Infinite-dimensional stochastic transforms and reproducing kernel Hilbert space

Palle E. T. Jorgensen¹ · Myung-Sin Song² · James Tian³

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Abstract
By way of concrete presentations, we construct two infinite-dimensional transforms at the crossroads of Gaussian fields and reproducing kernel Hilbert spaces (RKHS), thus leading to a new infinite-dimensional Fourier transform in a general setting of Gaussian processes. Our results serve to unify existing tools from infinite-dimensional analysis.

Keywords Positive-definite kernels · Fourier analysis · Probability · Stochastic processes · Reproducing kernel Hilbert space · Complex function-theory · Interpolation · Signal/image processing · Sampling · Frames · Moments · Machine learning · Embedding problems · Geometry · Information theory · Optimization · Algorithms · Kaczmarz · Karhunen–Loève · Factorizations · Splines · Principal Component Analysis · Dimension reduction · Digital image analysis · Covariance matrix · Gaussian process · Mathematical physics

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Myung-Sin Song
msong@siue.edu

Palle E. T. Jorgensen
palle-jorgensen@uiowa.edu

James Tian
jft@ams.org

¹ Department of Mathematics, The University of Iowa, Iowa City, IA 52242-1419, USA
² Department of Mathematics and Statistics, Southern Illinois University Edwardsville, Edwardsville, IL 62026, USA
³ Mathematical Reviews, 416 4th Street, Ann Arbor, MI 48103-4816, USA
Contents

1 Introduction ............................................. 2
2 A general transform for reproducing kernel Hilbert spaces (RKHS) ................. 3
  2.1 Effective sequences ....................................... 4
  2.2 Stochastic analysis and p.d. kernels ............................................................... 10
  2.3 The isomorphism $T_K : L^2(K) \rightarrow H(K)$ ..................................................... 14
3 An infinite-dimensional Fourier transform for Gaussian processes via kernel analysis ....... 20
  3.1 An Infinite-dimensional Fourier transform ....................................................... 21
References ................................................ 25

1 Introduction

Our present paper is motived by a host of applications of the general theory of kernels, and their corresponding reproducing kernel Hilbert spaces (RKHS). The list of these applications is long, and includes both brand new advances, and classical topics in analysis. And the following areas are included: Statistical inference, achieving separation of features in machine learning designs, PDEs, harmonic analysis, stochastic processes, mathematical physics and more [1, 2, 5]. While the various reproducing kernel Hilbert spaces involved constitute versatile tools, their realization has a drawback. Its definition and realization entails an abstract completion step. To overcome this, in Sect. 2, we present a general transform which applies in the general context of reproducing kernel Hilbert spaces (RKHS) but more concrete presentations. While in special cases, there are transforms which produce “concrete” presentations for a particular RKHS, these transforms tend to be ad hoc. For the benefit of the readers, we provide some example references: the paper [13] deals with sensitivity issues, [22] direct integration algorithms, [14] image processing, [3, 7, 8] pattern recognition and machine learning, [46] statistical properties, and finally [42] on selection of efficient parameterizations. In addition to earlier papers by the co-authors [24, 37], we also include here a partial list of other relevant and current citations; see e.g., the papers mentioned above, [10, 12, 13, 15, 30–32, 35, 36, 41, 44]. Our present general transform will serve to unify special cases which have appeared in the literature. In Sect. 3, we present a new infinite-dimensional Fourier transform in a general framework of Gaussian processes. The latter in turn is motivated by applications to stochastic differential equations (SDE), including generalized Ito calculus formulas. The links between the two main results involving general transforms are related because of a general fact about positive definite kernels (and the corresponding RKHSs): Every positive definite kernel $K$, defined on $D \times D$ where $D$ is a set, is the covariance kernel of a centered Gaussian process indexed by $D$. The latter fact then unifies the two settings.

For background references on kernel theory and Gaussian processes, we refer readers to the following [4, 16, 33, 34], but we caution that the literature is extensive. The book [9] offers a great overview of the subject and its applications. Our main results presented below build on the following earlier papers [23, 26–29] by the co-authors. In addition, there are multiple current and very active research teams which make use of diverse aspects of the kind of kernel methods discussed here. We have been especially motivated by the following recent papers, covering such diverse results as
machine learning, approximations, chaos, noisy data, Markov sampling, and neural nets, all making use of analysis, algorithms, and optimization with kernels and RKHSs, especially the papers [11, 19, 20, 38–40, 45].

2 A general transform for reproducing kernel Hilbert spaces (RKHS)

We present new frame-theoretic tools with view to learning and sampling from large data-sets. A key role in this endeavor is played by our use of infinite-dimensional Kaczmarz algorithms, and an analysis of systems of projections. However a more realistic approach to an analysis of large and non-linear data sets must be adapted to include an analysis of “noise” terms. More precisely, in order to incorporate stochastic tools, one is faced with choices among families of Gaussian processes, and probability spaces, and Karhunen–Loève expansions which will then be adapted to the Hilbert space analysis we introduced above. Please see [23, 24, 26–29] for examples. Such a stochastic path-space analysis is the focus of the section below.

