Metric on Random Dynamical Systems with Vector-valued Reproducing Kernel Hilbert Spaces

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Abstract

Development of metrics for structural data-generating mechanisms is fundamental in machine learning and the related fields. In this paper, we give a general framework to construct metrics on random nonlinear dynamical systems, defined with the Perron-Frobenius operators in vector-valued reproducing kernel Hilbert spaces (vvRKHSs). We employ vvRKHSs to design mathematically manageable metrics and also to introduce operator-valued kernels, which enables us to handle randomness in systems. Our metric provides an extension of the existing metrics for deterministic systems, and gives a specification of the kernel maximal mean discrepancy of random processes. Moreover, by considering the time-wise independence of random processes, we clarify a connection between our metric and the independence criteria with kernels such as Hilbert-Schmidt independence criteria. We empirically illustrate our metric with synthetic data, and evaluate it in the context of the independence test for random processes. We also evaluate the performance with real time series data via clustering tasks.

1 Introduction

Development of a metric for data-generating mechanisms is fundamental in machine learning and the related fields. This is because the development of an algorithm for respective learning problems according to the type of data structures in many cases is basically reduced to the design of an appropriate metric or kernel.

As for the context of dynamical systems, the majority of the existing metrics for dynamical systems have been developed with principal angles between some appropriate subspaces such as column subspaces of observability matrices [13, 4, 18]. Recently, several metrics on dynamical systems are developed with transfer operators such as Koopman operators and Perron-Frobenius operators [12]. Mezic et al. [15, 14] propose metrics of dynamical systems in the context of the ergodic theory via Koopman operators on $L^2$-spaces. Fujii et al. [7] developed metrics with Koopman operators as a generalization of the ones with Binet-Cauchy kernel proposed by Vishwanathan et al. [18]. And, Ishikawa et al. [11] gave metrics on nonlinear dynamical systems with Perron-Frobenius operators in RKHSs, which generalize the classical ones with principal angles mentioned above. However, the above existing metrics are basically defined for deterministic dynamical systems. And, to the best of our knowledge, few existing literature has addressed the design of metrics for random dynamical systems or stochastic processes despite its importance for data analysis. Vishwanathan et al. [18] mentioned their metrics for cases where systems include random noises by taking expectations over the randomness. And, Chwialkowski and Gretton [3] developed non-parametric test statistics for random processes by extending the Hilbert Schmidt independence criteria.

In this paper, we give a framework to construct metrics on random nonlinear dynamical systems, which are defined with the Perron-Frobenius operators in vector-valued reproducing kernel Hilbert spaces (vvRKHSs). Here, we employ vvRKHSs to design mathematically manageable metrics and also to introduce operator-valued kernels, which enable us to handle the randomness in systems. We first define the Perron-Frobenius operators in vvRKHSs and construct a dynamical system in a canonical way. And based on these, we define a metric on random dynamical systems as a positive definite operator-valued kernel. Our metric provides an extension of the existing metrics for deterministic systems to random ones, and gives a specification of the
kernel maximal mean discrepancy of random processes. Moreover, by considering the time-wise independence of random processes, we clarify a connection between our metric and the independence criteria with kernels such as Hilbert-Schmidt independence criteria. We empirically illustrate our metric using synthetic data, and evaluate it in the context of the independence test for random processes.

The remainder of this paper is organized as follows. In Section 2 we first briefly review the notions necessary in this paper such as the Perron-Frobenius operators in RKHSs, and a positive definite kernel on random processes by means of the kernel mean embeddings. In Section 3 we construct a vRKHS to treat random dynamical system, and define the Perron-Frobenius operators on the vRKHSs. Then, in Section 4 we give the definition of our metric for comparing deterministic nonlinear dynamical systems, which generalizes many of the existing metrics for dynamical systems [13, 11, 18].

2 Background

In this section, we briefly review the Perron-Frobenius operators in RKHSs in Subsection 2.1, and we introduce the notion of random dynamical systems in Subsection 2.2. In the end, we describe a way of defining a metric for comparing two random processes with the kernel mean embeddings in Subsection 2.3.

2.1 Perron-Frobenius Operators in RKHSs

Let \(X\) be a state space and \(k\) be a positive definite kernel on \(X\). For any \(a \in X\), we denote by \(k_a\) the function on \(X\) defined by \(k_a(x) = k(a, x)\). By Moore-Aronszajn’s theorem, there exists a unique Hilbert space \(H_k\) composed of functions of \(X\) such that for any \(a \in X\), the function \(k_a\) is contained in \(H_k\) and the reproducing property holds, namely, for any \(f \in H_k\), \(\langle f, k_a \rangle_{H_k} = f(a)\). The Gaussian kernel \(k(x, y) = e^{-\|x-y\|^2}\) for \(x, y \in \mathbb{R}^d\) is a typical example of the positive definite kernel.

Let \(T := \mathbb{Z}, \mathbb{Z}_0^+, \mathbb{R}, \) or \(\mathbb{R}_0^+\). We call a map \(\varphi : T \times X \to X\) a dynamical system if \(\varphi(0, x) = x\) and for any \(s, t \in T\) and \(x \in X\), \(\varphi(s + t, x) = \varphi(s, \varphi(t, x))\).

For \(t \in T\), we define the Perron-Frobenius operator \(K^t_\varphi : H_k \to H_k\) by a linear operator with a dense domain, \(\text{span}\{k_x | x \in X\}\), by

\[
K^t_\varphi k_x := k_{\varphi(t, x)}.
\]

As in the same manner as Proposition 2.1 in [11], \(K^t_\varphi\) is the adjoint operator of the Koopman operator in \(H_k\), which is a linear operator allocating \(g \in H_k\) to \(g(\varphi(t, \cdot))\). Note that, although the contents in [11] are considered only for the discrete time case, i.e., \(T = \mathbb{Z}\) or \(\mathbb{Z}_0^+\), we can consider the general case \(T\). Ishikawa et al. [11] define a positive definite kernel by using the Perron-Frobenius operators \(K^t_\varphi\) for comparing deterministic nonlinear dynamical systems, which generalizes many of the existing metrics for dynamical systems [13, 11, 18].

