega, \mathcal{F}, P)$ . Let  $\mathbf{W} = (\omega_1, \dots, \omega_N)$  be independently sampled from  $(\Omega, P)$ , which corresponds to N sample paths  $\xi_i(x) = \xi(\omega_i, x), 1 \leq i \leq N, x \in T$ . Let  $\mathbf{X} = (x_i)_{i=1}^m \in T^m$  be fixed. Consider the following  $m \times N$  data matrix

(5.1) 
$$\mathbf{Z} = \begin{pmatrix} \xi(\omega_1, x_1), \dots, \xi(\omega_N, x_1), \\ \dots \\ \xi(\omega_1, x_m), \dots, \xi(\omega_N, x_m) \end{pmatrix} = [\mathbf{z}(\omega_1), \dots \mathbf{z}(\omega_N)] \in \mathbb{R}^{m \times N}.$$

Here  $\mathbf{z}(\omega) = (\mathbf{z}_i(\omega))_{i=1}^m = (\xi(\omega, x_i))_{i=1}^m$ . Since  $(K[\mathbf{X}])_{ij} = \mathbb{E}[\xi(\omega, x_i)\xi(\omega, x_j)], 1 \le i, j \le m$ ,

(5.2) 
$$K[\mathbf{X}] = \mathbb{E}[\mathbf{z}(\omega)\mathbf{z}(\omega)^T] = \int_{\Omega} \mathbf{z}(\omega)\mathbf{z}(\omega)^T dP(\omega).$$

The empirical version of  $K[\mathbf{X}]$ , using the random sample  $\mathbf{W} = (\omega_i)_{i=1}^N$ , is then

(5.3) 
$$\hat{K}_{\mathbf{W}}[\mathbf{X}] = \frac{1}{N} \sum_{i=1}^{N} \mathbf{z}(\omega_i) \mathbf{z}(\omega_i)^T = \frac{1}{N} \mathbf{Z} \mathbf{Z}^T.$$

The convergence of  $K_{\mathbf{W}}[\mathbf{X}]$  to  $K[\mathbf{X}]$  is given by the following.

Proposition 5.1. Assume Assumptions 1-5. Let  $\xi \sim \operatorname{GP}(0, K)$  on  $(\Omega, \mathcal{F}, P)$  Let  $\mathbf{X} = (x_i)_{i=1}^m \in T^m$  be fixed. Then  $||K[\mathbf{X}]||_F \leq m\kappa^2$ . Let  $\mathbf{W} = (\omega_1, \ldots, \omega_N)$  be independently sampled from  $(\Omega, P)$ . For any  $0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

(5.4) 
$$||\hat{K}_{\mathbf{W}}[\mathbf{X}] - K[\mathbf{X}]||_F \le \frac{2\sqrt{3}m\kappa^2}{\sqrt{N}\delta}, \ ||\hat{K}_{\mathbf{W}}[\mathbf{X}]||_F \le \frac{2m\kappa^2}{\delta}$$

Let now  $\xi^i \sim \operatorname{GP}(0, K^i)$ , i = 1, 2, on the probability spaces  $(\Omega_i, \mathcal{F}_i, P_i)$ , respectively. Let  $\mathbf{W}^i = (\omega_j^i)_{j=1}^N$ , be independently sampled from  $(\Omega_i, P_i)$ , corresponding to the sample paths  $\{\xi_j^i(t) = \xi^i(\omega_j, t)\}_{j=1}^N$ ,  $t \in T$ , from  $\xi^i$ , i = 1, 2. Combining Proposition 5.1 and Theorem 2.2, we obtain the following empirical estimate of  $\operatorname{S}_2^{\epsilon} \left[ \mathcal{N} \left( 0, \frac{1}{m} K^1[\mathbf{X}] \right), \mathcal{N} \left( 0, \frac{1}{m} K^2[\mathbf{X}] \right) \right]$  from two finite samples of  $\xi^1 \sim \operatorname{GP}(0, K^1)$  and  $\xi^2 \sim \operatorname{GP}(0, K^2)$  given by  $\mathbf{W}^1, \mathbf{W}^2$ .

**Theorem 5.2.** Assume Assumptions 1-5. Let  $\mathbf{X} = (x_i)_{i=1}^m \in T^m$ ,  $m \in \mathbb{N}$  be fixed. Let  $\mathbf{W}^1 = (\omega_j^1)_{j=1}^N$ ,  $\mathbf{W}^2 = (\omega_j^2)_{j=1}^N$  be independently sampled from  $(\Omega_1, P_1)$  and  $(\Omega_2, P_2)$ , respectively. For any  $0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

$$\left| S_{2}^{\epsilon} \left[ \mathcal{N}\left(0, \frac{1}{m} \hat{K}_{\mathbf{W}^{1}}^{1}[\mathbf{X}]\right), \mathcal{N}\left(0, \frac{1}{m} \hat{K}_{\mathbf{W}^{2}}^{2}[\mathbf{X}]\right) \right] - S_{2}^{\epsilon} \left[ \mathcal{N}\left(0, \frac{1}{m} K^{1}[\mathbf{X}]\right), \mathcal{N}\left(0, \frac{1}{m} K^{2}[\mathbf{X}]\right) \right] \right|$$
  
(5.5) 
$$\leq \frac{12\sqrt{3}}{\epsilon\delta} \left[ \left(1 + \frac{4}{\delta}\right) \kappa_{1}^{4} + \left(3 + \frac{8}{\delta}\right) \kappa_{1}^{2} \kappa_{2}^{2} + \kappa_{2}^{4} \right] \frac{1}{\sqrt{N}}.$$

Here the probability is with respect to the product space  $(\Omega_1, P_1)^N \times (\Omega_2, P_2)^N$ .

Combing Theorem 5.2 with Theorem 4.5, we are finally led to the following empirical estimate of the theoretical Sinkhorn divergence  $S_2^{\epsilon}[\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})]$  from two finite samples  $\mathbf{Z}^1, \mathbf{Z}^2$  of  $\xi^1 \sim GP(0, K^1)$  and  $\xi^2 \sim GP(0, K^2)$ . Theorem 5.3 (Estimation of Sinkhorn divergence between Gaussian processes from finite samples - bounded kernels). Assume Assumptions 1-5. Let  $\mathbf{X} = (x_i)_{i=1}^m$  be independently sampled from  $(T, \nu)$ . Let  $\mathbf{W}^1 = (\omega_j^1)_{j=1}^N$ ,  $\mathbf{W}^2 = (\omega_j^2)_{j=1}^N$  be independently sampled from  $(\Omega_1, P_1)$  and  $(\Omega_2, P_2)$ , respectively. For any  $0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

$$\left| S_{2}^{\epsilon} \left[ \mathcal{N}\left(0, \frac{1}{m} \hat{K}_{\mathbf{W}^{1}}^{1}[\mathbf{X}]\right), \mathcal{N}\left(0, \frac{1}{m} \hat{K}_{\mathbf{W}^{2}}^{2}[\mathbf{X}]\right) \right] - S_{2}^{\epsilon} [\mathcal{N}(0, C_{K^{1}}), \mathcal{N}(0, C_{K^{2}})] \right|$$

$$(5.6) \qquad \leq \frac{6}{\epsilon} (\kappa_{1}^{2} + \kappa_{2}^{2})^{2} \left[ \frac{2\log \frac{12}{\delta}}{m} + \sqrt{\frac{2\log \frac{12}{\delta}}{m}} \right] + \frac{24\sqrt{3}}{\epsilon\delta} \left[ \left(1 + \frac{8}{\delta}\right) \kappa_{1}^{4} + \left(3 + \frac{16}{\delta}\right) \kappa_{1}^{2} \kappa_{2}^{2} + \kappa_{2}^{4} \right] \frac{1}{\sqrt{N}}.$$

Here the probability is with respect to the space  $(T,\nu)^m \times (\Omega_1, P_1)^N \times (\Omega_2, P_2)^N$ .

We note that if  $\kappa_1, \kappa_2$  are absolute constants, e.g. for exponential kernels, then the convergence rate in Theorem 5.3 is *completely dimension-independent*. Theorem 5.3 provides the theoretical justification for the Sinkhorn divergence estimation in Algorithm 5.1 (we set  $N_1 = N_2 = N$  in the theoretical analysis only for simplicity).

**Algorithm 5.1** Estimate Wasserstein distance and Sinkhorn divergence between centered Gaussian processes from finite samples

**Input**: Finite samples  $\{\xi_k^i(x_j)\}$ , from  $N_i$  realizations  $\xi_k^i$ ,  $1 \le k \le N_i$ , of processes  $\xi^i$ , i = 1, 2, sampled at m points  $x_j$ ,  $1 \le j \le m$ 

## Procedure:

Form  $m \times N_i$  data matrices  $Z_i$ , with  $(Z_i)_{jk} = \xi_k^i(x_j)$ ,  $i = 1, 2, 1 \le j \le m, 1 \le k \le N_i$ Compute  $m \times m$  empirical covariance matrices  $\hat{K}^i = \frac{1}{N} Z_i Z_i^T$ , i = 1, 2Compute  $W = W_2 \left[ \mathcal{N}\left(0, \frac{1}{m} \hat{K}^1\right), \mathcal{N}\left(0, \frac{1}{m} \hat{K}^2\right) \right]$  according to Eq.(2.3) Compute  $S = S_2^{\epsilon} \left[ \mathcal{N}\left(0, \frac{1}{m} \hat{K}^1\right), \mathcal{N}\left(0, \frac{1}{m} \hat{K}^2\right) \right]$  according to Eq.(2.7) **return** W and S

6. Estimation of Wasserstein distance between Gaussian processes. In contrast to the Sinkhorn divergence of centered Gaussian processes, which is continuous in the  $|| ||_{\text{HS}}$  norm, the 2-Wasserstein divergence is continuous in the  $|| ||_{\text{tr}}$  norm ([29, 2]). We note that Theorem 8 in [27], which claims that  $W_2$  is continuous in the operator norm || ||, is *not* correct in infinite-dimensional setting (see [29], Proposition 4 and discussion). More specifically ([35]),

(6.1) 
$$W_2^2[\mathcal{N}(0,C_1),\mathcal{N}(0,C_2)] \le ||C_1 - C_2||_{\mathrm{tr}}.$$

It is not clear if concentration results in e.g. [40], which require 2-smooth Banach space norms, can be extended to the  $|| ||_{tr}$  norm. We now present estimates of the 2-Wasserstein distance when  $\min\{\dim(\mathcal{H}_{K^i}), i = 1, 2\} < \infty$ , in which case  $|| ||_{tr(\mathcal{H}_{K^i})}$  and  $|| ||_{HS(\mathcal{H}_{K^i})}$  are equivalent for at least one i = 1, 2. They are *not* valid in the case  $\dim(\mathcal{H}_{K^1}) = \dim(\mathcal{H}_{K^2}) = \infty$ .