By a probability space, we mean a triple $(\Omega, \mathcal{F}, \mathbb{P})$ where

- $\Omega$: set of sample points,
- $\mathcal{F}$: $\sigma$-algebra of events (subsets of $\Omega$),
- $\mathbb{P}$: a probability measure defined on $\mathcal{F}$.

A random variable

$$K : \Omega \to \mathbb{R} \text{ (C, or a Hilbert space)}$$

(2.1)

is a measurable function defined on $(\Omega, \mathcal{F})$, i.e., we require that for Borel sets $B$ (in $\mathbb{R}$, or $\mathbb{C}$), and cylinder sets (referring to a fixed Hilbert space $\mathcal{H}$) we have $K^{-1}(B) \in \mathcal{F}$ where

$$K^{-1}(B) = \{\omega \in \Omega : K(\omega) \in B\}.$$  

(2.2)

The distribution $\mu_K$ of $K$ is the measure

$$\mu_K := \mathbb{P} \circ K^{-1}.$$  

(2.3)

If $\mu_K$ is Gaussian, we say that $K$ is a Gaussian random variable. A Gaussian process is a system $\{K_x : x \in X\}$ of random variables (refer to $(\Omega, \mathcal{F}, \mathbb{P})$), indexed by some set $X$.

Here we shall restrict to the case of a Gaussian process, and we shall assume

$$\mathbb{E}(K_x) = 0, \quad \forall x \in X;$$  

(2.4)

where

$$\mathbb{E}(\cdot) = \int_\Omega (\cdot) \, d\mathbb{P}$$  

(2.5)

denotes expectation w.r.t. $\mathbb{P}$.
If \( \mu_K \in N(0, 1) \), i.e.,

\[
\mu_K(t) = \frac{1}{\sqrt{2\pi}} e^{-t^2/2}, \quad t \in \mathbb{R},
\]

we say that \( K \) (or \( \mu_K \)) is a standard Gaussian.

### 2.1 Effective sequences

We now turn to a general framework dealing with an approximation-algorithm but couched in the context of projections in Hilbert space. Starting with a sequence \( (P_n) \) of projections, in the premise of Theorem 2.1, we define an associated approximation-algorithm. Our algorithm is in terms of a new system, defined as a sequence of operator products (2.8). And we then present necessary and sufficient conditions for the algorithm to converge. When it does, we say that the system is effective, see (2.7) and (2.9). This general setting and framework are inspired by (but different from) such well known algorithms as Gram–Schmidt, and Kaczmarz, see also [17, 18].

Our first applications of effective sequences, Corollary 2.4, Proposition 2.7, are to stochastic processes. In Theorem 2.5 (Kolmogorov) we recall the correspondence between positive definite kernels on the one hand, and Gaussian processes, Gaussian fields on the other. Our discussion of transforms will then resume in Sects. 2.2 and 2.3 below.

**Theorem 2.1** Let \( \{P_j\}_{j \in \mathbb{N}_0} \) be a sequence of orthogonal projections in a Hilbert space \( \mathcal{H} \). Set

\[
T_n = (1 - P_n)(1 - P_{n-1}) \cdots (1 - P_0), \quad (2.7)
\]

\[
Q_n = P_n(1 - P_{n-1}) \cdots (1 - P_0), \quad (2.8)
\]

where \( Q_0 = P_0 \).

For all \( n \in \mathbb{N} \), we have

\[
\|x\|^2 = \|T_n x\|^2 + \sum_{k=0}^{n} \|Q_k x\|^2, \quad x \in \mathcal{H}.
\]

The combination of (2.7) and (2.9) yields a condition for when the algorithm yields a direct sum representation for the Hilbert space \( \mathcal{H} \). Equation (2.9) expresses this in the form of a resolution of the identity operator for \( \mathcal{H} \) in terms of the generalized Kaczmarz operators \( Q_n \) introduced in 2.8. Equations (2.10) and (2.11) yield equivalent forms of this sum expansion. Hence \( T_n \xrightarrow{s} 0 \) if and only if

\[
I = \sum_{j \in \mathbb{N}_0} Q_j^* Q_j. \tag{2.9}
\]
More precisely, \((2.9)\) means that,
\[
\langle x, y \rangle = \sum_{j \in \mathbb{N}_0} \langle Q_j x, Q_j y \rangle, \quad x, y \in \mathcal{H}.
\] (2.10)

In particular,
\[
\|x\|^2 = \sum_{j \in \mathbb{N}_0} \| Q_j x \|^2, \quad x \in \mathcal{H}.
\] (2.11)