2.2 Random Dynamical Systems (RDS)

Let \((\Omega, P)\) be a probability space, where \(\Omega\) is a measurable space, and \(P\) is a probability measure. Let \(T := \mathbb{Z}, \mathbb{Z}_0^+, \mathbb{R}, \) or \(\mathbb{R}_0^+\), and \(X\) be a state space. We fix a semi-group of measure preserving measurable maps \(\Theta := \{\theta_t\}_{t \in T}\) on \(\Omega\), namely, \(\theta_s \circ \theta_t = \theta_{s+t}\) for all \(s, t \in T\). Here, \(\theta_0\) is the push-forward measure of \(P\).

**Definition 2.1.** (Random dynamical system) Let \(M \subset X\) be an open subset. A random dynamical system on \(\Omega\) with respect to \(\Theta\) is a measurable map

\[
\Phi : T \times \Omega \times M \to M
\]

such that \(\Phi(0, \omega, x) = x\) and \(\Phi(t + s, \omega, x) = \Phi(t, \theta_s(\omega), \Phi(s, \omega, x))\) for any \(x \in M\).

Random dynamical systems include many kinds of stochastic processes, and typically appear as solutions of stochastic differential equations. In the case where \(\Omega\) is an one point set, a random dynamical system is reduced to a deterministic one.

**Example 2.2.** An auto-regressive (AR) model \("x_{t+1} = Ax_t + v_t"\) is given as a special case of the random dynamical system as follows. Let \(T := \mathbb{Z}, X := \mathbb{R}^d\). Let \(\Omega_0\) be a probability space and \(\nu : \Omega_0 \to X\) be the Gaussian noise \(N(0, \Sigma)\) for some \(\Sigma > 0\). Let \(\Omega := \Omega_0^T\).

We define \(\theta_n : \Omega \to \Omega; (x_n) \mapsto (x_{n+t})_n\). Put \(v_m : \Omega \to \mathbb{R}^d; (x_n) \mapsto v_m\). Then, the function

\[
\Phi(n, \omega, x) := A(x; \cdot(\cdot Ax + v_0(\omega)) + v_1(\omega)) + \ldots + v_{n-1}(\omega)
\]

is a random dynamical system with respect to \(\{\theta_n\}_{n \in T}\).

Therefore, the \(t\)-th sample \(x_t\) determined by the AR model \("x_{t+1} = Ax_t + v_t"\) is given by \(\Phi(t, \cdot, x_0)\).

(reason for putting the following definition) We remark that random dynamical systems induce dynamical systems on random variables as in the following definition, which plays a main role to define Perron-Frobenius operators for RDS.

**Definition 2.3.** Let \(\Phi\) be a random dynamical system in \(M\) with respect to \(\Theta = \{\theta_t\}_{t \in T}\). We define \(\varphi : T \times M(\Omega, M) \to M(\Omega, M)\) by \(\varphi(t, \omega)(x) := \Phi(t, \theta_t(\omega), X(\theta_{-t}(\omega)))\).
2.3 Comparison of Two Random Processes

Here we describe a common method to define a metric for comparing two random processes \[1\]. A random dynamical system \( \Phi \) in \( M \) gives a random processes \( \{ \Phi(t, \cdot, x) \}_{t \in \mathbb{T}} \) for each \( x \in M \), thus, in particular, this method provides us with a metric for random dynamical systems. We give its generalization in Theorem 4.3 in terms of the operator theoretic method.

Let \( X : \Omega \to C^0(\mathbb{T}, \mathcal{X}) \) be a stochastic process with continuous paths (for simplicity, we only consider continuous path in the case of \( \mathbb{T} = \mathbb{R} \) or \( \mathbb{R}_{>0} \)). Let \( \mathcal{L}(X) \) be the law of \( X \), namely, the push-forward measure \( X_\ast P \) on \( C^0(\mathbb{T}, \mathcal{X}) \). The common strategy to define a metric between stochastic processes is to define the metric between the laws of the stochastic processes by the metric of a probability measure, for example, kernel maximal mean discrepancy (KMMMD), Wasserstein distance, and Kullback–Leibler (KL) divergence (cf. \[9\]).

Let \( \kappa \) be a positive definite kernel on \( C^0(\mathbb{T}, \mathcal{X}) \). For a probability measure \( \nu \), we denote by \( \mu_\nu \in \mathcal{H}_k \) the kernel mean embedding of \( \nu \), which is given by \( \int_{\Omega} \kappa_x \, d\nu(x) \in \mathcal{H}_k \). Then for two stochastic processes \( X \) and \( Y \), we can define the metric

\[
\left\langle \mu_{\mathcal{L}(X)}, \mu_{\mathcal{L}(Y)} \right\rangle_{\mathcal{H}_k} = \int_{\Omega} \kappa(\cdot, \omega, Y(\cdot, \eta)) \, dP(\omega) \, dP(\eta).
\]

If a positive definite kernel \( k \) on \( \mathcal{X} \) is given, we naturally define a positive definite kernel for \( g, h \in C^0(\mathbb{T}, \mathcal{X}) \) by \( \kappa_{k, \mu}(g, h) := \int_{\mathbb{T}} k(f(t), g(t)) \, d\mu(t) \). We give a generalization of \( \kappa_{k, \mu} \) in Theorem 4.3 in the case where the kernel \( \kappa = \kappa_{k, \mu} \) for some \( k \) and \( \mu \).

3 Perron-Frobenius operators for random dynamical systems

In this section, we define a Perron-Frobenius operator for random dynamical systems, which is a natural generalization of the operator defined in \([11]\) in Subsection 3.3. vvrRKHSs are employed to introduce operator-valued positive definite kernels, which enables us to incorporate the effects of random variables. These notions are generalizations of the corresponding deterministic case (namely, the case where \( \Omega \) is an one point set). For simplicity, in this section, we assume \( \mathbb{T} = \mathbb{R} \) or \( \mathbb{Z} \).