Theorem 6.1 (Estimation of 2-Wasserstein distance from finite covariance matrices). Under Assumptions 1-5, let  $\mathbf{X} = (x_i)_{i=1}^m$  be independently sampled from  $(T, \nu)$ . Then

(6.2) 
$$W_2^2[\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})] = \operatorname{tr}(L_{K^1}) + \operatorname{tr}(L_{K^2}) - 2\operatorname{tr}[(R_{12}^* R_{12})^{1/2}].$$

(6.3) 
$$W_2^2\left[\mathcal{N}\left(0,\frac{1}{m}K^1[\mathbf{X}]\right), \mathcal{N}\left(0,\frac{1}{m}K^2[\mathbf{X}]\right)\right] = \operatorname{tr}(L_{K^1,\mathbf{X}}) + \operatorname{tr}(L_{K^2,\mathbf{X}}) - 2\operatorname{tr}[(R_{12,\mathbf{X}}^*R_{12,\mathbf{X}})^{1/2}].$$

Assume further that  $\dim(\mathcal{H}_{K^2}) < \infty$ .  $\forall 0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

$$\left| W_2^2 \left[ \mathcal{N}\left(0, \frac{1}{m} K^1[\mathbf{X}]\right), \mathcal{N}\left(0, \frac{1}{m} K^2[\mathbf{X}]\right) \right] - W_2^2[\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})] \right|$$

$$(6.4) \qquad \leq (\kappa_1^2 + \kappa_2^2) \left[ \frac{2\log\frac{6}{\delta}}{m} + \sqrt{\frac{2\log\frac{6}{\delta}}{m}} \right] + 2\sqrt{2\kappa_1\kappa_2}\sqrt{\dim(\mathcal{H}_{K^2})} \sqrt{\frac{2\log\frac{6}{\delta}}{m}} + \sqrt{\frac{2\log\frac{6}{\delta}}{m}}.$$

**Theorem 6.2.** Assume Assumptions 1-5. Let  $\mathbf{X} = (x_i)_{i=1}^m \in T^m$ ,  $m \in \mathbb{N}$  be fixed. Let  $\mathbf{W}^1 = (\omega_j^1)_{j=1}^N$ ,  $\mathbf{W}^2 = (\omega_j^2)_{j=1}^N$  be independently sampled from  $(\Omega_1, P_1)$  and  $(\Omega_2, P_2)$ , respectively. For any  $0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

$$\left| W_2 \left[ \mathcal{N} \left( 0, \frac{1}{m} \hat{K}_{\mathbf{W}^1}^1[\mathbf{X}] \right), \mathcal{N} \left( 0, \frac{1}{m} \hat{K}_{\mathbf{W}^2}^2[\mathbf{X}] \right) \right] - W_2 \left[ \mathcal{N} \left( 0, \frac{1}{m} K^1[\mathbf{X}] \right), \mathcal{N} \left( 0, \frac{1}{m} K^2[\mathbf{X}] \right) \right] \right|$$
  
(6.5) 
$$\leq 3(\kappa_1 + \kappa_2) \sqrt{\frac{4}{N\delta^2} + \frac{\sqrt{m}}{\sqrt{N\delta}} \left( 3 + \frac{4}{\sqrt{N\delta}} \right)}.$$

Theorem 6.3 (Estimation of 2-Wasserstein distance from finite samples). Assume Assumptions 1-5. Let  $\mathbf{X} = (x_i)_{i=1}^m$  be independently sampled from  $(T, \nu)$ . Let  $\mathbf{W}^1 = (\omega_j^1)_{j=1}^N$ ,  $\mathbf{W}^2 = (\omega_j^2)_{j=1}^N$  be independently sampled from  $(\Omega_1, P_1)$  and  $(\Omega_2, P_2)$ , respectively. For any  $0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

$$\left| W_2 \left[ \mathcal{N} \left( 0, \frac{1}{m} \hat{K}_{\mathbf{W}^1}^1[\mathbf{X}] \right), \mathcal{N} \left( 0, \frac{1}{m} \hat{K}_{\mathbf{W}^2}^2[\mathbf{X}] \right) \right] - W_2(\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})) \right|$$

$$(6.6) \leq \left( (\kappa_1^2 + \kappa_2^2) \left[ \frac{2 \log \frac{12}{\delta}}{m} + \sqrt{\frac{2 \log \frac{12}{\delta}}{m}} \right] + 2\sqrt{2}\kappa_1\kappa_2\sqrt{\dim(\mathcal{H}_{K^2})} \sqrt{\frac{2 \log \frac{12}{\delta}}{m}} + \sqrt{\frac{2 \log \frac{12}{\delta}}{m}} \right)^{1/2} + 3(\kappa_1 + \kappa_2) \sqrt{\frac{16}{N\delta^2} + \frac{2\sqrt{m}}{\sqrt{N\delta}} \left( 3 + \frac{8}{\sqrt{N\delta}} \right)}.$$

In contrast to Theorems 4.5 and 5.3, the convergence rates in Theorems 6.1 and 6.3 both depend on dim( $\mathcal{H}_{K^2}$ ). As an example, if  $T = [0,1]^d$  and  $K^2(x,y) = \langle x,y \rangle^D$ ,  $D \in \mathbb{N}$ , then [5] dim( $\mathcal{H}_{K^2}$ ) =  $\binom{D+d-1}{d-1}$ . Theorem 6.3 provides the theoretical justification for the estimation of the 2-Wasserstein distance in Algorithm 5.1 when dim( $\mathcal{H}_{K^2}$ ) <  $\infty$ .

**7. Estimation of Sinkhorn divergence via sample covariance operators.** For comparison, we now estimate the Sinkhorn divergence via sample covariance operators, which is a standard

approach in functional data analysis (see e.g. [37, 21]). For  $\xi \sim GP(0, K)$  on the probability space  $(\Omega, \mathcal{F}, P)$ , define the rank-one operator  $\xi(\omega, .) \otimes \xi(\omega, .) \in \mathcal{L}(\mathcal{L}^2(T, \nu))$  by  $[\xi(\omega, .) \otimes \xi(\omega, .)]f(x) = \xi(\omega, x) \int_T \xi(\omega, t) f(t) d\nu(t), \ \omega \in \Omega, \ f \in \mathcal{L}^2(T, \nu)$ . Then

(7.1) 
$$||\xi(\omega,.) \otimes \xi(\omega,.)||_{\mathrm{HS}(\mathcal{L}^2(T,\nu))} = \int_T \xi(\omega,t)^2 d\nu(t) < \infty \ P\text{-almost surely}$$

Thus  $[\xi(\omega, .) \otimes \xi(\omega, .)] \in HS(\mathcal{L}^2(T, \nu))$  *P*-almost surely. By Fubini Theorem (Lemma 10.7),

(7.2) 
$$C_K = \mathbb{E}[\xi \otimes \xi], \quad C_K f(x) = \mathbb{E} \int_T \xi(\omega, x)\xi(\omega, t)f(t)d\nu(t) = \int_T K(x, t)f(t)d\nu(t).$$

Let  $\mathbf{W} = (\omega_j)_{j=1}^N$  be independently sampled from  $(\Omega, P)$ , corresponding to the samples  $\{\xi_j(t) = \xi(\omega_j, t)\}_{j=1}^N$  from  $\xi$ . It defines the pair of sample covariance function/operator

(7.3) 
$$K_{\mathbf{W}}(x,y) = \frac{1}{N} \sum_{i=1}^{N} \xi(\omega_i, x) \xi(\omega_i, y), \quad C_{K,\mathbf{W}} = \frac{1}{N} \sum_{i=1}^{N} \xi(\omega_i, .) \otimes \xi(\omega_i, .),$$

(7.4) 
$$C_{K,\mathbf{W}}f(x) = \frac{1}{N} \sum_{i=1}^{N} \int_{T} \xi(\omega_i, x) \xi(\omega_i, t) f(t) d\nu(t) = \int_{T} K_{\mathbf{W}}(x, t) f(t) d\nu(t)$$

For each fixed  $\mathbf{W}$ ,  $K_{\mathbf{W}}$  is symmetric, positive definite. It is continuous if the sample paths  $\xi(\omega, .)$  are continuous *P*-almost surely, but not necessarily uniformly bounded over  $\mathbf{W}$  even if K is bounded. We always have, however, that  $\mathcal{H}_{K_{\mathbf{W}}} = \operatorname{span} \{\xi(\omega_j, .)\}_{j=1}^N \subset \mathcal{L}^2(T, \nu)$  is a vector space of dimension at most N,  $C_{K,\mathbf{W}}$  is a finite-rank operator, together with the following

Lemma 7.1. Under Assumptions 1-4 and 6, taking expectation with respect to W gives

(7.5) 
$$\mathbb{E}\int_{T} K_{\mathbf{W}}(x,x)^{2} d\nu(x) \leq 3 \int_{T} K(x,x)^{2} d\nu(x) \leq 3\kappa^{4}.$$

In particular  $\mathbb{P}\{\mathbf{W} \in (\Omega, P)^N : \int_T K_{\mathbf{W}}(x, x)^2 d\nu(x) \leq \frac{3\kappa^4}{\delta}\} \geq 1 - \delta$  for any  $0 < \delta < 1$ .

**Proposition 7.2.** Assume Assumptions 1-4 and 6. Let  $\mathbf{W} = (\omega_j)_{j=1}^N$  be independently sampled from  $(\Omega, P)$ . For any  $0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

(7.6) 
$$||C_{K,\mathbf{W}}||_{\mathrm{HS}(\mathcal{L}^{2}(T,\nu))} \leq \frac{2\kappa^{2}}{\delta}, \quad ||C_{K,\mathbf{W}} - C_{K}||_{\mathrm{HS}(\mathcal{L}^{2}(T,\nu))} \leq \frac{2\sqrt{3}\kappa^{2}}{\sqrt{N}\delta}.$$

Combining Theorem 2.2 and Proposition 7.2, we obtain the following result.

Theorem 7.3 (Estimation of Sinkhorn divergence between Gaussian processes from sample covariance operators). Under Assumptions 1-4 and 6, let  $\mathbf{W}^i = (\omega_j^i)_{j=1}^N$ , i = 1, 2, be independently sampled from  $(\Omega_i, P_i)$ .  $\forall 0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

(7.7) 
$$\begin{aligned} \left| \mathbf{S}_{2}^{\epsilon} [\mathcal{N}(0, C_{K^{1}, \mathbf{W}^{1}}), \mathcal{N}(0, C_{K^{2}, \mathbf{W}^{2}})] - \mathbf{S}_{2}^{\epsilon} [\mathcal{N}(0, C_{K^{1}}), \mathcal{N}(0, C_{K^{2}})] \right| \\ &\leq \frac{12\sqrt{3}}{\epsilon\delta} \left( \left( 1 + \frac{4}{\delta} \right) \kappa_{1}^{4} + \left( 3 + \frac{8}{\delta} \right) \kappa_{1}^{2} \kappa^{2} + \kappa_{2}^{4} \right) \frac{1}{\sqrt{N}}. \end{aligned}$$

On a set  $\mathbf{X} = (x_i)_{i=1}^m \in T^m$ , the Gram matrix of  $K_{\mathbf{W}}$  is precisely  $\hat{K}_{\mathbf{W}}[\mathbf{X}]$ , as in Eq.(5.3). Combining Lemma 7.1, Theorem 4.7, and Theorem 7.3, we obtain the following result

Theorem 7.4 (Estimation of Sinkhorn divergence between Gaussian processes from finite samples - general kernels). Under Assumptions 1-4 and 6, let  $\mathbf{W}^1 = (\omega_j^1)_{j=1}^N$ ,  $\mathbf{W}^2 = (\omega_j^2)_{j=1}^N$  be independently sampled from  $(\Omega_1, P_1)$  and  $(\Omega_2, P_2)$ , respectively. Let  $\mathbf{X} = (x_i)_{i=1}^m$  be independently sampled from  $(T, \nu)$ . For any  $0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

$$\left| S_{2}^{\epsilon} \left[ \mathcal{N}\left(0, \frac{1}{m} \hat{K}_{\mathbf{W}^{1}}^{1}[\mathbf{X}]\right), \mathcal{N}\left(0, \frac{1}{m} \hat{K}_{\mathbf{W}^{2}}^{2}[\mathbf{X}]\right) \right] - S_{2}^{\epsilon} [\mathcal{N}(0, C_{K^{1}}), \mathcal{N}(0, C_{K^{2}})] \right|$$

$$(7.8) \qquad \leq \frac{48\sqrt{3}}{\epsilon\delta} \left( \left(1 + \frac{16}{\delta}\right) \kappa_{1}^{4} + \left(3 + \frac{32}{\delta}\right) \kappa_{1}^{2} \kappa^{2} + \kappa_{2}^{4} \right) \frac{1}{\sqrt{N}} + \frac{864}{\epsilon\delta} (\kappa_{1}^{2} + \kappa_{2}^{2})^{2} \left(1 + \frac{12}{\delta}\right) \frac{1}{\sqrt{m}}.$$

We note that a similar version of Theorem 7.4 can also be obtained from Theorem 4.7.

8. Divergences between covariance operators of stochastic processes. Assume that  $\xi^1, \xi^2$  are centered stochastic processes, not necessarily Gaussian, with covariance functions  $K^1, K^2$  and paths in  $\mathcal{L}^2(T, \nu)$ . Then  $W_2[\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})], S_2^{\epsilon}[\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})]$  are distance/divergence between the two covariance operators  $C_{K^1}, C_{K^2}$  associated with  $\xi^1, \xi^2$ .