Proof Note that
\[
\|T_n x\|^2 = \| (1 - P_n) (1 - P_{n-1}) \cdots (1 - P_0) x \|^2
= \| (1 - P_{n-1}) \cdots (1 - P_0) x \|^2 - \| P_n (1 - P_{n-1}) \cdots (1 - P_0) x \|^2
= \| T_{n-1} x \|^2 - \| Q_n x \|^2
= \| T_{n-2} x \|^2 - \| Q_{n-1} x \|^2 - \| Q_n x \|^2
\]
\[
\vdots
\]
\[
= \| (1 - P_0) x \|^2 - \| Q_1 x \|^2 - \| Q_{n-1} x \|^2 - \| Q_n x \|^2
= \| x \|^2 - \| Q_0 x \|^2 - \| Q_1 x \|^2 - \| Q_{n-1} x \|^2 - \| Q_n x \|^2.
\]
Therefore
\[
T_n \xrightarrow{\text{S}} 0 \iff \|x\|^2 = \sum_{j \in \mathbb{N}_0} \| Q_j x \|^2.
\]

Remark 2.2 The system of operators \(\{ Q_j \}_{j \in \mathbb{N}_0}\) in Theorem 2.1 has frame-like properties, see \((2.9)\)–\((2.11)\). Specifically, the mapping
\[
\mathcal{H} \ni x \mapsto (Q_j x) \in l^2(\mathbb{N}_0) \otimes \mathcal{H}
\]
plays the role of an analysis operator, and the synthesis operator \(V^*\) is given by
\[
l^2(\mathbb{N}_0) \otimes \mathcal{H} \ni \xi \mapsto \sum_{j \in \mathbb{N}_0} Q_j^* \xi_j.
\]
Note that \(1 = V^* V\), and \((2.11)\) is the generalized Parseval identity.

Lemma 2.3 Let \(\{ Z_n \}_{n \in \mathbb{N}_0}\) be a system of independent identically distributed \(N(0, 1)\)s \(\text{i.i.d } N(0, 1)\) on \(\mathbb{R}\). Let \(\mathcal{H}\) be a Hilbert space, and \(\{ Q_n \}_{n \in \mathbb{N}_0}\) a system of projections as in Theorem 2.1, i.e.,
\[
\sum_{n \in \mathbb{N}_0} \langle Q_n u, Q_n v \rangle_{\mathcal{H}} = \langle u, v \rangle_{\mathcal{H}}, \quad \forall u, v \in \mathcal{H}.
\] (2.12)
Then
\[
W(\cdot) = W(Q, \mathcal{H})(\cdot) := \sum_{n \in \mathbb{N}_0} Q_n Z_n (\cdot) \tag{2.13}
\]
defines an operator valued Gaussian process, and
\[
\mathbb{E} (\langle W(\cdot) u, W(\cdot) v \rangle_{\mathcal{H}}) = \langle u, v \rangle \quad \forall u, v \in \mathcal{H}. \tag{2.14}
\]

**Proof** (Proof sketch) Fix \(u, v \in \mathcal{H}\); then
\[
LHS_{(2.14)} = \sum_{n_0 \times n_0} \sum_{\mathbb{N}_0 	imes \mathbb{N}_0} \langle Q_n u, Q_m v \rangle_{\mathcal{H}} \mathbb{E}(Z_n Z_m) = \delta_{n, m}
\]
\[
= \sum_{n \in \mathbb{N}_0} \langle Q_n u, Q_n v \rangle_{\mathcal{H}}
\]
\[
= \langle u, v \rangle_{\mathcal{H}}. \tag{2.12}
\]

\(\square\)

**Corollary 2.4** Let \(\{Q_n\}_{n \in \mathbb{N}_0}\) be an effective system in \(\mathcal{H}_K\), where \(K : X \times X \rightarrow \mathbb{R}\) is a given p.d. kernel and \(\mathcal{H}_K\) the associated RKHS. Then \(W\) from (2.13) has the property that
\[
K(x, y) = \mathbb{E} \left( \langle W(\cdot) K_x, W(\cdot) K_y \rangle_{\mathcal{H}_K} \right).
\]

We recall the following theorem of Kolmogorov. It states that there is a 1–1 correspondence between p.d. kernels on a set and mean zero Gaussian processes indexed by the set. One direction is easy, and the other is the deep part:

**Theorem 2.5** (Kolmogorov) Let \(X\) be a set. A function \(K : X \times X \rightarrow \mathbb{C}\) is positive definite if and only if there is a Gaussian process \(\{W_x\}_{x \in X}\) realized in \(L^2(\Omega, \mathcal{F}, \mathbb{P})\) with mean zero, such that
\[
K(x, y) = \mathbb{E} \left[ \overline{W_x} W_y \right]. \tag{2.15}
\]

**Note:** This deals with the general framework of Gaussian processes: There are two sets where \(X\) is the indexed set for the Gaussian processes, for the classical case, \(X\) may be a real line. And \(\Omega\) is the probability space, also referred to as the sample space.