3.1 A brief review of vector-valued RKHSs

Let \( \mathcal{X} \) be a set and \( V \) be a Hilbert space. We denote by \( B(V) \) the space of bounded linear operators in \( V \). We define a \( B(V) \)-valued positive definite kernel \( k \) as a map \( k : \mathcal{X} \times \mathcal{X} \to B(V) \) satisfying the following two conditions: (1) for any \( x, y \in \mathcal{X} \), \( k(x, y) = k(y, x) \), and (2) for any \( r \in \mathbb{N} \), \( v_1, \ldots, v_r \in V \), and \( x_1, \ldots, x_r \in \mathcal{X} \),

\[
\sum_{i,j=1}^r \langle k(x_i, x_j) v_i, v_j \rangle_V \geq 0.
\]

We note that \( \mathcal{B}(V) \)-valued positive definite kernel \( \kappa \) is equivalent to \( \mathcal{V} \)-valued kernel of positive type in \([2]\). We define a linear map \( k_y : V \to V^X \) by \( (k_y v)(x) = k(y, x) v \) for \( v \in V \). We note that \( \mathcal{V} \)-valued positive definite kernel is the equivalent notion to the positive definite kernel in Section 2.4.

For any \( \mathcal{B}(V) \)-valued positive definite kernel \( k \), it is well known that there uniquely exists a Hilbert space \( \mathcal{H}_k \) in \( V^X \) such that for any \( x \in \mathcal{X} \) and \( v \in V \), \( k_x v \in \mathcal{H}_k \), and for any \( h \in \mathcal{H}_k \), \( \langle h, k_x v \rangle_{\mathcal{H}_k} = \langle h(x), v \rangle_V \) (see Proposition 2.3 in \([2]\)). We call \( \mathcal{H}_k \) the vector-valued reproducing kernel Hilbert space associated with \( k \) or the \( V \)-valued reproducing kernel Hilbert space associated with \( k \).

We note that we can canonically construct RKHSs from the vvrRKHS as in the following proposition:

**Proposition 3.1.** For any \( v \in V \), the kernel \( k_v(x, y) := \langle v, k(x, y) v \rangle_V \) is a \( \mathcal{V} \)-valued positive definite kernel. Moreover, the RKHS \( \mathcal{H}_k \), associated with \( k_v \) is isomorphic to the closed subspace of \( \mathcal{H}_k \) defined by the closure of the span\{\( k_v v : x \in \mathcal{X} \)\}.

3.2 vvrRKHS on random variables

Here, we gives vvrRKHS for random variables by specifying vvrRKHS described above, which plays a central role in the following parts of this paper.

Let \( k \) be a bounded and continuous \( \mathcal{V} \)-valued positive definite kernel on a topological space \( \mathcal{X} \), and let \( (\Omega, P) \) be a probability space with the probability measure \( P \). We denote by \( M(\Omega, \mathcal{X}) \) the space of \( \mathcal{X} \)-valued random variables. Now, we define a vvrRKHS on \( M(\Omega, \mathcal{X}) \) in terms of the given kernel \( k \).

**Definition 3.2.** We define the \( \mathcal{B}(L^2(\Omega)) \)-valued positive definite kernel \( k \) on \( M(\Omega, \mathcal{X}) \) by

\[
(k(X, Y) f)(\omega) := k(X(\omega), Y(\omega)) f(\omega),
\]

where \( X, Y \in M(\Omega, \mathcal{X}) \).

We note that \( k(X, Y) \) induces a bounded linear operator such that \( \|k(X, Y)\| := \sup_{\omega, \xi, \eta} \|k(X(\omega), Y(\omega))\| \). We may define a natural positive definite kernel for random variables as the expectation of \( k(X, Y) \), but, we can mathematically deduce this kernel in our framework: Let \( 1 \in L^2(\Omega) \) be a constant function valued 1. We see that we can construct the positive definite kernel \( k_1(X, Y) := \mathbb{E}(k(X, Y)) \) by Proposition 3.1.
3.3 Perron-Frobenius Operators for RDS

In this subsection, we construct Perron-Frobenius operators for random dynamical systems. Random dynamical systems include random effects in addition to the structure of dynamical systems. To this end, we utilize the vvRKHS in Section 2.2 and construct linear operators on the vvRKHS by means of the dynamical systems defined in Definition 2.3.

First, let $\mathcal{X}$ be a topological space and let $k$ be the $B(L^2(\Omega))$-valued positive definite kernel on $\mathcal{X}$ as in Proposition 2.2. For any subspace $\mathcal{M} \subset \mathcal{X}$, and random dynamical system $\Phi$ in $\mathcal{M}$, we define a closed subspace $\mathcal{H}_{k,\Phi} \subset \mathcal{H}_k$ as the closure of span $\{ k_\mathcal{X}h \mid X = \Phi(t,\cdot,x), x \in \mathcal{M}, t \in T, h \in L^2(\Omega) \}$.

**Definition 3.3** (Perron-Frobenius operators for RDS). For $t \in T$, we define the $t$-th Perron-Frobenius operator for RDS $\Phi$ by the linear operator $K^t_{\Phi} : \mathcal{H}_{k,\Phi} \rightarrow \mathcal{H}_{k,\Phi}$ with the domain span $\{ k_\mathcal{X}h \mid X = \Phi(t,\cdot,x), x \in \mathcal{M}, t \in T, h \in L^2(\Omega) \}$ such that $K^t_{\Phi}k_\mathcal{X}h = k_\mathcal{X}\Phi(t,x)h$, where $\Phi$ is the dynamical system defined in Definition 2.3.

We give some connections between our operators and other existing operators:

**Proposition 3.4.** For any $x \in \mathcal{X}$, we have

$$t^* K^t_{\Phi} f(k_x) = \int_{\Omega} k_{\Phi(t,\omega,x)} dP(\omega).$$

**Connection to Koopman operators on vvRKHS**

Here, we show the relation between existing operators in vvRKHS and our operator. In the case where a dynamical system is deterministic ($\Omega$ is an one-point set), discrete-time ($T = \mathbb{Z}$ or $\mathbb{Z}_{>0}$). Then $K^t_{\Phi}$ is the same one defined in [11]. Let $\mathcal{M} = \mathcal{X}$. In [9], they define the Koopman operator for a discrete-time dynamical system by the linear operator $g \mapsto g \circ f$ for $g \in \mathcal{H}_k$, where we put $f := \varphi(1,\cdot)$. As stated in the following proposition, their operator is given as the adjoint of the Perron-Frobenius operator:

**Proposition 3.5.** We have $(K^t_{\Phi})^* = K^t_{\Phi}$, where $K^t_{\Phi}$ is the Koopman operator defined in [9] (we give a rigorous definition of the Koopman operator in the proof of this proposition).