Assumption 6(\*)  $\xi, \xi^i, i = 1, 2$ , are centered stochastic processes and  $\exists \kappa, \kappa_i > 0$  with

(8.1) 
$$\mathbb{E}\int_{T}\xi(\omega,x)^{4}d\nu(x) \leq 3\kappa^{4}, \quad \mathbb{E}\int_{T}\xi^{i}(\omega,x)^{4}d\nu(x) \leq 3\kappa_{i}^{4}.$$

For  $\xi \sim \mathcal{N}(0, K)$ ,  $\xi^i \sim \mathcal{N}(0, K^i)$ , Assumption 6(\*) reduces to Assumption 6, as follows.

Lemma 8.1. Under Assumption 6(\*),  $\xi(\omega, .) \in \mathcal{L}^2(T, \nu)$  P-almost surely. Furthermore,  $\int_T K(x, x)^2 d\nu(x) \leq 3\kappa^4$  and  $\mathbb{E}||\xi||^4_{\mathcal{L}^2(T, \nu)} \leq 3\kappa^4$ . In particular, if  $\xi \sim \mathcal{N}(0, K)$ , then

(8.2) 
$$\mathbb{E}[\xi(.,x)^4] = 3K(x,x)^2 \ \forall x \in T, \ \mathbb{E}\int_T \xi(\omega,x)^4 d\nu(x) = 3\int_T K(x,x)^2 d\nu(x)$$

Hence, Proposition 4.6, 7.2, and Theorems 4.7 7.3, 7.4 for  $S_2^{\epsilon}$  carry over virtually unchanged, except for some absolute constant factors. We note that condition  $\mathbb{E}||\xi||_{\mathcal{L}^2(T,\nu)}^4 \leq 3\kappa^4$  is sufficient for proving Proposition 7.2 and Theorem 7.3. Similar results also hold for  $W_2$ .

**9.** Numerical experiments. We demonstrate  $W_2$  and  $\mathcal{S}_2^{\epsilon}$  on the following Gaussian processes  $\xi^i = \operatorname{GP}(0, K^i), i = 1, 2, \text{ on } T = [0, 1]^d \subset \mathbb{R}^d$ , where d = 1, 5, 50, with

(9.1) 
$$K^{1}(x,y) = \exp(-a||x-y||), \quad K^{2}(x,y) = \exp\left(-\frac{1}{\sigma^{2}}||x-y||^{2}\right),$$

In the experiments, we fix  $a = 1, \sigma = 0.1$ . Figure 1 shows samples of these processes for d = 1.

(i) Let  $\mathbf{X} = (x_i)_{i=1}^m$  be randomly chosen from T, where  $m = 10, 20, 30, \ldots, 1000$ . We plot in Figures 1 and 2 the following divergences between  $(1/m)K^1[\mathbf{X}]$  and  $(1/m)K^2[\mathbf{X}]$ :  $|| \ ||_{\text{HS}}^2$ (squared Hilbert-Schmidt),  $W_2^2$  (squared Wasserstein), and  $S_2^{\epsilon}$  (Sinkhorn,  $\epsilon = 0.1$  and  $\epsilon = 0.5$ ).

(ii) Consider two sets of N sample paths from each process, each path sampled at m = 500 points  $\mathbf{X} = (x_i)_{i=1}^m$ , which are randomly chosen and fixed in advance from T. We then compute the different divergences using Algorithm 5.1, for  $N = 10, 20, \ldots, 1000$  (Figure 3).

In agreement with theory, the convergence of the Sinkhorn divergence and Hilbert-Schmidt distance, being dimension-independent, is consistent across different dimensions, whereas the convergence of the Wasserstein distance is slower the larger the dimension d is.

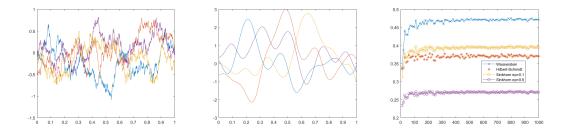


Figure 1: Samples of the centered Gaussian processes defined in Eq.(9.1) on T = [0, 1] and approximations of divergences/squared distances between them. Left:  $K^1(x, y) = \exp(-a||x-y||)$ , a = 1. Right:  $K^2(x, y) = \exp(-||x-y||^2/\sigma^2)$ ,  $\sigma = 0.1$ . Here  $m = 10, 20, \ldots, 1000$ .

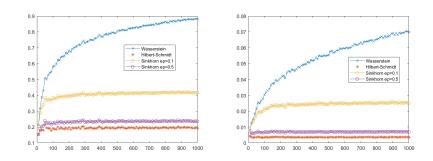


Figure 2: Approximate divergences/squared distances between the Gaussian processes defined in Eq.(9.1), using normalized  $m \times m$  covariance matrices, on  $T = [0, 1]^d \subset \mathbb{R}^d$ . Left: d = 5. Right: d = 50. Here  $m = 10, 20, \ldots, 1000$ .

## 10. Proofs of main results.

**Proof of Lemma 3.3.** It suffices to prove this for the case i = 1, j = 2. Let  $\{e_k\}_{k \in \mathbb{N}}$  be any orthonormal basis in  $\mathcal{H}_{K^2}$ , then

$$\begin{split} ||R_{12}||^{2}_{\mathrm{HS}(\mathcal{H}_{K^{2}},\mathcal{H}_{K^{1}})} &= \sum_{k=1}^{\infty} ||R_{12}e_{k}||^{2}_{\mathcal{H}_{K^{1}}} = \sum_{k=1}^{\infty} \left\| \int_{T} K_{x}^{1} \langle e_{k}, K_{x}^{2} \rangle_{\mathcal{H}_{K^{2}}} d\nu(x) \right\|^{2}_{\mathcal{H}_{K^{1}}} \\ &\leq \sum_{k=1}^{\infty} \left( \int_{T} ||K_{x}^{1}||_{\mathcal{H}_{K^{1}}} ||\langle e_{k}, K_{x}^{2} \rangle_{\mathcal{H}_{K^{2}}} |d\nu(x) \right)^{2} \leq \sum_{k=1}^{\infty} \int_{T} ||K_{x}^{1}||^{2}_{\mathcal{H}_{K^{1}}} d\nu(x) \int_{T} |\langle e_{k}, K_{x}^{2} \rangle_{\mathcal{H}_{K^{2}}} |^{2} d\nu(x) \\ &= \int_{T} ||K_{x}^{1}||^{2}_{\mathcal{H}_{K^{1}}} d\nu(x) \int_{T} \sum_{k=1}^{\infty} |\langle e_{k}, K_{x}^{2} \rangle_{\mathcal{H}_{K^{2}}} |^{2} d\nu(x) \text{ by the Monotone Convergence Theorem} \\ &= \int_{T} ||K_{x}^{1}||^{2}_{\mathcal{H}_{K^{1}}} d\nu(x) \int_{T} ||K_{x}^{2}||^{2}_{\mathcal{H}_{K^{2}}} d\nu(x) = \int_{T} K^{1}(x, x) d\nu(x) \int_{T} K^{2}(x, x) d\nu(x) \leq \kappa_{1}^{2} \kappa_{2}^{2}. \end{split}$$

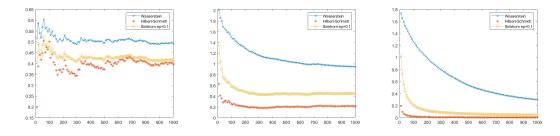


Figure 3: Approximate divergences/squared distances between the Gaussian processes defined in Eq.(9.1) on  $T = [0, 1]^d \subset \mathbb{R}^d$ . Left: d = 1. Middle: d = 5. Right: d = 50. The estimation is obtained using N realizations of each process, sampled at m = 500 points, according to Algorithm 5.1. Here  $N = 10, 20, \ldots, 1000$ .

**Proof of Lemma 3.4.** For any  $f \in \mathcal{H}_{K^2}$ ,  $g \in \mathcal{H}_{K^1}$ ,

$$\langle g, R_{12,\mathbf{X}}f \rangle_{\mathcal{H}_{K^1}} = \left\langle g, \frac{1}{m} \sum_{i=1}^m f(x_i) K_{x_i}^1 \right\rangle_{\mathcal{H}_{K^1}} = \frac{1}{m} \sum_{i=1}^m f(x_i) g(x_i) = \langle R_{21,\mathbf{X}}g, f \rangle_{\mathcal{H}_{K^2}}$$

showing that  $R_{12,\mathbf{X}}^* = R_{21,\mathbf{X}}$ . It follows that for any  $f \in \mathcal{H}_{K^2}$ ,

$$\begin{split} R_{12,\mathbf{X}}^* R_{12,\mathbf{X}} f &= \frac{1}{m} \sum_{i=1}^m R_{12,\mathbf{X}}^* f(x_i) K_{x_i}^1 = \frac{1}{m^2} \sum_{i,j=1}^m f(x_i) K_{x_j}^2 \langle K_{x_i}^1, K_{x_j}^1 \rangle_{\mathcal{H}_{K^1}} \\ &= \frac{1}{m^2} \sum_{i,j=1}^m f(x_i) K^1(x_i, x_j) K_{x_j}^2. \\ R_{12,\mathbf{X}}^* R_{12,\mathbf{X}} K_{x_k}^2 &= \frac{1}{m^2} \sum_{i,j=1}^m K^2(x_k, x_i) K^1(x_i, x_j) K_{x_j}^2 = \frac{1}{m^2} \sum_{j=1}^m (K^2[\mathbf{X}] K^1[\mathbf{X}])_{kj} K_{x_j}^2. \end{split}$$

It follows that, in the span $\{K_{x_i}^2\}_{i=1}^m$ , the matrix representation of  $R_{12,\mathbf{X}}^*R_{12,\mathbf{X}} : \mathcal{H}_{K^2,\mathbf{X}} \to \mathcal{H}_{K^2,\mathbf{X}}$  is  $\frac{1}{m^2}(K^2[\mathbf{X}]K^1[\mathbf{X}])^T = \frac{1}{m^2}K^1[\mathbf{X}]K^2[\mathbf{X}]$ .

Lemma 10.1 (Corollary 5 in [35]). For  $A, B \in \text{Sym}^+(\mathcal{H}) \cap \text{Tr}(\mathcal{H})$ ,

(10.1) 
$$||(I+A)^r - (I+B)^r||_{\rm tr} \le r||A-B||_{\rm tr}, \ 0 \le r \le 1.$$

Corollary 10.2. For  $A, B \in \text{Sym}^+(\mathcal{H}) \cap \text{Tr}(\mathcal{H})$ ,

(10.2) 
$$|\operatorname{tr}[-I + (I+A)^{1/2}] - \operatorname{tr}[-I + (I+B)^{1/2}]| \le \frac{1}{2}||A-B||_{\operatorname{tr}}$$

Lemma 10.3 (Corollary 6 in [35]). For  $A, B \in \text{Sym}^+(\mathcal{H}) \cap \text{Tr}(\mathcal{H})$ ,

(10.3) 
$$\left|\log \det \left(\frac{1}{2}I + \frac{1}{2}(I+A)^{1/2}\right) - \log \det \left(\frac{1}{2}I + \frac{1}{2}(I+B)^{1/2}\right)\right| \le \frac{1}{4}||A-B||_{\rm tr}.$$

**Proof of Proposition 4.2.** (i) For  $A, B \in \text{Sym}^+(\mathcal{H}) \cap \text{Tr}(\mathcal{H})$ ,

$$\begin{aligned} |G(A) - G(B)| &\leq |\operatorname{tr}[M(A)] - \operatorname{tr}[M(B)]| + \left| \log \det \left( I + \frac{1}{2}M(A) \right) - \log \det \left( I + \frac{1}{2}M(B) \right) \right| \\ &= |\operatorname{tr}[-I + (I + c^2 A)^{1/2}] - \operatorname{tr}[-I + (I + c^2 B)^{1/2}]| \\ &+ \left| \log \det \left( \frac{1}{2}I + \frac{1}{2}(I + c^2 A)^{1/2} \right) - \log \det \left( \frac{1}{2}I + \frac{1}{2}(I + c^2 B)^{1/2} \right) \right| \\ &\leq \frac{c^2}{2} ||A - B||_{\operatorname{tr}} + \frac{c^2}{4} ||A - B||_{\operatorname{tr}} = \frac{3c^2}{4} ||A - B||_{\operatorname{tr}}, \text{ by Corollary 10.2 and Lemma 10.3.} \end{aligned}$$