Starting with a set \(X\), and a positive definite (p.d) kernel on \(X \times X\), there are then two approaches to fleshing out the desired Gaussian process \(W = W^{(K)}\) indexed by \(X\), centered, and having \(K\) as its covariance kernel. Both are useful, and they serve different purposes.

The first approach is based on an application of the Kolmogorov extension principle; and its validity can be established with the use of the assumed p.d. property for \(K\); we refer to [2, 4, 21, 28].

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The other approach is different, stating with a fixed p.d. kernel $K$ as above, one then proceeds as follows: (i) pass to the corresponding reproducing kernel Hilbert space (RKHS) $H(K)$; (ii) pick an orthonormal basis (ONB) in $H(K)$, and (iii) build the desired Gaussian process $W = W^{(K)}$ from it with an application of a choice of an i.i.d. system of $N(0,1)$ random variables; and (iv) an application of the Central Limit Theorem; see e.g., [9, 16, 27, 40]. In both cases, we make use of the general fact that a centered Gaussian process is determined by its covariance kernel, see e.g., [29]. For the details of this approach, we also refer to Lemma 2.3 above, especially equations (2.13) and (2.14).

Proof We refer to [34] for the fact that very p.d. function $K$ on $X \times X$ can be realized as the covariance kernel of a Gaussian process in some probability space. Conversely, to stress the idea, we include a proof that $K$, as defined in (2.15), is positive definite: Let $\{c_i\}_{i=1}^n \subset \mathbb{C}$ and $\{x_i\}_{i=1}^n \subset X$, then we have

$$\sum_i \sum_j \overline{c_i} c_j K(x_i, x_j) = \mathbb{E} \left[ \left| \sum_i c_i W_{x_i} \right|^2 \right] \geq 0,$$

i.e., $K$ is p.d. \(\Box\)

Let $(X, \mathcal{B}, \nu)$ be a $\sigma$-finite measure space, and let $\mathcal{B}_{fin} = \{E \in \mathcal{B} : \nu(E) < \infty\}$. Below we consider the following kernel $K$ on $\mathcal{B}_{fin} \times \mathcal{B}_{fin}$: Set

$$K(A, B) = \nu(A \cap B), \quad A, B \in \mathcal{B}_{fin}$$

(2.16)

and let $\mathcal{H}_{K(\nu)}$ denote the associated RKHS.

This particular classes of Gaussian processes and RKHSs play an important role in our approach to manifold learning, and to approximation via Monte Carlo simulations and associated Karhunen–Loève expansions. We also note that the resulting stochastic analysis is of interest for the same purpose. It is further outlined in the remaining two subsections below.

Proposition 2.6 (1) $K = K^{(\nu)}$ in (2.16) is positive definite.

(2) $K^{(\nu)}$ is the covariance kernel for the stationary Wiener process $W = W^{(\nu)}$ indexed by $\mathcal{B}_{fin}$, i.e., Gaussian, mean zero, and

$$\mathbb{E}(W_A W_B) = K^{(\nu)}(A, B) = \nu(A \cap B).$$

(2.17)

(3) If $f \in L^2(\nu)$, and $W_f = \int_X f(x) \, dW_x$ denotes the corresponding Wiener integral, then

$$\mathbb{E}\left(\left|W_f\right|^2\right) = \int_X |f|^2 \, d\nu;$$

in particular, if $f = \sum_i \alpha_i \chi_{A_i}$, then

$$\sum_i \sum_j \alpha_i \alpha_j K^{(\nu)}(A_i, A_j) = \int_X \left| \sum_i \alpha_i \chi_{A_i} \right|^2 \, d\nu.$$
The RKHS $\mathcal{H}_K(\nu)$ of the positive definite kernel in (2.16) consists of functions $F$ on $\mathcal{B}_{fin}$ represented by $f \in L^2(\nu)$ via

$$F(A) = F_f(A) = \int_A f \, d\nu, \quad A \in \mathcal{B}_{fin};$$

(2.18)

and

$$\|F_f\|^2_{\mathcal{H}_K(\nu)} = \|f\|^2_{L^2(\nu)} = \int_X |f|^2 \, d\nu.$$ (2.19)

The map specified by

$$\Psi(K^{(\nu)}(\cdot, A)) = \Psi(\nu ((\cdot) \cap A)) = \chi_A, \quad \forall A \in \mathcal{B}_{fin};$$

(2.20)

extends by linearity and by limits to an isometry

$$\Psi : \mathcal{H}(K^{(\nu)}) \rightarrow L^2(\nu).$$ (2.21)

More generally if $F_f \in \mathcal{H}(K^{(\nu)})$ is as in (2.18), then $\Psi(F_f) = f \in L^2(\nu)$.