4 Metrics on Random Dynamical Systems

As in the previous section, we fix a bounded positive definite kernel $k$, and suppose $T$ is $\mathbb{R}$ or $\mathbb{Z}$. In this section, we construct a metric to compare two random dynamical systems. At first, we specify the rigorous definition of the domain where our metric is defined, which we call triples of random dynamical systems with respect to $k$. Then we define the metric on the triples of the random dynamical systems. Our metric is given as a positive definite $V$-kernel for some Hilbert space (we specify $V$ later), namely it is an linear operator on $V$. When we evaluate this metric with a linear functional, for example the trace, it becomes a usual positive definite kernel. Then we see our metric gives a generalization of KMMD for random processes introduced in Section 2.3 and define two metrics which we use in empirical computation in Section 6.

4.1 Definition of our metrics

Let $\nu$ be a Borel measure on $T$, and let $\mathcal{H}_{\text{in}}$ and $\mathcal{H}_{\text{ob}}$ be Hilbert spaces. We define triples of a random dynamical system with respect to $k$ and $\nu$ by $D = (L, \Phi, \mathcal{I})$, where $\Phi$ is a random dynamical system on $\mathcal{M} \subset \mathcal{X}$, and $\mathcal{I} : \mathcal{H}_{\text{in}} \rightarrow \mathcal{H}_{k,\Phi}$ and $L : \mathcal{H}_{k,\Phi} \rightarrow \mathcal{H}_{\text{ob}}$ such that $LK^t_{\Phi} \mathcal{I}$ is a Hilbert-Schmidt operator for $t \in T$, and for any $v \in \mathcal{H}_{\text{in}}$, the function of $t \mapsto \|LK^t_{\Phi} \mathcal{I}||h|_{\mathcal{H}_{\text{in}}} \in L^2(T, \nu)$. We call $\mathcal{I}$ and $L$ an initial value operator and an observable operator, respectively. Intuitively, the operator $L$ corresponds to an observable that gives an output at $\mathcal{H}_{\text{ob}}$, and $\mathcal{I}$ describes an initial condition for data. We denote by

$$\mathcal{F}_k(\mathcal{H}_{\text{in}}, \mathcal{H}_{\text{ob}}; \nu)$$

the set of the triples of random dynamical systems.

Now, we give the definition of our metric on random dynamical systems as follows:

**Definition 4.1** (Metrics for RDS’s). For $i = 1, 2$, we fix a triple $D_i := (L_i, \Phi_i, \mathcal{I}_i) \in \mathcal{F}_k(\mathcal{H}_{\text{in}}, \mathcal{H}_{\text{ob}}; \nu)$. For $m \in \mathbb{N}$, $T \in \mathbb{T}$, we define a Hilbert-Schmidt operator by

$$\mathcal{K}^{(m)}(D_1, D_2) := \bigwedge_{T} \left(L_2 K_{\Phi_2}^t \mathcal{I}_2 \right)^* L_1 K_{\Phi_1}^t \mathcal{I}_1 d\nu(t),$$

and we define

$$\varphi^T(m)(D_1, D_2) := \text{tr} \left(\mathcal{K}^{(m)}(D_1, D_2)\right).$$

Here, $\bigwedge^m$ is the $m$-th exterior product (cf. Appendix B).
Then we have the following theorem:

**Theorem 4.2.** The kernel \( \mathcal{K}_k^{(m)} \) is a \( \mathcal{B}(\bigwedge^m \mathcal{H}_{in}) \)-valued positive definite kernel on \( \mathcal{T}_k(\mathcal{H}_{in}, \mathcal{H}_{ob}, \nu) \) for each \( \nu \).

We note that \( \mathcal{K}_m \) becomes the positive definite kernel introduced in [11] in the special case where random dynamical systems are not random but deterministic.

### 4.2 Estimation of the metric

Here we give estimation formula [(5) and (6)] below for our metric. The proof of these formula is given in Appendix C. We use these formula to carry out the numerical experiment in Section 6. For \( i = 1, 2 \), let \( \Phi_i \) be a random dynamical system in \( \mathcal{M}_i \) and let \( x^1_i, \ldots, x^m_i \in \mathcal{M}_i \). In the case of \( \mathcal{H}_{in} = \mathbb{C}^m, \mathcal{H}_{ob} = \mathcal{H}_k, L_i((a_p)_{p=1}^m) := \sum_{p=1}^m a_p (\phi(x^p_1)) \) (here, \( i \) is defined in (2)), we define

\[
I_{m}^T ((\Phi_1, x_1), (\Phi_2, x_2)) := \mathcal{K}_m((\Phi_1, x_1), (\Phi_2, x_2)),
\]

where \( x_i := (x^1_i, \ldots, x^m_i) \in \mathcal{M}_i^m \). Then, we have the computation formula as follows:

\[
I_{m}^T ((\Phi_1, x_1), (\Phi_2, x_2)) = \int \det (k(\Phi_1(t_p, \omega_p, x^p_1), \Phi_2(t_q, \eta_q, x^q_2)))_{p,q=1, \ldots, m}
\]

where the variable \( (t_1, \ldots, t_m, \omega_1, \ldots, \omega_m, \eta_1, \ldots, \eta_j) \) in the integral runs over \( [0, T]^m \times \Omega^m \times \Omega^m \). In particular, our metric is a generalization of KMMD for an integral type kernel, which is given through the following theorem:

**Theorem 4.3.** Let

\[
\kappa_T(g, h) := \int_0^T k(g(t), h(t)) d\nu(t)
\]

be an integral type kernel on \( C^0(\mathbb{T}, \mathcal{X}) \), then we have

\[
I_1^T ((\Phi_1, x_1), (\Phi_2, x_2)) = \left\langle \mu_{\mathcal{L}}(\phi_1, \ldots, \phi_j), \mu_{\mathcal{L}}(\phi_2, \ldots, \phi_j) \right\rangle_{\mathcal{H}(\mathcal{M})}
\]

where the variable \( (t_1, \ldots, t_m, \omega_1, \ldots, \omega_m, \eta_1, \ldots, \eta_j) \) in the integral runs over \( [0, T]^m \times \Omega^m \times \Omega^m \).