(ii) For  $A, B \in \text{Sym}(\mathcal{H}) \cap \text{HS}(\mathcal{H})$ , using the first part,

$$|G(A^{2}) - G(B^{2})| \leq \frac{3c^{2}}{4} ||A^{2} - B^{2}||_{tr} \leq \frac{3c^{2}}{4} ||A(A - B) + (A - B)B||_{tr}$$
$$\leq \frac{3c^{2}}{4} [||A||_{HS} + ||B||_{HS}]||A - B||_{HS}.$$

(iii) For  $A, B \in \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ , by Proposition 12.1,  $A^*A, B^*B \in \mathrm{Sym}^+(\mathcal{H}_1) \cap \mathrm{Tr}(\mathcal{H}_1)$  and

$$|G(A^*A) - G(B^*B)| \le \frac{3c^2}{4} ||A^*A - B^*B||_{\operatorname{tr}(\mathcal{H}_1)} \text{ from part (i)} \le \frac{3c^2}{4} [||A||_{\operatorname{HS}(\mathcal{H}_1, \mathcal{H}_2)} + ||B||_{\operatorname{HS}(\mathcal{H}_1, \mathcal{H}_2)}]||A - B||_{\operatorname{HS}(\mathcal{H}_1, \mathcal{H}_2)}.$$

**Proof of Proposition 4.4.** It suffices to prove this for the case i = 1, j = 2. Define the random variable  $\xi : (T, \nu) \to \operatorname{HS}(\mathcal{H}_{K^2}, \mathcal{H}_{K^1})$  by  $\xi(x) = K_x^1 \otimes K_x^2 : \mathcal{H}_{K^2} \to \mathcal{H}_{K^1}, \ \xi(x)f = K_x^1 \langle f, K_x^2 \rangle = f(x)K_x^1 \ \forall f \in \mathcal{H}_{K^2}.$  Then  $\mathbb{E}[\xi(x)] = \int_T (K_x^1 \otimes K_x^2) d\nu(x) = R_{12}, \quad \frac{1}{m} \sum_{i=1}^m \xi(x_i) = \frac{1}{m} \sum_{i=1}^m K_{x_i}^1 \otimes K_{x_i}^2 = R_{12,\mathbf{X}}.$  By Lemma 12.3,

$$\begin{split} ||\xi(x)||_{\mathrm{HS}(\mathcal{H}_{K^{2}},\mathcal{H}_{K^{1}})} &= ||K_{x}^{1}||_{\mathcal{H}_{K^{1}}} ||K_{x}^{2}||_{\mathcal{H}_{K^{2}}} = \sqrt{K^{1}(x,x)K^{2}(x,x)} \leq \kappa_{1}\kappa_{2}, \quad \forall x \in T, \\ ||R_{12,\mathbf{X}}||_{\mathrm{HS}(\mathcal{H}_{K^{2}},\mathcal{H}_{K^{1}})} \leq \frac{1}{m} \sum_{i=1}^{m} ||K_{x_{i}}^{1} \otimes K_{x_{i}}^{2}||_{\mathrm{HS}(\mathcal{H}_{K^{2}},\mathcal{H}_{K^{1}})} \leq \kappa_{1}\kappa_{2}, \\ E||\xi||_{\mathrm{HS}(\mathcal{H}_{K^{2}},\mathcal{H}_{K^{1}})} = \int_{T} K^{1}(x,x)K^{2}(x,x)d\nu(x) \leq \kappa_{1}^{2}\kappa_{2}^{2}. \end{split}$$

The bound for  $||R_{12,\mathbf{X}} - R_{12}||_{\mathrm{HS}(\mathcal{H}_{K^2},\mathcal{H}_{K^1})}$  follows from Proposition 4.3. By Corollary 12.2,

$$\begin{split} &||R_{12,\mathbf{X}}^*R_{12,\mathbf{X}} - R_{12}^*R_{12}||_{\operatorname{tr}(\mathcal{H}_{K^2})} \\ &\leq (||R_{12,\mathbf{X}}||_{\operatorname{HS}(\mathcal{H}_{K^2},\mathcal{H}_{K^1})} + ||R_{12}||_{\operatorname{HS}(\mathcal{H}_{K}^2,\mathcal{H}_{K^1})})||R_{12,\mathbf{X}} - R_{12}||_{\operatorname{HS}(\mathcal{H}_{K^2},\mathcal{H}_{K^1})}, \end{split}$$

which gives the desired bound for  $||R_{12,\mathbf{X}}^*R_{12,\mathbf{X}} - R_{12}^*R_{12}||_{\operatorname{tr}(\mathcal{H}_{K^2})}$ .

**Proof of Theorem 4.5**. By Proposition 4.1, let  $c = \frac{4}{\epsilon}$ , then

$$\Delta = \left| S_2^{\epsilon} [\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})] - S_2^{\epsilon} \left[ \mathcal{N}\left(0, \frac{1}{m} K^1[\mathbf{X}]\right), \mathcal{N}\left(0, \frac{1}{m} K^2[\mathbf{X}]\right) \right] \right| \\ \leq \frac{1}{c} \left[ |G(L_{K^1, \mathbf{X}}^2) - G(L_{K^1}^2)| + |G(L_{K^2, \mathbf{X}}^2) - G(L_{K^2}^2)| + 2|G(R_{12, \mathbf{X}}^* R_{12, \mathbf{X}}) - G(R_{12}^* R_{12})| \right].$$

We now combine Proposition 4.2 with Propositions 4.4. For  $0 < \delta < 1$ , define

$$U_{i} = \left\{ \mathbf{X} \in T^{m} : |G(L_{K^{i},\mathbf{X}}^{2}) - G(L_{K^{i}}^{2})| \le \frac{3c^{2}}{2}\kappa_{i}^{4} \left( \frac{2\log\frac{6}{\delta}}{m} + \sqrt{\frac{2\log\frac{6}{\delta}}{m}} \right) \right\}, \quad i = 1, 2,$$
$$U_{3} = \left\{ \mathbf{X} \in T^{m} : |G(R_{12,\mathbf{X}}^{*}R_{12,\mathbf{X}}) - G(R_{12}^{*}R_{12})| \le \frac{3c^{2}}{2}\kappa_{1}^{2}\kappa_{2}^{2} \left[ \frac{2\log\frac{6}{\delta}}{m} + \sqrt{\frac{2\log\frac{6}{\delta}}{m}} \right] \right\}.$$

Then  $\nu^m(U_1) \ge 1 - \frac{\delta}{3}$ ,  $\nu^m(U_2) \ge 1 - \frac{\delta}{3}$ ,  $\nu^m(U_3) \ge 1 - \frac{\delta}{3}$ . From the Inclusion-Exclusion Principle, using the property  $\nu^m(U_i \cup U_j) = \nu^m(U_i) + \nu^m(U_j) - \nu^m(U_i \cap U_j)$ ,

$$\nu^{m}(U_{1} \cap U_{2} \cap U_{3}) = \nu^{m}(U_{1} \cup U_{2} \cup U_{3}) + \nu^{m}(U_{1}) + \nu^{m}(U_{2}) + \nu^{m}(U_{3}) - [\nu^{m}(U_{1} \cup U_{2}) + \nu^{m}(U_{1} \cup U_{3}) + \nu^{m}(U_{2} \cup U_{3})] \ge 1 + 3(1 - \frac{\delta}{3}) - 3 = 1 - \delta.$$

Thus for any  $0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

$$\Delta \leq \frac{3c}{2} (\kappa_1^2 + \kappa_2^2)^2 \left[ \frac{2\log\frac{6}{\delta}}{m} + \sqrt{\frac{2\log\frac{6}{\delta}}{m}} \right] = \frac{6}{\epsilon} (\kappa_1^2 + \kappa_2^2)^2 \left[ \frac{2\log\frac{6}{\delta}}{m} + \sqrt{\frac{2\log\frac{6}{\delta}}{m}} \right].$$

**Proof of Propositions 4.6.** Define the random variables  $Y_j : (T, \nu)^m \to \operatorname{HS}(\mathcal{H}_{K^2}, \mathcal{H}_{K^1})$ by  $Y_j(\mathbf{X}) = K_{x_j}^1 \otimes K_{x_j}^2$ ,  $1 \leq j \leq m$ , where  $\mathbf{X} = (x_j)_{j=1}^m$  is independently sampled from  $(T, \nu)$ . The  $Y_j$ 's are IID, with  $\mathbb{E}Y_j = R_{12}$  and  $\frac{1}{m} \sum_{j=1}^m Y_j(\mathbf{X}) = R_{12,\mathbf{X}}$ . By Lemma 12.3,

$$\begin{split} \mathbb{E}||Y_{j}||_{\mathrm{HS}(\mathcal{H}_{K^{2}},\mathcal{H}_{K^{1}})} &= \int_{T} ||K_{x}^{1}||_{\mathcal{H}_{K^{1}}} ||K_{x}^{2}||_{\mathcal{H}_{K^{2}}} d\nu(x) = \int_{T} \sqrt{K^{1}(x,x)} \sqrt{K^{2}(x,x)} d\nu(x) \\ &\leq \sqrt{\int_{T} K^{1}(x,x) d\nu(x)} \sqrt{\int_{T} K^{2}(x,x) d\nu(x)} \leq \kappa_{1}\kappa_{2}, \\ \mathbb{E}||Y_{j}||_{\mathrm{HS}(\mathcal{H}_{K^{2}},\mathcal{H}_{K^{1}})}^{2} &= \int_{T} ||K_{x}^{1}||_{\mathcal{H}_{K^{1}}}^{2} ||K_{x}^{2}||_{\mathcal{H}_{K^{2}}}^{2} = \int_{T} K^{1}(x,x) K^{2}(x,x) d\nu(x) \\ &\leq \sqrt{\int_{T} [K^{1}(x,x)]^{2} d\nu(x)} \sqrt{\int_{T} [K^{2}(x,x)]^{2} d\nu(x)} \leq \kappa_{1}^{2}\kappa_{2}^{2}. \end{split}$$

Define the random variable  $\eta : (T, \nu)^m \to \mathbb{R}$  by  $\eta(\mathbf{X}) = \left\| \frac{1}{m} \sum_{j=1}^m Y_j(\mathbf{X}) - \mathbb{E}Y_j \right\|_{\mathrm{HS}(\mathcal{H}_{K^2}, \mathcal{H}_{K^1})} = ||R_{12,\mathbf{X}} - R_{12}||_{\mathrm{HS}(\mathcal{H}_{K^2}, \mathcal{H}_{K^1})}$ . Since the  $Y_j$ 's are IID,

$$\mathbb{E}\eta^{2} = \mathbb{E}\left\|\frac{1}{m}\sum_{j=1}^{m}Y_{j} - \mathbb{E}Y_{j}\right\|_{\mathrm{HS}}^{2} = \frac{1}{m^{2}}\sum_{j=1}^{m}\mathbb{E}||Y_{j} - EY_{j}||_{\mathrm{HS}}^{2} = \frac{1}{m^{2}}\sum_{j=1}^{m}(\mathbb{E}||Y_{j}||_{\mathrm{HS}}^{2} - ||EY_{j}||_{\mathrm{HS}}^{2}) \le \frac{\kappa_{1}^{2}\kappa_{2}^{2}}{m}.$$

By Chebyshev inequality, for any t > 0,  $\mathbb{P}(\eta \ge t) \le \frac{\mathbb{E}\eta}{t} \le \frac{\sqrt{\mathbb{E}\eta^2}}{t} \le \frac{\kappa_1\kappa_2}{\sqrt{mt}}$ . Let  $\delta = \frac{\kappa_1\kappa_2}{\sqrt{mt}} \iff t = \frac{\kappa_1\kappa_2}{\sqrt{m\delta}}$ , then  $\mathbb{P}\{\mathbf{X} : ||R_{12,\mathbf{X}} - R_{12}||_{\mathrm{HS}} = \eta(\mathbf{X}) \le \frac{\kappa_1\kappa_2}{\sqrt{m\delta}}\} \ge 1 - \delta$ . Similarly, since  $\mathbb{E}||R_{12,\mathbf{X}}||_{\mathrm{HS}} \le \frac{1}{m}\sum_{j=1}^m \mathbb{E}||Y_j||_{\mathrm{HS}} \le \kappa_1\kappa_2$ , we have  $\mathbb{P}\{\mathbf{X} : ||R_{12,\mathbf{X}}||_{\mathrm{HS}} \le \frac{\kappa_1\kappa_2}{\delta}\} \ge 1 - \delta$ . Computing the intersection of these two sets of events and replacing  $\delta$  by  $\frac{\delta}{2}$ , we obtain the desired bounds.