Proof (1) One checks that

$$\sum_i \sum_j \alpha_i \alpha_j K^{(\nu)}(A_i, A_j) = \int \left| \sum_i \alpha_i 1_{A_i} \right|^2 \, d\nu \geq 0,$$

which holds for all $\{\alpha_i\}_n$ and $\{A_i\}_n$ with $\alpha_i \in \mathbb{R}, A_i \in \mathcal{B}_{fin}$, and for all $n \in \mathbb{N}$. Here we assume that $\alpha_i \in \mathbb{R}$. Note that a real symmetric matrix $T$ is p.d. if and only if $\langle Tx, x \rangle \geq 0$, for all real vectors $x$. (cf N.N. Vakhania, V.I. Tarieladze, S.A. Chobayan, Probability distributions on Banach spaces (1987) [43], Kluwer; the proof of Theorem 1.1, page 128 in Russian original edition).

(2) Follows from Theorem 2.5.

(3) One first verifies that

$$\sum_i \sum_j \alpha_i \alpha_j K^{(\nu)}(A_i, A_j) = \int_X \left| \sum_i \alpha_i \chi_{A_i} \right|^2 \, d\nu.$$

Then use density and standard approximation by simple functions to get the desired conclusion.

(4) Note that every $F \in \mathcal{H}(K^{(\nu)})$ is a $\sigma$-additive signed measure, and $dF \ll d\nu$. Moreover, for $A, B \in \mathcal{B}_{fin}$, one has

$$K^{(\nu)}(A, B) = \int_B 1_A(x) \, d\nu(x) = \mu(B \cap A),$$

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so that
\[
\frac{dK^{(v)}(\cdot, A)}{dv} = 1_A. \tag{2.22}
\]

Now, for all \( B \in \mathcal{B}_{fin} \), we have
\[
F(B) = \int_B \left( \frac{dF}{dv} \right) dv. \tag{2.23}
\]

The function \( F \) on \( \mathcal{B}_{fin} \) is in \( \mathcal{H}(K^{(v)}) \) if and only if the following supremum, on all positions \( \{A_i\}_1^n, A_i \in \mathcal{B}_{fin}, A_i \cap A_j = \emptyset, \) for \( i \neq j, \) is finite with the upper bound depending on \( F \)
\[
\sup \sum \frac{|F(A_i)|^2}{\mu(A_i)} < \infty.
\]

Indeed, from the reproducing property, we get that
\[
F(B) = \langle K(B, \cdot), F \rangle_{\mathcal{H}(K^{(v)})} = \int \frac{dK(B, \cdot)}{dv} \left( \frac{dF}{dv} \right) dv = \int \chi_B \left( \frac{dF}{dv} \right) dv = \int_B \left( \frac{dF}{dv} \right) dv.
\]

Therefore, if \( F_i \in \mathcal{H}(K^{(v)}), i = 1, 2, \) then
\[
\langle F_1, F_2 \rangle_{\mathcal{H}(K^{(v)})} = \int \left( \frac{dF_1}{dv} \right) \left( \frac{dF_2}{dv} \right) dv.
\]

A more detailed discussion of this part of stochastic calculus can be found at various places in the literature; see e.g., [4, 25, 27, 29].

(5) This follows from the fact that (i) \( \Psi \) is isometric by its very definition; (ii) the linear spans, span \( \{ K^{(v)}(\cdot, A) : A \in \mathcal{B}_{fin} \} \), and span \( \{ \chi_A : A \in \mathcal{B}_{fin} \} \) are dense in the respective Hilbert spaces, and (iii) an application of standard approximation by simple functions in \( L^2 \)-spaces.

\begin{proposition}
Let \( \mathcal{B}_{fin} \times \mathcal{B}_{fin} \overset{K}{\rightarrow} \mathbb{R} \) be the p.d. kernel as in (2.16), and \( \mathcal{H}_{K^{(v)}} \) the RKHS of \( K \). Suppose \( \{Q_n\}_{n \in \mathbb{N}_0} \) is an effective system in \( \mathcal{H}_{K^{(v)}} \), and let \( \Psi \) be the isometry specified in (2.20)–(2.21). Then
\[
\{\Psi Q_n\}_{n \in \mathbb{N}_0}
\]
is effective in the closed subspace
\[
\Psi \left( \mathcal{H}_{K^{(v)}} \right) \subset L^2(\Omega, \mathbb{P}).
\]
\end{proposition}
Proof For all $F, G \in \mathcal{H}_{K(v)}$, we have
\[
E[\Psi(F) \Psi(G)] = (F, G)_{\mathcal{H}_{K(v)}} = \sum_{n \in \mathbb{N}_0} (Q_n F, Q_n G)_{\mathcal{H}_{K(v)}} = \sum_{n \in \mathbb{N}_0} E[\Psi(Q_n F) \Psi(Q_n G)].
\]
\[\Box\]