### 5 Connection to Hilbert-Schmidt Independence Criteria

In this section, we argue a relation between our operator-valued positive definite kernel and Hilbert-Schmidt independence criteria (HSIC). We first define a independence criterion for random dynamical systems based on the above contexts, and then give its estimator. Our independence criterion measures a pairwise independence of random dynamical systems. Although our metric is constructed in the context of the dynamical system, it can also be used to extract the information about the independence of two systems. This is a main reason to introduce the vRKHS above.

#### 5.1 A brief review of Hilbert-Schmidt independence criterion

We first briefly review HSIC [10]. Let \( X, Y : \Omega \to \mathcal{X} \) be two random variables. And, let \( k \) be a positive definite kernel on \( \mathcal{X} \). Here, we assume that \( k \) is characteristic, namely, the kernel mean embedding is injective [10]. Also, we define the cross covariance operator \( C_k(X,Y) : \mathcal{H}_k \to \mathcal{H}_k \) by

\[
C_k(X,Y) := \int_0^T (k_X(\omega) - \mu_X) \otimes (k_Y(\omega) - \mu_Y) \ dP(\omega),
\]

where \( \mu_X, \mu_Y \in \mathcal{H}_k \) are the kernel mean embeddings of the laws \( X, P \) of \( X \) and \( Y, P \) of \( Y \), respectively. We regard any element of \( \mathcal{H}_k \otimes \mathcal{H}_k \) as a bounded linear operator on \( \mathcal{H}_k \), namely, for any \( \varphi \otimes \psi \in \mathcal{H}_k \otimes \mathcal{H}_k \), we define \( \varphi \otimes \psi \in \mathcal{B}(\mathcal{H}_k) \) by \( (\varphi \otimes \psi)(x) := \langle \varphi, \psi(x) \rangle_v \). We note that via the identification, \( \mathcal{H}_k \otimes \mathcal{H}_k \) is equal to the space of Hilbert-Schmidt operators, in particular, the cross-covariance operator \( C_k(X,Y) \) is also a Hilbert-Schmidt operator. Straightforward computations show that

\[
C_k(X,Y) = \mu_{[X|Y]} - \mu_X \otimes \mu_Y,
\]

where \( [X|Y] : \Omega \to \mathcal{X} \times \mathcal{X} : \omega \to (X(\omega), Y(\omega)) \). The characteristic property of \( k \) shows that \( C_k(X,Y) = 0 \) if and only if \( X \) and \( Y \) are independent. The HSIC is defined to be\(^{\text{HSIC}} \)

\[
\text{HSIC}_k(X,Y) := \left\| C_k(X,Y) \right\|_{\text{HS}}^2 := \text{tr}(C_k(X,Y)^* C_k(X,Y)),
\]

which is the Hilbert-Schmidt norm of \( C_k(X,Y) \). The value \( \text{HSIC}_k(X,Y) \) can be estimated via the evaluation of kernel functions over samples (see [10] Lemma 1).

#### 5.2 HSIC for random dynamical systems

Let us consider the independence of random dynamical systems in our context. For \( i = 1, 2 \), let \( \Phi_i \) be a
Figure 1: Orbits of rotation dynamics by (a) just multiplying $\alpha = |\alpha|e^{2\pi i\theta}$ with same initial values, (b): multiplying $\alpha$ and perturb it by Gaussian noise with variance $\sigma^2$.

random dynamical system on $X$. We fix $x_1, x_2 \in X$, and let $X := \{X_t\}_{t \in T} = \{\Phi_t(x_1), x_2\}_{t \in T}$, $Y := \{Y_t\}_{t \in T} = \{\Phi_t(x_2), x_1\}_{t \in T}$. We set $\mathcal{H}_\text{in} := L^2(\Omega)$ and $\mathcal{H}_{cb} := \mathcal{H}_k$. We define $\mathcal{H}_k(h) := k_x(h - \int_t h)$. Set $D_t := (\Phi_t, \mathcal{H}_k) \in \mathcal{K}(\mathcal{H}_\text{in}, \mathcal{H}_{cb}, \nu_1)$. We define the independent criteria for random dynamical systems by

$$C_k((\Phi_1, x_1, \nu_1), (\Phi_2, x_2, \nu_2)) := \text{tr} \left( \mathcal{K}_k^1(D_1, D_1, \mathcal{K}_k^1(D_2, D_2)) \right).$$

Then, we have the following relation:

**Theorem 5.1.** We have

$$C_k((\Phi_1, x_1, \nu_1), (\Phi_2, x_2, \nu_2)) = \int_{T} \int_{T} C_k(X_t, Y_t) d\nu_1(s) d\nu_2(t).$$

Next we consider the estimation of $C_k$. Let $\{X_t^{(1)}\}_{t \in T}$, $\{X_t^{(2)}\}_{t \in T}$ and $\{Y_t^{(1)}\}_{t \in T}$, $\{Y_t^{(2)}\}_{t \in T}$ be independent $n$ sample paths for $X$ and $Y$, respectively.

Set $Z := X$ or $Y$, $Z_t^{(p)} := X_t^{(p)}$ or $Y_t^{(p)}$, $D := D_t$, and $\nu := \nu_t$. We define

$$\hat{c}_D^{(n)}(t; x, y) := c(x, y) - \frac{1}{n} \sum_{p=1}^{n} k(x, Z_t^{(p)})$$

$$- \frac{1}{n} \sum_{i=p}^{n} k(Z_t^{(p)}, y) + \frac{1}{n^2} \sum_{i=p}^{n} k(Z_t^{(p)}, Z_t^{(q)}).$$

Let $G_k^{(n)}(t ; p, q) := \left( \hat{c}_D^{(n)}(Z_t^{(p)}, Z_t^{(q)}) \right)_{p,q=1}^{1,n}$ be a matrix of size $n$. By Theorem 5.1 and Theorem 1 in [10], we have an estimator of $C_k((\Phi_1, x_1, \nu_1), (\Phi_2, x_2, \nu_2))$ as

$$\hat{C}_k((\Phi_1, x_1, \nu_1), (\Phi_2, x_2, \nu_2)) := \frac{1}{(n-1)^2 S_1 S_2} \sum_{(s,t) \in S_1 \times S_2} \text{tr} \left( G_k^{(n)}(s) G_k^{(n)}(t) \right),$$

where $S_1$ and $S_2$ are finite samples according to $\nu_1$ and $\nu_2$, respectively.