**Proof of Theorem 4.7.** Define  $\Delta$  as in the proof of Theorem 4.5. We now combine Proposition 4.2 with Propositions 4.6. For  $0 < \delta < 1$ , define

$$U_{i} = \left\{ \mathbf{X} \in T^{m} : |G(L_{K^{i},\mathbf{X}}^{2}) - G(L_{K^{i}}^{2})| \le \frac{3c^{2}}{2}\kappa_{i}^{4}\left(1 + \frac{6}{\delta}\right)\frac{3}{\sqrt{m\delta}} \right\}, \quad i = 1, 2,$$
  
$$U_{3} = \left\{ \mathbf{X} \in T^{m} : |G(R_{12,\mathbf{X}}^{*}R_{12,\mathbf{X}}) - G(R_{12}^{*}R_{12})| \le \frac{3c^{2}}{2}\kappa_{1}^{2}\kappa_{2}^{2}\left(1 + \frac{6}{\delta}\right)\frac{3}{\sqrt{m\delta}} \right\}$$

Then  $\nu^m(U_i) \ge 1 - \frac{\delta}{3}$ , i = 1, 2, 3. Thus for any  $0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

$$\Delta \leq \frac{3c}{2}(\kappa_1^2 + \kappa_2^2)^2 \left(1 + \frac{6}{\delta}\right) \frac{3}{\sqrt{m\delta}} = \frac{18}{\epsilon}(\kappa_1^2 + \kappa_2^2)^2 \left(1 + \frac{6}{\delta}\right) \frac{1}{\sqrt{m\delta}}.$$

**Proof of Lemma 8.1.** Since  $\mathbb{E}||\xi||_{\mathcal{L}^2(T,\nu)}^4 = \mathbb{E}\left(\int_T \xi(\omega,x)^2 d\nu(x)\right)^2 \leq \mathbb{E}\int_T \xi(\omega,x)^4 d\nu(x)$   $\leq 3\kappa^4$ , we have  $\mathbb{E}||\xi||_{\mathcal{L}^2(T,\nu)}^2 \leq \sqrt{\mathbb{E}}||\xi||_{\mathcal{L}^2(T,\nu)}^4 \leq \sqrt{3\kappa^2}$ , thus  $\xi(\omega,.) \in \mathcal{L}^2(T,\nu)$  *P*-almost surely. By Hölder Theorem and Tonelli Theorem,

$$\int_T K(x,x)^2 d\nu(x) = \int_T \left( \int_\Omega \xi(\omega,x)^2 dP(\omega) \right)^2 d\nu(x) \le \int_\Omega \int_T \xi(\omega,x)^4 dP(\omega) d\nu(x) \le 3\kappa^4.$$

If  $\xi \sim \mathcal{N}(0, K)$ , then for each fixed  $x \in T$ , we have  $\xi(., x) \sim \mathcal{N}(0, K(x, x))$ . Thus

$$\mathbb{E}\xi(.,x)^4 = \int_{\Omega} \xi(\omega,x)^4 dP(\omega) = \int_{\mathbb{R}} t^4 d\mathcal{N}(0,K(x,x))(t) = 3K(x,x)^2$$

by using the integral  $\int_{\mathbb{R}} t^4 d\mathcal{N}(0,\lambda)(t) = 3\lambda^2$  (see Formula 7.4.4 in [1]).

**Proof of Proposition 5.1.** We have  $||K[\mathbf{X}]||_F = m||L_{K,\mathbf{X}}||_{\mathrm{HS}(\mathcal{H}_K)} \leq m\kappa^2$  by Proposition 4.4. Define the map  $\mathbf{z} : \Omega \to \mathbb{R}^m$  by  $\mathbf{z}(\omega) = (\xi(\omega, x_i))_{i=1}^m \in \mathbb{R}^m$ . Let  $Y_j : (\Omega, P)^N \to \mathrm{Sym}^+(m), \ 1 \leq j \leq N$ , be IID  $\mathrm{Sym}^+(m)$ -valued random variables defined by  $Y_j(\mathbf{W}) = \mathbf{z}(\omega_j)\mathbf{z}(\omega_j)^T$ , where  $\mathbf{W} = (\omega_1, \ldots, \omega_N)$  is independently sampled from  $(\Omega, P)^N$ . Then

$$\begin{split} K[\mathbf{X}] &= \int_{\Omega} \mathbf{z}(\omega) \mathbf{z}(\omega)^T dP(\omega) = \mathbb{E}Y_j, \quad \hat{K}_{\mathbf{W}}[\mathbf{X}] = \frac{1}{N} \sum_{j=1}^N \mathbf{z}(\omega_j) \mathbf{z}(\omega_j)^T = \frac{1}{N} \sum_{j=1}^N Y_j(\mathbf{W}), \\ \mathbb{E}||Y_j||_F &= \mathbb{E}||\mathbf{z}(\omega)||^2 = \int_{\Omega} \sum_{i=1}^m \xi(\omega, x_i)^2 dP(\omega) = \sum_{i=1}^m K(x_i, x_i) \le m\kappa^2, \\ \mathbb{E}||Y_j||_F^2 &= \mathbb{E}||\mathbf{z}||^4 = \mathbb{E}\left[(\sum_{i=1}^m \xi(\omega, x_i)^2)^2\right] \le m \sum_{i=1}^m \mathbb{E}\left[\xi(\omega, x_i)^4\right] = 3m \sum_{i=1}^m K(x_i, x_i)^2 \le 3m^2\kappa^4 \end{split}$$

by Lemma 8.1. Define  $\eta : (\Omega, P)^N \to \mathbb{R}$  by  $\eta(\mathbf{W}) = \left\| \frac{1}{N} \sum_{j=1}^N Y_j(\mathbf{W}) - \mathbb{E}Y_j \right\|_F = \left\| \hat{K}_{\mathbf{W}}[\mathbf{X}] - K[\mathbf{X}] \right\|_F$ . Since the  $Y_j$ 's are independent, identically distributed,

$$\mathbb{E}\eta^2 = \mathbb{E}\left\|\frac{1}{N}\sum_{j=1}^N Y_j - \mathbb{E}Y_j\right\|_F^2 = \frac{1}{N^2}\sum_{j=1}^N \mathbb{E}||Y_j - EY_j||_F^2 = \frac{1}{N^2}\sum_{j=1}^N (\mathbb{E}||Y_j||_F^2 - ||EY_j||_F^2) \le \frac{3m^2\kappa^4}{N}.$$

By Chebyshev inequality, for any t > 0,  $\mathbb{P}(\eta \ge t) \le \frac{\mathbb{E}\eta}{t} \le \frac{\sqrt{\mathbb{E}\eta^2}}{t} \le \frac{\sqrt{3}m\kappa^2}{\sqrt{Nt}}$ . Let  $\delta = \frac{\sqrt{3}m\kappa^2}{\sqrt{Nt}} \iff t = \frac{\sqrt{3}m\kappa^2}{\sqrt{N\delta}}$ , then  $\mathbb{P}\{\mathbf{W} : ||\hat{K}_{\mathbf{W}}[\mathbf{X}] - K[\mathbf{X}]||_F = \eta(\mathbf{W}) \le \frac{\sqrt{3}m\kappa^2}{\sqrt{N\delta}}\} \ge 1 - \delta$ . Similarly,  $\mathbb{E}||\hat{K}_{\mathbf{W}}[\mathbf{X}]||_F \le \frac{1}{N}\sum_{j=1}^{N} \mathbb{E}||Y_j||_F = m\kappa^2 \Rightarrow \mathbb{P}\{\mathbf{W} : ||\hat{K}_{\mathbf{W}}[\mathbf{X}]||_F \le \frac{m\kappa^2}{\delta}\} \ge 1 - \delta$ . Computing the intersection of these two events and replacing  $\delta$  by  $\frac{\delta}{2}$ , we obtain the desired bounds.

**Proof of Theorem 5.2.** With each pair  $(\mathbf{W}^1, \mathbf{W}^2)$ , by Theorem 2.2,

$$\begin{split} \Delta &= \Delta(\mathbf{W}^{1}, \mathbf{W}^{2}) = \left| \mathbf{S}_{2}^{\epsilon} \left[ \mathcal{N} \left( 0, (1/m) \hat{K}_{\mathbf{W}^{1}}^{1}[\mathbf{X}] \right), \mathcal{N} \left( 0, (1/m) \hat{K}_{\mathbf{W}^{2}}^{2}[\mathbf{X}] \right) \right] \\ &- \mathbf{S}_{2}^{\epsilon} \left[ \mathcal{N} \left( 0, (1/m) K^{1}[\mathbf{X}] \right), \mathcal{N} \left( 0, (1/m) K^{2}[\mathbf{X}] \right) \right] \right| \\ &\leq \frac{3}{\epsilon m^{2}} [||\hat{K}_{\mathbf{W}^{1}}^{1}[\mathbf{X}]||_{F} + ||K^{1}[\mathbf{X}]||_{F} + 2||K^{2}[\mathbf{X}]||_{F}]||\hat{K}_{\mathbf{W}^{1}}^{1}[\mathbf{X}] - K^{1}[\mathbf{X}]||_{F} \\ &+ \frac{3}{\epsilon m^{2}} [2||\hat{K}_{\mathbf{W}^{1}}^{1}[\mathbf{X}]||_{F} + ||K^{1}[\mathbf{X}]||_{F} + ||K^{2}[\mathbf{X}]||_{F}]||\hat{K}_{\mathbf{W}^{2}}^{2}[\mathbf{X}] - K^{2}[\mathbf{X}]||_{F} \end{split}$$

For  $0 < \delta < 1$ , by Proposition 5.1, the following sets satisfy  $P_i^N(U_i) \ge 1 - \frac{\delta}{2}, i = 1, 2,$ 

$$U_i = \left\{ \mathbf{W}^i \in \Omega_i^N : ||\hat{K}_{\mathbf{W}^i}^i[\mathbf{X}] - K^i[\mathbf{X}]||_F \le \frac{4\sqrt{3}m\kappa_i^2}{\sqrt{N}\delta}, ||\hat{K}_{\mathbf{W}^i}^i[\mathbf{X}]||_F \le \frac{4m\kappa_i^2}{\delta} \right\}$$

Let  $U = (U_1 \times \Omega_2) \cap (\Omega_1 \times U_2)$ , then  $(P_1 \otimes P_2)^N(U) \ge 1 - \delta$  and  $\forall (\mathbf{W}^1, \mathbf{W}^2) \in U$ ,

$$\Delta(\mathbf{W}^1, \mathbf{W}^2) \le \frac{3}{\epsilon m^2} \left[ \frac{4m\kappa_1^2}{\delta} + m\kappa_1^2 + 2m\kappa_2^2 \right] \frac{4\sqrt{3}m\kappa_1^2}{\sqrt{N}\delta} + \frac{3}{\epsilon m^2} \left[ \frac{8m\kappa_1^2}{\delta} + m\kappa_1^2 + m\kappa_2^2 \right] \frac{4\sqrt{3}m\kappa_2^2}{\sqrt{N}\delta} \\ = \frac{12\sqrt{3}}{\epsilon\delta} \left[ \left( 1 + \frac{4}{\delta} \right) \kappa_1^4 + \left( 3 + \frac{8}{\delta} \right) \kappa_1^2 \kappa_2^2 + \kappa_2^4 \right] \frac{1}{\sqrt{N}}.$$

**Proof of Theorem 5.3.** For each fixed  $\mathbf{X} \in (T, \nu)^m$ , define

$$\Delta_1 = \left| \mathbf{S}_2^{\epsilon} \left[ \mathcal{N} \left( 0, (1/m) K^1[\mathbf{X}] \right), \mathcal{N} \left( 0, (1/m) K^2[\mathbf{X}] \right) - \mathbf{S}_2^{\epsilon} \left[ \mathcal{N} (0, C_{K^1}), \mathcal{N} (0, C_{K^2}) \right] \right] \right|.$$