2.2 Stochastic analysis and p.d. kernels

Consider a suitable transform for the more general class of positive definite function $K : S \times S \to \mathbb{R}$ (or $\mathbb{C}$). We can introduce a $\sigma$-algebra on $S$ generated by $\{K(\cdot, t)\}_{t \in S}$ such that $\mu \mapsto \int \mu(ds) K(s, \cdot)$ makes sense, where $\mu$ is a suitable signed measure (i.e., $\mu K \mu < \infty$; see (2.9)); but it is more useful to consider linear functionals $l$ on $\mathcal{H}(K)$.

Definition 2.8 We say that $l \in L^2(K)$ if, there exists $C = C_l < \infty$ such that $|l(G)| \leq C_l \|G\|_{\mathcal{H}(K)}$, for all $G \in \mathcal{H}(K)$. On $L^2(K)$, introduce the Hilbert inner product
\[
lKl := \langle l, l \rangle_{L^2} = l(\text{acting in } s) K(s, t) l(\text{acting in } t).
\]

Definition 2.9 Given $K : S \times S \to \mathbb{R}$ p.d., let $\mathcal{B}(S, K)$ be the cylinder $\sigma$-algebra on $S$ and consider signed measures $\mu$ on $\mathcal{B}(S, K)$. More precisely, $\mathcal{B}(S, K)$ is the weakest $\sigma$-algebra with respect to which $K$ is measurable. Let
\[
\mathfrak{M}_2(K) := \left\{ \mu \mid \mu K \mu := \langle \mu, \mu \rangle_{\mathfrak{M}_2} = \iint \mu(ds) K(s, t) \mu(dt) < \infty \right\}
\]
where $\langle \mu, \mu \rangle_{\mathfrak{M}_2}$ is a Hilbert pre-inner.

The general idea in Definition 2.9 here is to make use of a fixed p.d. kernel $K$ on $S \times S$, and then from this introduce a new pre-Hilbert inner product on signed measures as follows. The construction will be in three steps: (i) we use $K$ to create a metric on $S$, and we then consider the corresponding Borel $\sigma$-algebra; (ii) and we may therefore introduce the real vector space of all the corresponding signed Borel measures $\mu, \nu$ etc. (iii) In our definition of the $K$-pre-Hilbert inner product we make it precise as a pre-Hilbert inner product via the formula $\mu K \nu$ where $K$ now takes the form of an integral kernel.

The basic idea with the approach using linear functionals, $l : \mathcal{H}(K) \to \mathbb{R}$, is to extend from the case of finite atomic measures to a precise completion.
Example 2.10 For \( \{ c_i \}_{i=1}^n \), \( \{ s_i \}_{i=1}^n \) \( c_i \in \mathbb{R} \), let

\[
1 (G) := \sum_i c_i G(s_i), \quad \forall G \in \mathcal{H}(K); \tag{2.24}
\]

which is the case when \( \mu = \sum_i c_i \delta_{s_i} \), with \( \delta_{s_i} \) denoting the Dirac measure. Setting

\[
T_K (\mu) = \sum_i c_i K(s_i, \cdot) \in \mathcal{H}(K),
\]

we then get

\[
1 (G) = \langle T_K (\mu), G \rangle_{\mathcal{H}(K)}, \quad \forall G \in \mathcal{H}(K). \tag{2.25}
\]

Moreover, the following isometric property holds for all finite atomic measures \( \mu \):

\[
\| T_K (\mu) \|_{\mathcal{H}(K)} = \| \mu \|_{\mathcal{M}_2(K)}.
\]

We include some basic facts about \( \mathcal{M}_2(K) \) and \( L_2(K) \).

Theorem 2.11 Suppose the p.d. function \( K : X \times X \rightarrow \mathbb{R} \) has the representation

\[
K(s, t) = \sum_{n \in \mathbb{N}} e_n(s) e_n(t) \tag{2.26}
\]

(pointwise convergence) for some functions \( \{ e_n \}_{n \in \mathbb{N}} \).

1. Then \( \{ e_n \} \subset \mathcal{H}(K) \), and for all \( G \in \mathcal{H}(K) \),

\[
\| G \|_{\mathcal{H}(K)}^2 = \sum_{n \in \mathbb{N}} | \langle G, e_n \rangle_{\mathcal{H}(K)} |^2.
\]

That is, \( \{ e_n \} \) is a Parseval frame in \( \mathcal{H}(K) \).