**6 Empirical Evaluations**

We first empirically illustrate how our metric behaves by using synthetic data from rotation dynamics with noise on the unit disk in the complex plane in Subsection 6.1 and then evaluate it in the context of the independence test for random processes in Subsection 6.2.

In the end, we carry out clustering task with real time series data in Subsection 6.3. The codes for generating the results are included in the supplementary.

**6.1 Illustrative Example of Rotation Dynamics with Noise**

We used synthetic data from the rotation dynamics $R_{|\alpha|}: z \mapsto \alpha z$ for $\alpha \in \mathbb{C}$ with $|\alpha| \leq 1$ with a noise $\epsilon_t$ on the unit disk $\{z \in \mathbb{C}; |z| \leq 1\}$ in the complex plane, where the variance of the noise is $\sigma^2$, i.e. $\epsilon_t \sim N(0, \sigma^2)$ (i.i.d.). We prepared $3 \times 3$ combination of parameters $\alpha = |\alpha|e^{2\pi i\theta}$ with $|\alpha| \in \{1, 0, 0.9, 0.3\}$ and $\theta \in \{1/3, 1/4, 1/6\}$. The graphs in Figure 1 show the deterministic case and 10 independent paths for the case with $\sigma = 0$ from the identical initial condition $z_0$ with $|z_0| = 0.9$, where the lines of different colors show different sample paths. Then, we calculated the normalized variant of our metric defined by

$$L_{\text{m}^T}((\Phi_1, x_1), (\Phi_2, x_2)) = \lim_{\epsilon \to 0} \left[ \frac{1}{2} \sum_{i=1}^{n} \left| L_{\text{m}^T}^{(i)}((\Phi_1, x_1), (\Phi_2, x_2)) + \epsilon \right|^2 \right]$$

(10)

with an empirical approximation of $L_{m}^{(i)}$ defined in [4]. We also define $L_{\text{m}^T}$ by replacing $L_{\text{m}^T}$ with $L_{\text{m}^T}$, whose
empirical estimation is given by [6]. We computed $L_1^T$ and $L_2^T$ here. The graphs in Figure 2 show numerical results for some cases. As can be seen in (b), if the number of samples $N_s$ is rather small compared with the strength of the noise $\epsilon_t$, we observe that $L_1^T$ only captures rough similarity and $L_2^T$ judges all dynamics are different. However, it tend to improved in (c) as the number of samples $N_s$ get larger. Also, $L_2^T$ gives similar results with the deterministic case. As for (d) where the noise level is stronger, $L_2^T$ again seems to judge all dynamics are different.

6.2 Independence between Two Time-series Data

We empirically evaluated the effectiveness of our metric as an independence criterion. For this purpose, we first generated $N_s=20$ pairs of complex valued time-series data with total time $T=20$ by

\[
\begin{align*}
x_{t+1} &= 0.3\exp(-\pi i) x_t (1 - 0.01x_t) + \epsilon_t^X, \\
y_{t+1} &= 0.9\exp(-\pi i) y_t (1 - 0.01y_t) + \epsilon_t^Y,
\end{align*}
\]

where noises are sampled from complex normal distribution: $\epsilon_t^X, \epsilon_t^Y \sim \mathcal{CN}(0, 0.1^2)$. We denote by $X = [x_1, x_2, \ldots, x_{T=20}]$ and $Y = [y_1, y_2, \ldots, y_{T=20}]$ the generated sequences. Then, we created different data pairs as

\[
\begin{align*}
X_\varphi &:= X \cos \varphi + Y \sin \varphi, \\
Y_\varphi &:= -X \sin \varphi + Y \cos \varphi.
\end{align*}
\]

By the definitions, $X_\varphi$ and $Y_\varphi$ are independent for $\varphi = 0$, and correlated for $\varphi \neq 0$. The two subplots in $\varphi = 0$ column in the graphs of the left-hand side in Figure 3 show 10 independently generated samples for $X$ and $Y$, where the lines of different colors show different sample paths. On the other hand, samples of $X_\varphi=0.35$ and $Y_\varphi=0.35$ share the square shapes and seem to be correlated.

And, the graph of the right-hand side in Figure 3 shows the calculated $\hat{C}_k(X_\varphi, Y_\varphi)$ (blue) and $L_m^T(X_\varphi, Y_\varphi)$ (red) with these sample paths. As a baseline, we also calculated the mean value of shift HSICs among $20 \times 20$ paths (green) with head=10 and tail=15 [3]. All values are normalized so that the maximum value is 1.0 and the minimum value is 0.

As one can see, the both graphs for Shift HSIC and $\hat{C}_k(X_\varphi, Y_\varphi)$ are monotone along the independence of the random processes. It is consistent to their ability to measure the independence of the systems. In contrast, the metric $1 - L_1^T$ has a peak between 0.3 and 0.5. It reflects that $L_m^T$ detects not the independence of the random behavior but the difference of the dynamics, which can be seen in Section 6.1 as well.

6.3 Clustering real data

As an experiment using real-world data, we used UCR Archive in 2018 [6]. We show results for TEST data in BME, and StarLightCurves in Figure 4. Each data is composed of $N_c$-class pairs of $N_{\text{paths}}$ paths with time-length $T$. To apply our method and compare it to the existing one, we first take $n_{\text{paths}} < N_{\text{paths}}$ paths from each class and divide it to $n_{\text{pairs}}$ pairs of $n_{\text{sub-paths}}$ paths, and calculate $(N_c \cdot n_{\text{pairs}}) \times (N_c \cdot n_{\text{pairs}})$ distance matrix using Eq. (10), i.e. $1 - L_1^T$. We used $n_{\text{paths}} = 50, n_{\text{pairs}} = 5$, i.e. $n_{\text{sub-paths}} = 10$ in BME.
and StarLightCurves data. We also calculated \((N_c \cdot n_{\text{paths}}) \times (N_c \cdot n_{\text{paths}})\) distance matrix using \(1 - A^T_1\) proposed in [11] and applied tSNE [17]. To reduce the computational costs, we took skipped time series \(X^{\text{skipped}} = [x_1, x_{s+1}, x_{2s+1}, \ldots]\). We used sBME = 1, ad sStarLightCurves = 100.