By Theorem 4.5, the following set  $U_1 \subset (T,\nu)^m$  satisfies  $\nu^m(U_1) \ge 1 - \frac{\delta}{2}$ 

$$U_1 = \left\{ \mathbf{X} \in (T, \nu)^m : \Delta_1 \le \frac{6}{\epsilon} (\kappa_1^2 + \kappa_2^2)^2 \left[ \frac{2\log\frac{12}{\delta}}{m} + \sqrt{\frac{2\log\frac{12}{\delta}}{m}} \right] \right\}.$$

For each fixed  $\mathbf{X} \in (T, \nu)^m, \mathbf{W}^1 \in (\Omega_1, P_1)^N, \mathbf{W}^2 \in (\Omega_2, P_2)^N$ , define

$$\Delta_2 = \left| \mathbf{S}_2^{\epsilon} \left[ \mathcal{N}\left( 0, (1/m) \hat{K}_{\mathbf{W}^1}^1[\mathbf{X}] \right), \mathcal{N}\left( 0, (1/m) \hat{K}_{\mathbf{W}^2}^2[\mathbf{X}] \right) \right] - \mathbf{S}_2^{\epsilon} \left[ \mathcal{N}\left( 0, (1/m) K^1[\mathbf{X}] \right), \mathcal{N}\left( 0, (1/m) K^2[\mathbf{X}] \right) \right] \right|.$$

By Theorem 5.2, the following set  $U_2 \in (\Omega_1, P_1)^N \times (\Omega_2, P_2)^N$  satisfies  $(P_1 \otimes P_2)^N (U_2) \ge 1 - \frac{\delta}{2}$ 

$$U_2 = \left\{ (\mathbf{W}^1, \mathbf{W}^2) : \Delta_2 \le \frac{24\sqrt{3}}{\epsilon\delta} \left[ \left( 1 + \frac{8}{\delta} \right) \kappa_1^4 + \left( 3 + \frac{16}{\delta} \right) \kappa_1^2 \kappa_2^2 + \kappa_2^4 \right] \frac{1}{\sqrt{N}} \right\}.$$

Let  $U = (U_1 \times (\Omega_1, P_1)^N \times (\Omega_2, P_2)^N) \cap ((T, \nu)^m \times U_2)$ , then  $(\nu^m \otimes P_1^N \otimes P_2^N)(U) \ge 1 - \delta$  and

$$\begin{split} \Delta_1 + \Delta_2 &\leq \frac{6}{\epsilon} (\kappa_1^2 + \kappa_2^2)^2 \left[ \frac{2\log\frac{12}{\delta}}{m} + \sqrt{\frac{2\log\frac{12}{\delta}}{m}} \right] \\ &+ \frac{24\sqrt{3}}{\epsilon\delta} \left[ \left( 1 + \frac{8}{\delta} \right) \kappa_1^4 + \left( 3 + \frac{16}{\delta} \right) \kappa_1^2 \kappa_2^2 + \kappa_2^4 \right] \frac{1}{\sqrt{N}}, \ \forall (\mathbf{X}, \mathbf{W}^1, \mathbf{W}^2) \in U. \end{split}$$

Lemma 10.4. Under Assumptions 1-5, let  $\mathbf{X} = (x_i)_{i=1}^m$  be independently sampled from  $(T, \nu)$ . For any  $0 < \delta < 1$ , with probability at least  $1-\delta$ ,

(10.4) 
$$|\operatorname{tr}(L_{K,\mathbf{X}}) - \operatorname{tr}(L_{K})| \le \kappa^{2} \left( \frac{2\log\frac{2}{\delta}}{m} + \sqrt{\frac{2\log\frac{2}{\delta}}{m}} \right)$$

**Proof.** Define the random variable  $\eta : (T, \nu) \to \mathbb{R}$  by  $\eta(x) = K(x, x)$ , then  $||\eta||_{\infty} \leq \kappa^2$  and  $\operatorname{tr}(L_{K,\mathbf{X}}) = \frac{1}{m} \operatorname{tr} \left[\sum_{i=1}^m K_{x_i} \otimes K_{x_i}\right] = \frac{1}{m} \sum_{i=1}^m K(x_i, x_i) = \frac{1}{m} \sum_{i=1}^m \eta(x_i)$ ,  $\operatorname{tr}(L_K) = \int_T K(x, x) d\nu(x) = \mathbb{E}\xi$ ,  $\mathbb{E}|\eta^2| = \int_T K(x, x)^2 d\nu(x) \leq \kappa^4$ . The desired bound then follows from Proposition 4.3.

Lemma 10.5 (Lemma 4.1 in [41]). For  $A, B \in \text{Sym}^+(\mathcal{H}) \cap \text{Tr}(\mathcal{H})$ ,

(10.5) 
$$||A^{1/2} - B^{1/2}||_{\text{HS}}^2 \le ||A - B||_{\text{tr}}.$$

**Proof of Theorem 6.1.** Eqs.(6.2) and (6.3) follow as in the case of the Sinkhorn divergence. By Lemma 10.4,  $\forall 0 < \delta < 1$ , the following sets satisfy  $\nu^m(U_i) \ge 1 - \frac{\delta}{3}$ , i = 1, 2,

$$U_i = \left\{ \mathbf{X} \in (T, \nu)^m : |\operatorname{tr}(L_{K^i, \mathbf{X}}) - \operatorname{tr}(L_{K^i})| \le \kappa_i^2 \left[ \frac{2\log \frac{6}{\delta}}{m} + \sqrt{\frac{2\log \frac{6}{\delta}}{m}} \right] \right\}.$$

Under the assumption  $\dim(\mathcal{H}_{K^2}) < \infty$ , we have by Lemma 10.5,

$$\begin{aligned} |\operatorname{tr}[(R_{12,\mathbf{X}}^*R_{12,\mathbf{X}})^{1/2}] &- \operatorname{tr}[(R_{12}^*R_{12})^{1/2}]| \leq ||(R_{12,\mathbf{X}}^*R_{12,\mathbf{X}})^{1/2} - (R_{12}^*R_{12})^{1/2}||_{\operatorname{tr}(\mathcal{H}_{K^2})} \\ &\leq \sqrt{\dim(\mathcal{H}_{K^2})} ||(R_{12,\mathbf{X}}^*R_{12,\mathbf{X}})^{1/2} - (R_{12}^*R_{12})^{1/2}||_{\operatorname{HS}(\mathcal{H}_{K^2})} \\ &\leq \sqrt{\dim(\mathcal{H}_{K^2})} \sqrt{||(R_{12,\mathbf{X}}^*R_{12,\mathbf{X}}) - (R_{12}^*R_{12})||_{\operatorname{tr}(\mathcal{H}_{K^2})}}.\end{aligned}$$

By Proposition 4.1, the following set satisfies  $\nu^m(U_3) \ge 1 - \frac{\delta}{3}$ ,

$$U_{3} = \left\{ \mathbf{X} \in (T,\nu)^{m} : ||R_{12,\mathbf{X}}^{*}R_{12,\mathbf{X}} - R_{12}^{*}R_{12}||_{\operatorname{tr}(\mathcal{H}_{K^{2}})} \le 2\kappa_{1}^{2}\kappa_{2}^{2} \left[ \frac{2\log\frac{6}{\delta}}{m} + \sqrt{\frac{2\log\frac{6}{\delta}}{m}} \right] \right\}.$$

Let  $U = U_1 \cap U_2 \cap U_3$ . As in the proof of Theorem 4.5,  $\nu^m(U) \ge 1 - \delta$  and  $\forall \mathbf{X} \in U$ ,

$$\begin{aligned} \left| W_2^2 \left[ \mathcal{N}\left(0, (1/m)K^1[\mathbf{X}]\right), \mathcal{N}\left(0, (1/m)K^2[\mathbf{X}]\right) - W_2^2[\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})] \right] \right| \\ \leq \left(\kappa_1^2 + \kappa_2^2\right) \left[ \frac{2\log\frac{6}{\delta}}{m} + \sqrt{\frac{2\log\frac{6}{\delta}}{m}} \right] + 2\sqrt{2}\kappa_1\kappa_2\sqrt{\dim(\mathcal{H}_{K^2})} \sqrt{\frac{2\log\frac{6}{\delta}}{m} + \sqrt{\frac{2\log\frac{6}{\delta}}{m}}}. \end{aligned}$$

The following is a special case of Corollary 4 in [35], where  $\mu_{\mathbf{X}}$  and  $C_{\mathbf{X}}$  are the sample mean and sample covariance matrix, respectively, based on the sample  $\mathbf{X} = (x_i)_{i=1}^N$ .

Proposition 10.6 (Estimation of 2-Wasserstein distance between Gaussian measures on  $\mathbb{R}^d$ ). Let  $\rho_i = \mathcal{N}(\mu_i, C_i)$  on  $\mathbb{R}^d$ , i = 1, 2. Let  $\mathbf{X} = (x_i)_{i=1}^N$  and  $\mathbf{Y} = (y_j)_{j=1}^N$  be independently sampled from  $(\mathbb{R}^d, \rho_1)$  and  $(\mathbb{R}^d, \rho_2)$ , respectively.  $\forall 0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

(10.6) 
$$|W_{2}[\mathcal{N}(\mu_{\mathbf{X}}, C_{\mathbf{X}}), \mathcal{N}(\mu_{\mathbf{Y}}, C_{\mathbf{Y}})] - W_{2}(\mathcal{N}(\mu_{1}, C_{1}), \mathcal{N}(\mu_{2}, C_{2}))|$$
$$\leq 2(\eta_{1} + \eta_{2})\sqrt{\frac{4}{N\delta^{2}} + \frac{\sqrt{d}}{\sqrt{N}\delta}\left(3 + \frac{4}{\sqrt{N}\delta}\right)},$$

where  $\eta_i = (2||C_i||_{\text{HS}}^2 + 4\langle \mu_i, C_i\mu_i \rangle + (\text{tr}C_i + ||\mu_i||^2)^2)^{1/4}, i = 1, 2.$ 

**Proof of Theorem 6.2.** Apply Proposition 10.6 with d = m,  $\mu_i = 0$ ,  $C_i = \frac{1}{m} K^i[\mathbf{X}]$ , and  $\operatorname{tr}(C_i) = \frac{1}{m} \operatorname{tr}(K^i[\mathbf{X}]) = \frac{1}{m} \sum_{j=1}^m K^i(x_j, x_j) \le \kappa_i^2$ ,  $||C_i||_{\operatorname{HS}}^2 \le [\operatorname{tr}(C_i)]^2 \le \kappa_i^4$ . Thus  $\eta_i = (2||C_i||_{\operatorname{HS}}^2 + [\operatorname{tr}(C_i)]^2)^{1/4} \le 3^{1/4} \kappa_i < \frac{3}{2} \kappa_i$ .