2. We have

\[
1 \in L_2(K) \iff \sum_{n \in \mathbb{N}} |1(e_n)|^2 < \infty,
\]

i.e., \( 1 \in L_2(K) \iff (1(e_n))_{n \in \mathbb{N}} \in l^2(\mathbb{N}) \).

Proof Part (1). It suffices to check that, for all \( N \), \( \{ c_i \}_{i=1}^N \subset \mathbb{R} \), and all \( \{ x_i \}_{i=1}^N \subset X \), one has

\[
\left| \sum_i c_i e_{n_0}(x_i) \right|^2 \leq \sum_i \sum_j c_i c_j K(x_i, x_j), \quad \forall n_0 \in \mathbb{N}.
\]
Indeed,

\[
0 \leq \left| \sum_i c_i e_{n_0} (x_i) \right|^2 = \sum_i \sum_j c_i c_j e_{n_0} (x_i) e_{n_0} (x_j)
\]

\[
\leq \sum_i \sum_j c_i c_j \sum_{n \in \mathbb{N}} e_n (x_i) e_n (x_j)
\]

\[
= \sum_i \sum_j c_i c_j K (x_i, x_j).
\]

This implies that \(e_{n_0} \in \mathcal{H} (K)\), for all \(n_0 \in \mathbb{N}\). Now, for all \(G = \sum_{\text{finite}} c_i K (\cdot, x_i) \in \mathcal{H} (K)\), it follows that

\[
\sum_{n \in \mathbb{N}} \left| \left\langle G, e_n \right\rangle_{\mathcal{H}(K)} \right|^2 = \|G\|^2_{\mathcal{H}(K)} = \sum c_i c_j K (x_i, x_j),
\]

which extends by density and linearity to all \(G \in \mathcal{H} (K)\).

Part (2). Given (2.26), if \(G \in \mathcal{H} (K)\), then

\[
G (t) = \sum \left\langle G, e_n \right\rangle_{\mathcal{H}(K)} e_n (t),
\]

(norm convergence) and

\[
\|l (G)\|^2 = \left| \sum \left\langle G, e_n \right\rangle_{\mathcal{H}(K)} l (e_n) \right|^2
\]

\[
\leq \sum \left| \left\langle G, e_n \right\rangle_{\mathcal{H}(K)} \right|^2 \sum \|l (e_n)\|^2
\]

\[
\leq C_l \|G\|^2_{\mathcal{H}(K)}
\]

using the Cauchy–Schwarz inequality.

Define \(V : \mathcal{H} (K) \to l^2 (\mathbb{N})\) by

\[
V (G) = \left( \left\langle G, e_n \right\rangle_{\mathcal{H}(K)} \right)_{n \in \mathbb{N}}.
\]

Then \(V\) is isometric by (1). Moreover, the adjoint \(V^* : l^2 (\mathbb{N}) \to \mathcal{H} (K)\) is given by

\[
V^* ((a_n)) (t) = \sum a_n e_n (t) \in \mathcal{H} (K),
\]

so that \(V^* V = I_{\mathcal{H}(K)}\). Note that (2.27) is a canonical representation, but it is not unique unless \((e_n)\) is assumed to be an ONB and not just a Parseval frame.

More details: Suppose \(l\) is a linear functional on \(\mathcal{H} (K)\) and \((l (e_n)) \in l^2\), then

\[
F = F_l = \sum l (e_n) e_n \in \mathcal{H} (K)
\]
is well defined, since \( \{ e_n \} \) is a Parseval frame. We also have

\[
\begin{align*}
l (G) &= \sum \langle G, e_n \rangle \mathcal{H}(K) l (e_n) \\
&= \left\langle \sum l (e_n) e_n, G \right\rangle \mathcal{H}(K) = \langle F_l, G \rangle \mathcal{H}(K),
\end{align*}
\]

which is the desired conclusion, i.e., \( T_K (l) = F_l \) and \( T_K^* (F_l) = l \). \( \square \)

**Example 2.12** Let \( S = [0, 1] \), \( K (s, t) = s \wedge t \). This is a relative kernel, since we specify

\[
\mathcal{H}(K) = \left\{ F : F' \in L^2 (0, 1), F (0) = 0 \right\},
\]

with \( \| F \|^2 \mathcal{H}(K) = \int_0^1 |F' (s)|^2 ds \), and we then get

\[
\begin{align*}
\langle F (\cdot), \cdot \wedge t \rangle \mathcal{H}(K) &= \int_0^1 F' (s) \chi_{[0,t]} (s) ds \\
&= \int_0^t F' (s) ds \\
&= F (t) - F (0) = F (t).
\end{align*}
\]

In this example,

\[
(T_K \mu) (t) = \int \mu (ds) s \wedge t = t - \frac{1}{2} t^2,
\]

\[
\mu K \mu = \| T_K \mu \|^2 \mathcal{H}(K) = \int_0^1 |(T_K \mu)' (t)|^2 dt = \frac{1}{3},
\]

where \( (T_K \mu)' (t) = \mu ([t, 1]) \).