In the left side of the Figure [1] we suppose the time series data purely comes from deterministic dynamical systems and do not take random effects into account. On the other hand, in the right hand side, we suppose it is generated by random systems. Since our metric includes an averaging process, it could cluster BME data perfectly. However, regarding StarLightCurves data, it seems not to be able to clearly separate two classes (red and green). This would imply the latent dynamics behind the two classes are quite similar.

7 Conclusions

In this paper, we developed a general framework for constructing metrics on random nonlinear dynamical systems with the Perron-Frobenius operators in vvRKHSs. vvRKHSs were employed to design mathematically manageable metrics and also to introduce \(B(L^2(\Omega))\)-valued kernels, which enables us to handle the randomness in systems. Our metric is an extension of the existing metrics for deterministic systems. Also, we generalized the Hilbert-Schmidt independence criteria to time series data. We empirically showed the effectiveness of our metric using examples of rotation dynamics with noise in the unit disk in the complex plane and clustering tasks for real time series data. We also evaluated our metric in the context of the independence test for random processes.

A Proofs

A.1 Proposition 3.4

For any \(X \in M(\Omega, \mathcal{X})\) and \(v \in L^2(\Omega)\), we claim that \(\nu^*(k_Xv)(x) = \int_{\Omega} k_X(\omega)v(\omega)d\mu(\omega)\). In fact, denote by \(\alpha\) the right hand side of this claim, then, by straightforward computations, we have

\[
\langle k_x, \nu^*(k_Xv) \rangle_{\mathcal{H}_k} = \langle k_x, \alpha \rangle_{\mathcal{H}_k}, \tag{15}
\]

which proves the claim. Since \(\langle k_x \rangle = k_x, 1\) for any \(t \in T\) and \(x \in M\), we have \(K^t_{k}(k_x) = k_x, 1\). By combining this with \(\langle 15 \rangle\), we see that \(\nu^*K^t_{k}(k_x) = \int_{\Omega} k_{\Phi(t,\omega,x)}d\mu(\omega)\).

A.2 Proposition 3.5

Set \(v := \varphi(1, \cdot)\). The definition of the Koopman operator \(K_k\) for vvRKHS is given as follows: \(K_k : \mathcal{H}_k \rightarrow \mathcal{H}_k\) is a linear operator with domain \(\mathcal{D}(K_k) := \{h \in \mathcal{H}_k | h \circ f \in \mathcal{H}_k\}\) such that for any \(h \in \mathcal{H}_k\), \(K_k h = h \circ f\). Then we see that \((K_k^r)^* = K_k^*\) since for any \(v \in \mathcal{V}, x \in \mathcal{X}, \) and \(h \in \mathcal{D}(K_f)\),

\[
\langle K^r_k(k_xv, h)_{\mathcal{H}_k} = \langle h(f(x)), v \rangle_{\mathcal{H}_k} = \langle k_xv, K_k h \rangle_{\mathcal{H}_k}.
\]

A.3 Theorem 4.2

We denote by \(L^2(\mathbb{T}, \nu; V)\) the space of \(L^2\)-integrable \(V\)-valued functions with respect to the measure \(\nu\), where \(V\) is any Hilbert space. Let \(Q(t) := i_t K_{\Phi,W} I_i\). Let \(R_{D} : \mathcal{H}_n \rightarrow L^2(\mathbb{T}, \nu; \mathcal{H}_{ob}); v \mapsto [t \mapsto Q(t)\nu] \). Then we see that the adjoint operator of \(R_{D}\) is given by

\[
R_{D}^* h = \int_{\mathbb{T}} Q(t)^* h(t) d\nu(t).
\]

Therefore, we see that \(\mathcal{X}_k^{(1)}(D_1, D_2) = R_{D_2}^* R_{D_1}\).

For general \(m\), let \(R_{D,m} := \wedge^m R_{D_1}\). Then we see that \(\mathcal{X}_k^{(m)}(D_1, D_2) = R_{D_2}^* R_{D_1,m}\). Therefore, we have \(\mathcal{X}_k^{(m)}(D_1, D_2) = \mathcal{X}_k^{(m)}(D_2, D_1)^*\), and for \(D_1, \ldots, D_r \in \mathcal{F}_k(\mathcal{H}_{in}, \mathcal{H}_{ob}, \nu)\), and \(v_1 \cdots v_r \in \wedge^m \mathcal{H}_{in}\),

\[
\sum_{i,j=1}^{r} \langle \mathcal{X}_k^{(m)}(D_1, D) v_i, v_j \rangle_{\wedge^m \mathcal{H}_{in}} = \sum_{i=1}^{r} R_{D_i} v_i \|_{\wedge^m \mathcal{H}_{in}} \geq 0,
\]

namely, \(\mathcal{X}_k^{(m)}\) is a \(B(\wedge^m \mathcal{H}_{in})\)-valued positive definite kernel.

A.4 Theorem 4.3

This theorem follows from the formula \(10\) and the definition of the kernel mean embedding.

A.5 Theorem 5.1

For \(i = 1, 2\), put \(E_i = (\Phi_i, x_i, \nu_i)\). Set \(Q(t) := \nu^* K_{\Phi_i} I_{X_i}\). Then, we see that

\[
C_i(E_1, E_2) = \int_{\mathbb{T}} \int_{\mathbb{T}} \|Q(t)Q_1(s)^*\|_{H^2} d\nu_1(s) d\nu_2(t).
\]