**Proof of Theorem 6.3.** This follows by combining Theorems 6.1 and 6.2, as in Theorem 5.3. Here we make use of the elementary inequality  $|a - b|^2 \le |a^2 - b^2|$  for  $a \ge 0, b \ge 0$ . Lemma 10.7. Under Assumptions 1-4,  $\forall x \in T, \forall f \in \mathcal{L}^2(T, \nu)$ ,

(10.7)  $\mathbb{E}[\xi \otimes \xi] f(x) = \mathbb{E} \int \xi(\omega, x)\xi(\omega, t) f(t)d\nu(t) = \int K(x, t) f(t)d\nu(t).$ 

$$\mathbb{E}[\zeta \otimes \zeta] f(x) = \mathbb{E} \int_{T} \zeta(\omega, x) \zeta(\omega, t) f(t) d\nu(t) = \int_{T} K(x, t) f(t) d\nu(t)$$

$$\mathbb{P}[\zeta \otimes \zeta] f(x) = \mathbb{E} \int_{T} \zeta(\omega, x) \zeta(\omega, t) f(t) d\nu(t) = \int_{T} K(x, t) f(t) d\nu(t)$$

*Proof.* By Hölder Theorem and Tonelli Theorem,  $\forall f \in \mathcal{L}^2(T, \nu), \forall x \in T$ ,

$$\left( \int_{\Omega} \int_{T} |\xi(\omega, x)\xi(\omega, t)f(t)| d\nu(t) dP(\omega) \right)^{2}$$
  
$$\leq \int_{\Omega \times T} \xi(\omega, t)^{2} d\nu(t) dP(\omega) \int_{\Omega \times T} \xi(\omega, x)^{2} f(t)^{2} dP(\omega) d\nu(t)$$
  
$$= ||f||^{2}_{\mathcal{L}^{2}(T,\nu)} K(x, x) \int_{T} K(t, t) d\nu(t) \leq \kappa^{2} ||f||^{2}_{\mathcal{L}^{2}(T,\nu)} K(x, x) < \infty.$$

Thus  $\xi(., x)\xi(., .)f \in \mathcal{L}^1(\Omega \times T, P \times \nu)$ . By Fubini Theorem,

$$\mathbb{E} \int_{T} \xi(\omega, x)\xi(\omega, t)f(t)d\nu(t) = \int_{\Omega} \left( \int_{T} \xi(\omega, x)\xi(\omega, t)f(t)d\nu(t) \right) dP(\omega)$$
$$= \int_{T} \left( \int_{\Omega} \xi(\omega, x)\xi(\omega, t)f(t)dP(\omega) \right) d\nu(t) = \int_{T} K(x, t)f(t)d\nu(t).$$

**Proof of Lemma 7.1.** By definition of  $K_{\mathbf{W}}$ , Lemma 8.1, and Tonelli Theorem,

$$\begin{split} &\mathbb{E}\int_{T} K_{\mathbf{W}}(x,x)d\nu(x) = \int_{T} \mathbb{E}[\xi(\omega,x)^{2}]d\nu(x) = \int_{T} K(x,x)d\nu(x) \le \kappa^{2}, \\ &\int_{T} K_{\mathbf{W}}(x,x)^{2}d\nu(x) = \frac{1}{N^{2}}\int_{T} \left(\sum_{i=1}^{N} \xi(\omega_{i},x)^{2}\right)^{2}d\nu(x) \le \frac{1}{N}\int_{T} \sum_{i=1}^{N} \xi(\omega_{i},x)^{4}d\nu(x), \\ &\mathbb{E}\int_{T} K_{\mathbf{W}}(x,x)^{2}d\nu(x) \le \int_{T} \mathbb{E}[\xi(\omega,x)^{4}]d\nu(x) = 3\int_{T} K(x,x)^{2}d\nu(x) \le 3\kappa^{4}. \end{split}$$

**Proof of Proposition 7.2.** Define random variable  $Y_j : (\Omega, P)^N \to \operatorname{HS}(\mathcal{L}^2(T, \nu))$  by  $Y_j(\mathbf{W}) = \xi(\omega_j, .) \otimes \xi(\omega_j, .)$ , where  $\mathbf{W} = (\omega_1, \ldots, \omega_N)$  is independently sampled from  $\Omega$ . Then the  $Y_j$ 's are IID and  $C_K = \mathbb{E}Y_j$ ,  $C_{K,\mathbf{W}} = \frac{1}{N} \sum_{j=1}^N Y_j(\mathbf{W})$ , and

$$\begin{split} ||Y_j||_{\mathrm{HS}(\mathcal{L}^2(T,\nu))} &= ||\xi(\omega_j,.)||_{\mathcal{L}^2(T,\nu)}^2 = \int_T \xi(\omega_j,t)^2 d\nu(t),\\ \mathbb{E}||Y_j||_{\mathrm{HS}(\mathcal{L}^2(T,\nu))} &= \int_\Omega \int_T \xi(\omega,t)^2 d\nu(t) dP(\omega) = \int_T K(t,t) d\nu(t) \le \kappa^2,\\ \mathbb{E}||Y_j||_{\mathrm{HS}(\mathcal{L}^2(T,\nu))}^2 &= \int_\Omega \left( \int_T \xi(\omega,t)^2 d\nu(t) \right)^2 dP(\omega) = \mathbb{E}||\xi||_{\mathcal{L}^2(T,\nu)}^4\\ &\leq \int_\Omega \int_T \xi(\omega,t)^4 d\nu(t) dP(\omega) = 3 \int_T K(t,t)^2 d\nu(t) \le 3\kappa^4 \text{ by Lemma 8.1.} \end{split}$$

Define the random variable  $\eta : (\Omega, P)^N \to \mathbb{R}$  by  $\eta(\mathbf{W}) = \left\| \frac{1}{N} Y_j(\mathbf{W}) - \mathbb{E} Y_j \right\|_{\mathrm{HS}}^2 = \left\| C_{K,\mathbf{W}} - C_K \right\|_{\mathrm{HS}}^2$ . Since the  $Y_j$ 's are independent, identically distributed,

$$\mathbb{E}\eta^{2} = \mathbb{E}\left\|\frac{1}{N}\sum_{j=1}^{N}Y_{j} - \mathbb{E}Y_{j}\right\|_{\mathrm{HS}}^{2} = \frac{1}{N^{2}}\sum_{j=1}^{N}\mathbb{E}||Y_{j} - EY_{j}||_{\mathrm{HS}}^{2} = \frac{1}{N^{2}}\sum_{j=1}^{N}(\mathbb{E}||Y_{j}||_{\mathrm{HS}}^{2} - ||EY_{j}||_{\mathrm{HS}}^{2}) \le \frac{3\kappa^{4}}{N}.$$

By the Chebyshev inequality, for any t > 0,  $\mathbb{P}(\eta \ge t) \le \frac{\mathbb{E}\eta}{t} \le \frac{\sqrt{\mathbb{E}\eta^2}}{t} \le \frac{\sqrt{3}\kappa^2}{\sqrt{N}t}$ . Let  $\delta = \frac{\sqrt{3}\kappa^2}{\sqrt{N}t} \iff t = \frac{\sqrt{3}\kappa^2}{\sqrt{N}\delta}$ , then  $\mathbb{P}\{\mathbf{W} : ||C_{K,\mathbf{W}} - C_K||_{\mathrm{HS}} = \eta(\mathbf{W}) \le \frac{\sqrt{3}\kappa^2}{\sqrt{N}\delta}\} \ge 1 - \delta$ . Similarly, since  $\mathbb{E}||C_{K,\mathbf{W}}||_{\mathrm{HS}} \le \frac{1}{N} \sum_{j=1}^N \mathbb{E}||Y_j||_F = \kappa^2$ , we have  $\mathbb{P}\{\mathbf{W} : ||C_{K,\mathbf{W}}||_{\mathrm{HS}} \le \frac{\kappa^2}{\delta}\} \ge 1 - \delta$ . Computing the intersection of these two sets, replacing  $\delta$  with  $\frac{\delta}{2}$ , gives us the desired result.

Proof of Theorem 7.3. By Theorem 2.2,

$$\begin{split} \Delta &= \left| \mathbf{S}_{2}^{\epsilon} [\mathcal{N}(0, C_{K^{1}, \mathbf{W}^{1}}), \mathcal{N}(0, C_{K^{2}, \mathbf{W}^{2}})] - \mathbf{S}_{2}^{\epsilon} [\mathcal{N}(0, C_{K^{1}}), \mathcal{N}(0, C_{K^{2}})] \right| \\ &\leq \frac{3}{\epsilon} [||C_{K^{1}, \mathbf{W}^{1}}||_{\mathrm{HS}} + ||C_{K^{1}}||_{\mathrm{HS}} + 2||C_{K^{2}}||_{\mathrm{HS}}]||C_{K^{1}, \mathbf{W}^{1}} - C_{K^{1}}||_{\mathrm{HS}} \\ &+ \frac{3}{\epsilon} [2||C_{K^{1}, \mathbf{W}^{1}}||_{\mathrm{HS}} + ||C_{K^{1}}||_{\mathrm{HS}} + ||C_{K^{2}}||_{\mathrm{HS}}]||C_{K^{2}, \mathbf{W}^{2}} - C_{K^{2}}||_{\mathrm{HS}}. \end{split}$$

For  $0 < \delta < 1$ , by Proposition 7.2, the following sets satisfy  $P_i^N(U_i) \ge 1 - \frac{\delta}{2}, i = 1, 2,$ 

$$U_i = \left\{ \mathbf{W}^i \in (\Omega_i, P_i)^N : ||C_{K^i, \mathbf{W}^i}||_{\mathrm{HS}} \le \frac{4\kappa_i^2}{\delta}, ||C_{K^i, \mathbf{W}^i} - C_{K^i}||_{\mathrm{HS}} \le \frac{4\sqrt{3}\kappa_i^2}{\sqrt{N}\delta} \right\}.$$

Then  $U = (U_1 \times \Omega_2^N) \cap (\Omega_1^N \times U_2)$  satisfies  $(P_1^N \times P_2^N)(U) \ge 1 - \delta$ . For  $(\mathbf{W}^1, \mathbf{W}^2) \in U$ ,

$$\begin{split} \Delta &\leq \frac{3}{\epsilon} \left[ \frac{4\kappa_1^2}{\delta} + \kappa_1^2 + 2\kappa_2^2 \right] \frac{4\sqrt{3}\kappa_1^2}{\sqrt{N}\delta} + \frac{3}{\epsilon} \left[ \frac{8\kappa_1^2}{\delta} + \kappa_1^2 + \kappa_2^2 \right] \frac{4\sqrt{3}\kappa_2^2}{\sqrt{N}\delta} \\ &\leq \frac{12\sqrt{3}}{\epsilon\sqrt{N}\delta} \left( \left( 1 + \frac{4}{\delta} \right) \kappa_1^4 + \left( 3 + \frac{8}{\delta} \right) \kappa_1^2 \kappa^2 + \kappa_2^4 \right). \end{split}$$

**Proof of Theorem 7.4.** This is similar to Theorem 5.3. By Lemma 7.1,  $\forall 0 < \delta < 1$ ,

$$\mathbb{P}\left\{ (\mathbf{W}^{1}, \mathbf{W}^{2}) \in (\Omega_{1}, P_{1})^{N} \times (\Omega_{2}, P_{2})^{N} : \int_{T} K_{\mathbf{W}^{1}}(x, x)^{2} d\nu(x) \leq \frac{24\kappa_{1}^{4}}{\delta}, \\ \int_{T} K_{\mathbf{W}^{2}}(x, x)^{2} d\nu(x) \leq \frac{24\kappa_{2}^{4}}{\delta} \right\} \geq 1 - \frac{\delta}{4}$$

Let  $\Delta_1 = \left| S_2^{\epsilon} [\mathcal{N}(0, C_{K^1, \mathbf{W}^1}), \mathcal{N}(0, C_{K^2, \mathbf{W}^2})] - S_2^{\epsilon} [\mathcal{N}(0, C_{K^1}), \mathcal{N}(0, C_{K^2})] \right|$ . By Theorem 7.3,  $\mathbb{P} \left\{ (\mathbf{W}^1 \ \mathbf{W}^2) \in (\Omega_1 \ P_1)^N \times (\Omega_2 \ P_2)^N \right\}$ 

$$\left\{ (\mathbf{W}^{1}, \mathbf{W}^{2}) \in (\Omega_{1}, P_{1})^{N} \times (\Omega_{2}, P_{2})^{N} : \Delta_{1} \leq \frac{48\sqrt{3}}{\epsilon\delta} \left( \left( 1 + \frac{16}{\delta} \right) \kappa_{1}^{4} + \left( 3 + \frac{32}{\delta} \right) \kappa_{1}^{2} \kappa^{2} + \kappa_{2}^{4} \right) \frac{1}{\sqrt{N}} \right\} \geq 1 - \frac{\delta}{4}.$$

It follows that the following set satisfies  $\mathbb{P}(U_1) \ge 1 - \frac{\delta}{2}$ ,

$$U_{1} = \left\{ (\mathbf{W}^{1}, \mathbf{W}^{2}) \in (\Omega_{1}, P_{1})^{N} \times (\Omega_{2}, P_{2})^{N} : \int_{T} K_{\mathbf{W}^{1}}(x, x)^{2} d\nu(x) \le \frac{24\kappa_{1}^{4}}{\delta}, \\ \int_{T} K_{\mathbf{W}^{2}}(x, x)^{2} d\nu(x) \le \frac{24\kappa_{2}^{4}}{\delta}, \Delta_{1} \le \frac{48\sqrt{3}}{\epsilon\delta} \left( \left( 1 + \frac{16}{\delta} \right) \kappa_{1}^{4} + \left( 3 + \frac{32}{\delta} \right) \kappa_{1}^{2} \kappa^{2} + \kappa_{2}^{4} \right) \frac{1}{\sqrt{N}} \right\}.$$