Thus, it suffices to show that \(Q_2(t)Q_1(s)^* = C_k(X_s, Y_t)\). Set \(F = \Phi_1, x = x_i, Q(t) = Q(t)_1, \) and let \(h := h - \int_{\Omega} b(\omega) d\mu(\omega)\). A straight computation shows that

\[
Q(t) h = \int_{\Omega} (k_{\Phi_i(\omega)} - \mu_{Z_i} h(\omega) d\mu(\omega),
\]

where \(Z_i = X_i \) or \(Y_i\). Thus we see that \(Q(t)^* v(\omega) = \langle v, k_{\Phi_i(\omega)} - \mu_{Z_i} \rangle_{\mathcal{H}_k}\). Therefore, we have

\[
Q_2(t)Q_1(s)v = \int_{\Omega} (k_{\Phi_i(\omega)} - \mu_{Z_i}) v(\omega, k_{\Phi_i(\omega)} - \mu_{X_i}) d\mu(\omega),
\]

namely, \(Q_2(t)Q_1(s)^* = C_k(X_s, Y_t)\).
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B Exterior product of Hilbert spaces

Let $H$ be a Hilbert space with inner product $\langle \cdot, \cdot \rangle$. Let $H^\otimes m$ be a $m$-tensor product as an abstract complex linear space. Then for $x_1 \otimes \ldots \otimes x_m, y_1 \otimes \ldots \otimes y_m \in H^\otimes m$,

$$\langle x_1 \otimes \ldots \otimes x_m, y_1 \otimes \ldots \otimes y_m \rangle_{H^\otimes m} := \prod_{i=1}^{m} \langle x_i, y_i \rangle$$

induces an inner product on $H^\otimes m$. We denote by $\otimes^m H$ the completion via the norm induced by the inner product $\langle \cdot, \cdot \rangle_{H^\otimes m}$.

We define a linear operator $\mathcal{E}: \otimes^m H \to \otimes^m H$ by

$$\mathcal{E}(x_1 \otimes x_m) := \sum_{\sigma \in S_m} \text{sgn}(\sigma)x_{\sigma(1)} \otimes \cdots \otimes x_{\sigma(m)},$$

where $S_m$ is the $m$-th symmetric group, and $\text{sgn} : S_m \to \{\pm 1\}$ is the sign homomorphism. We define the $m$-th exterior product of $H$ by

$$\wedge^m H := \mathcal{E}(\otimes^m H).$$

For $x_1, \ldots, x_m \in H$, we also define

$$x_1 \wedge \ldots \wedge x_m := \mathcal{E}(x_1 \otimes \cdots \otimes x_m).$$

The inner product on $\wedge^m H$ is described as

$$\langle x_1 \wedge \cdots \wedge x_m, y_1 \wedge \cdots \wedge y_m \rangle_{\wedge^m H} = \det(\langle x_i, y_j \rangle)_{i,j=1,\ldots,m}.$$

(16)

We note that there exists an isomorphism

$$\bigoplus_{r+s=m} \wedge^r H \otimes \wedge^s H' \cong \wedge^m (H \oplus H'); \sum_{r+s=m} x_r \otimes y_s \mapsto \sum_{r+s=m} x_r \wedge y_s.$$

Let $L : H \to H'$ be a linear operator. Then $L$ induces a linear operator $\otimes^m L : \otimes^m H \to \otimes^m H'$ defined by $\otimes^m L(x_1 \otimes \cdots \otimes x_m) := Lx_1 \otimes \cdots \otimes Lx_m$.

The operator $\otimes^m L$ induces an operator on $\wedge^m H$, namely, $\otimes^m L(\wedge^m H) \subset \wedge^m H'$, and we define

$$\wedge^m L := \otimes^m L|_{\wedge^m H'}.$$

C Proof of (5) and (6)

The proof of (5) and (6) are done in a similar way, so we only give the proof of (5) here. By the proof of Lemma 3.7 in [11] (see also Appendix E of [11]), we see the following formula:

$$T^m_m([\Phi_1, x_1], [\Phi_2, x_2]) = \int_{\mathbb{T}} \langle t^* \kappa_{\Phi_1}^i t \phi(x_1^1) \wedge \cdots \wedge t^* \kappa_{\Phi_2}^\otimes m t \phi(x_1^m),$$

$$t^* \kappa_{\Phi_2}^i t \phi(x_2^1) \wedge \cdots \wedge t^* \kappa_{\Phi_2}^\otimes m t \phi(x_2^m) \rangle_{\wedge^m \mathcal{H}_k}.$$

Thus, by Proposition 3.4 and the definition of the inner product for $\wedge^m \mathcal{H}_k$ (16), we have the formula (5).

D Other experiments in Subsection 6.2

In Subsection 6.2, we only show an experiment for independence criterion with a particular pair of random dynamical series $X$ and $Y$. Here, we show results of experiments using $9 \times 9$ combinations of $X^{(i)}$ and $X^{(j)}$ defined by

$$x_{i+1} = |\alpha^{(i)}| \epsilon_1 \phi^{(i)}x_{i+1} (1 - 0.01x_{i+1}) + \epsilon_i,$$

where $\epsilon_i \sim \mathcal{CN}(0, 0.1^2)$ and each pair of parameters $(|\alpha^{(i)}|, \phi^{(i)})$ is defined by the following table.

| $i$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|-----|---|---|---|---|---|---|---|---|---|
| $|\alpha^{(i)}|$ | 1 | 0.9 | 0.3 | 1 | 0.9 | 0.3 | 1 | 0.9 | 0.3 |
| $\theta^{(i)}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | $\frac{1}{4}$ |

We pick up two parameter indices $i$ and $j$, and sample $110$ independent paths with total time $T = 10$. From these sample paths, we define another pairs of paths

$$X_{\phi}^{(i)} = X^{(i)} \cos \phi + X^{(j)} \sin \phi,$$

$$X_{\phi}^{(j)} = -X^{(i)} \sin \phi + X^{(j)} \cos \phi,$$

and calculate $\text{shiftHSIC}(X_{\phi}^{(i)}, X_{\phi}^{(j)})$, $C_k(X_{\phi}^{(i)}, X_{\phi}^{(j)})$ and $L_1^T(X_{\phi}^{(i)}, X_{\phi}^{(j)})$ with $k$ as the Gaussian kernel. We plot these values in Figure [a] for $\phi \in [0, \pi/4]$ with all combinations of $i, j$. 
Figure 5: Plots of normalized shiftHSIC($X_i^{(i)}, X_j^{(j)}$) (green) $\hat{C}_k(X_i^{(i)}, X_j^{(j)})$ (blue) and $L_1^T (X_i^{(i)}, X_j^{(j)})$ (red) for $\varphi \in [0, \pi/4]$. 