Let  $\Delta_2 = \left| S_2^{\epsilon}[\mathcal{N}(0, \frac{1}{m} \hat{K}_{\mathbf{W}^1}^1[\mathbf{X}]), \mathcal{N}(0, \frac{1}{m} \hat{K}_{\mathbf{W}^2}^2[\mathbf{X}]) \right| - S_2^{\epsilon}[\mathcal{N}(0, C_{K^1, \mathbf{W}^1}), \mathcal{N}(0, C_{K^2, \mathbf{W}^2})] \right|$ . Theorem 4.7 implies that for  $(\mathbf{W}^1, \mathbf{W}^2) \in U_1$  fixed, the following set satisfies  $\mathbb{P}(U_2) \ge 1 - \frac{\delta}{2}$ ,

$$U_{2} = \left\{ \mathbf{X} \in (T,\nu)^{m} : \Delta_{2} \leq \frac{18}{\epsilon} (((24/\delta)^{1/4}\kappa_{1})^{2} + ((24/\delta)^{1/4}\kappa_{2})^{2})^{2} \left(1 + \frac{12}{\delta}\right) \frac{2}{\sqrt{m}\delta} \\ = \frac{864}{\epsilon\delta} (\kappa_{1}^{2} + \kappa_{2}^{2})^{2} \left(1 + \frac{12}{\delta}\right) \frac{1}{\sqrt{m}} \right\}.$$

Let  $U = (U_1 \times (T, \nu)^m) \cap (((\Omega_1, P_1)^N \times (\Omega_2, P_2)^N) \times U_2)$ , then  $\mathbb{P}(U) \ge 1 - \delta$ .

11. Estimation of Hilbert-Schmidt distance. For completeness, we present the finite sample estimate of  $||C_{K^1} - C_{K^2}||_{\mathrm{HS}(\mathcal{L}^2(T,\nu))}$ . For this, it is *not* necessary to assume that  $C_{K^i}$ , i = 1, 2 are self-adjoint, positive. The only requirement is that  $C_{K^i} \in \mathrm{HS}(\mathcal{L}^2(T,\nu))$ .

**Assumption 7.** Let T be a complete, separable metric space,  $\nu$  a Borel probability measure on T. Let  $K, K^1, K^2: T \to \mathbb{R}$  be pointwise defined. Assume  $\exists \kappa, \kappa_1, \kappa_2 > 0$  such that

(11.1) 
$$\sup_{x,y\in T\times T} |K(x,y)| \le \kappa^2, \ \sup_{(x,y)\in T\times T} |K^i(x,y)| \le \kappa_i^2, \ i=1,2.$$

It is well-known (see e.g. Theorem VI.23 in [44]) that the following operator  $C_K : \mathcal{L}^2(T,\nu) \to \mathcal{L}^2(T,\nu)$  (similarly  $C_{K^i}$ , i = 1, 2) is Hilbert-Schmidt

(11.2) 
$$(C_K f)(x) = \int_T K(x, y) f(y) d\nu(y)$$
, with  $||C_K||^2_{\mathrm{HS}(\mathcal{L}^2(T,\nu))} = \int_{T \times T} K(x, y)^2 d\nu(x) d\nu(y)$ .

Theorem 11.1 (Estimation of Hilbert-Schmidt distance). Under Assumption 7, let  $\mathbf{X} = (x_i)_{i=1}^m$ ,  $\mathbf{Y} = (y_j)_{j=1}^n$  be independently sampled from  $(T, \nu)$ . Let  $K[\mathbf{X}, \mathbf{Y}] \in \mathbb{R}^{m \times n}$  be defined by  $(K[\mathbf{X}, \mathbf{Y}])_{ij} = K(x_i, y_j)$ ,  $1 \le i \le m$ ,  $1 \le j \le n$ .  $\forall 0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

(11.3) 
$$\left| \frac{1}{mn} ||K^{1}[\mathbf{X}, \mathbf{Y}] - K^{2}[\mathbf{X}, \mathbf{Y}]||_{F}^{2} - ||C_{K^{1}} - C_{K^{2}}||_{\mathrm{HS}(\mathcal{L}^{2}(T, \nu))}^{2} \right|$$
$$\leq (\kappa_{1}^{2} + \kappa_{2}^{2})^{2} \left( \frac{2\log\frac{2}{\delta}}{mn} + \sqrt{\frac{2\log\frac{2}{\delta}}{mn}} \right).$$

Lemma 11.2. Under Assumption 7, let  $\mathbf{X} = (x_i)_{i=1}^m$ ,  $\mathbf{Y} = (y_j)_{j=1}^n$  be independently sampled from  $(T, \nu)$ .  $\forall 0 < \delta < 1$ , with probability at least  $1 - \delta$ ,

(11.4) 
$$\left| \frac{1}{mn} ||K[\mathbf{X}, \mathbf{Y}]||_F^2 - ||C_K||_{\mathrm{HS}(\mathcal{L}^2(T, \nu))}^2 \right| \le \kappa^4 \left( \frac{2\log\frac{2}{\delta}}{mn} + \sqrt{\frac{2\log\frac{2}{\delta}}{mn}} \right)$$

*Proof.* Define the random variable  $\eta: (T \times T, \nu \otimes \nu) \to \mathbb{R}$  by  $\eta(x, y) = K(x, y)^2$ . Then

$$||\eta||_{\infty} \leq \kappa^{4}, \quad \mathbb{E}_{x,y}\eta = \int_{T \times T} K(x,y)^{2} d\nu(x) d\nu(y) = ||C_{K}||_{\mathrm{HS}(\mathcal{L}^{2}(T,\nu))}^{2},$$
$$\frac{1}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} \eta(x_{i},y_{j}) = \frac{1}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} K(x_{i},y_{j})^{2} = \frac{1}{mn} ||K[\mathbf{X},\mathbf{Y}]||_{F}^{2}.$$

The desired bound the follows from Proposition 4.4.

**Proof of Theorem 11.1.** We apply Lemma 11.2 to  $K^1 - K^2$ , noting that  $C_{K^1} - C_{K^2} = C_{K^1 - K^2}$  and  $||K^1 - K^2||_{\infty} \le ||K^1||_{\infty} + ||K^2||_{\infty} \le \kappa_1^2 + \kappa_2^2$ .

12. Hilbert-Schmidt operators between two Hilbert spaces. For completeness, we include here several properties of the set of Hilbert-Schmidt operators  $HS(\mathcal{H}_1, \mathcal{H}_2)$  between two separable Hilbert spaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$ . Many standard texts in functional analysis consider the set  $HS(\mathcal{H})$ , with  $\mathcal{H} = \mathcal{H}_1 = \mathcal{H}_2$ . The definition of  $HS(\mathcal{H}_1, \mathcal{H}_2)$  that we use here is from [23]

(12.1) 
$$\operatorname{HS}(\mathcal{H}_1, \mathcal{H}_2) = \{ A \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2) : ||A||_{\operatorname{HS}(\mathcal{H}_1, \mathcal{H}_2)} < \infty \},$$

where the Hilbert-Schmidt norm  $|| ||_{HS(\mathcal{H}_1,\mathcal{H}_2)}$  is defined by

(12.2) 
$$||A||_{\mathrm{HS}(\mathcal{H}_1,\mathcal{H}_2)}^2 = \sum_{k,j=1}^{\infty} \langle Ae_{k,1}, e_{j,2} \rangle_{\mathcal{H}_2}^2 = \sum_{k=1}^{\infty} ||Ae_{k,1}||_{\mathcal{H}_2}^2 = \mathrm{tr}(A^*A)$$

for any orthonormal bases  $\{e_{k,i}\}_{k\in\mathbb{N}}$  of  $\mathcal{H}_i$ , i=1,2, independently of the choice of bases.

Proposition 12.1. Let  $\mathcal{H}_1, \mathcal{H}_2$  be two separable Hilbert spaces. Let  $A, B \in \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ . Then  $A^*B \in \mathrm{Tr}(\mathcal{H}_1)$  and  $||A^*B||_{\mathrm{tr}(\mathcal{H}_1)} \leq ||A||_{\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)} ||B||_{\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)}$ . *Proof.* Consider the polar decomposition  $A^*B = U|A^*B|$  where U is a partial isometry on  $\mathcal{H}_1$ , i.e. an isometry on the closed subspace  $\mathcal{H}_U = \ker(U)^{\perp} = \ker(AB)^{\perp}$ . Let  $\{e_k\}_{k\in\mathbb{N}}$  be an orthonormal basis in  $\mathcal{H}_U$ , then  $\{Ue_k\}_{k\in\mathbb{N}}$  is also an orthonormal basis in  $\mathcal{H}_U$  and

$$tr|A^*B| = tr|A^*B|_{\mathcal{H}_U} = \sum_{k=1}^{\infty} \langle |A^*B|e_k, e_k \rangle_{\mathcal{H}_1} = \sum_{k=1}^{\infty} \langle U|A^*B|e_k, Ue_k \rangle_{\mathcal{H}_1}$$
$$= \sum_{k=1}^{\infty} \langle A^*Be_k, Ue_k \rangle_{\mathcal{H}_1} = \sum_{k=1}^{\infty} \langle Be_k, AUe_k \rangle_{\mathcal{H}_2} \le \sum_{k=1}^{\infty} ||Be_k||_{\mathcal{H}_2} ||AUe_k||_{\mathcal{H}_2}$$
$$\le \left(\sum_{k=1}^{\infty} ||Be_k||_{\mathcal{H}_2}^2\right) \left(\sum_{k=1}^{\infty} ||AUe_k||_{\mathcal{H}_2}^2\right)^{1/2} \le ||B||_{\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)} ||A||_{\mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)}$$

where the last inequality is an equality if  $\ker(AB)^{\perp} = \{0\}$ , i.e.  $\mathcal{H}_U = \mathcal{H}_1$ .

Corollary 12.2. Let  $\mathcal{H}_1, \mathcal{H}_2$  be two separable Hilbert spaces. Let  $A, B \in \mathrm{HS}(\mathcal{H}_1, \mathcal{H}_2)$ . Then  $A^*A, B^*B \in \mathrm{Tr}(\mathcal{H}_1)$  and

(12.3) 
$$||A^*A - B^*B||_{tr(\mathcal{H}_1)} \le (||A||_{HS(\mathcal{H}_1,\mathcal{H}_2)} + ||B||_{HS(\mathcal{H}_1,\mathcal{H}_2)})||A - B||_{HS(\mathcal{H}_1,\mathcal{H}_2)}.$$

Lemma 12.3. Let  $\mathcal{H}_1, \mathcal{H}_2$  be two separable Hilbert spaces. Let  $u_1 \in \mathcal{H}_1, u_2 \in \mathcal{H}_2$ . Then  $u_1 \otimes u_2 \in \mathrm{HS}(\mathcal{H}_2, \mathcal{H}_1)$  and  $||u_1 \otimes u_2||_{\mathrm{HS}(\mathcal{H}_2, \mathcal{H}_1)} = ||u_1||_{\mathcal{H}_1}||u_2||_{\mathcal{H}_2}$ .

*Proof.* Let  $\{e_k\}_{k\in\mathbb{N}}$  be any orthonormal basis in  $\mathcal{H}_2$ . By definition,  $||u_1 \otimes u_2||^2_{\mathrm{HS}(\mathcal{H}_2,\mathcal{H}_1)} = \sum_{k=1}^{\infty} ||u_1 \langle u_2, e_k \rangle_{\mathcal{H}_2}|^2_{\mathcal{H}_1} = ||u_1||^2_{\mathcal{H}_1} \sum_{k=1}^{\infty} |\langle u_2, e_k \rangle_{\mathcal{H}_2}|^2 = ||u_1||^2_{\mathcal{H}_1} ||u_2||^2_{\mathcal{H}_2} < \infty.$ 

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