The example below serves to illustrate that the functionals from Definition 2.9 and Theorem 2.11 might in fact be Schwartz distributions.

**Example 2.13** Let \( K (s, t) = \frac{1}{1-st}, s, t \in (-1, 1) \), and let \( \mathcal{H}(K) \) be the corresponding RKHS. The kernel \( K \) is p.d. since

\[
K (s, t) = \sum_0^\infty s^n t^n = \sum_0^\infty e_n (s) e_n (t),
\]

where \( e_n (t) = t^n \), and \( \{ e_n \} \) is an ONB in \( \mathcal{H}(K) \). Now fix \( n > 0 \) and consider the linear functional

\[
l (G) = \langle G, e_n (\cdot) \rangle \mathcal{H}(K).
\]

\( \square \)
Then $|l(\mathcal{G})| \leq \|G\|_{\mathcal{H}(K)} \|e_n\|_{\mathcal{H}(K)} \leq \|G\|_{\mathcal{H}(K)}$, by Schwarz and the fact that $\|e_n\|_{\mathcal{H}(K)} = 1$. It follows that $C_l = 1$.

However, the LHS of (2.28) cannot be realized by a measure on $(-1, 1)$. In fact, the unique solution is given by $l = \frac{1}{n!}\delta_0^{(n)} \in \mathcal{L}_2(K)$, where $\delta_0^{(n)}$ is the Schwartz distribution (not a measure of course): $\delta_0^{(n)}(\varphi) = (-1)^n \varphi^{(n)}(0), \varphi^{(n)} = \left(\frac{d}{dt}\right)^n \varphi$, for all $\varphi \in C_c(-1, 1)$.

In this example, $\delta_0^{(n)} \in \mathcal{L}_2(K)$, but not in $\mathcal{M}_2(K)$. However, it is in the closure of $\mathcal{M}_2(K)$. The plan is therefore to extend from the space of $\mu = \sum_i c_i \delta_{x_i}$ to the more general measures, and (in some examples) to the case of Schwartz distributions.

Moreover, we have

$$\delta_{x_0} = \sum_{n \in \mathbb{N}_0} \frac{x_0^n}{n!} \delta_0^{(n)}, \ |x_0| < 1. \hspace{1cm} (2.29)$$

One may apply $T_K$ to both sides of (2.29), and get

$$\text{LHS}(2.29) = T_K(\delta_{x_0})(t) = \frac{1}{1-x_0 t} = K(x_0, t),$$

$$\text{RHS}(2.29) = \sum_{n \in \mathbb{N}_0} \frac{x_0^n}{n!} \left( T_K(\delta_0^{(n)}) \right)(t) = \sum_{n \in \mathbb{N}_0} \frac{x_0^n}{n!} n! e_n(t) = \sum_{n \in \mathbb{N}_0} x_0^n t^n = K(x_0, t).$$

Note that (2.29) lives in $\mathcal{L}_2(K)$ and so depends on $K$. We will later consider the case $K(s, t) = e^{s t}$.

### 2.3 The isomorphism $T_K : \mathcal{L}_2(K) \rightarrow \mathcal{H}(K)$

**Motivation.** The RKHS $\mathcal{H}(K)$ is defined abstractly whereas $\mathcal{M}_2(K)$ and $\mathcal{L}_2(K)$ are explicit (see Definitions 2.8 and 2.9), and more “natural”. Starting with a p.d. kernel $K$ on $S$, then the goal is to identify Hilbert spaces of measures $\mathcal{M}_2(K)$, or Hilbert spaces of Schwartz distributions, say $\mathcal{L}_2(K)$, which can give a more explicit norm, with a natural isometry $\mathcal{L}_2(K) \xrightarrow{T_K} \mathcal{H}(K)$.

The mapping $T_K$ may be defined for measures $\mu$, viewed as elements in $\mathcal{L}_2(K)$, as the generalized integral operator:

**Definition 2.14** For $\mu \in \mathcal{M}_2(K)$, set

$$(T_K \mu)(t) = \int \mu(ds) K(s, t), \ \mu \in \mathcal{M}_2(K). \hspace{1cm} (2.30)$$

For $l \in \mathcal{L}_2(K)$, by Riesz there exists a unique $F = F_l \in \mathcal{H}(K)$ such that $l(G) = \langle F_l, G \rangle_{\mathcal{H}(K)}$, for all $G \in \mathcal{H}(K)$.
Definition 2.15 For $l \in \mathcal{L}_2(K)$, set

$$T_K(l) = F_l, \text{ and so } T_K^*(F_l) = l. \quad (2.31)$$

Alternatively, one may define

$$F_l := T_K(l) = l \text{ (acting ins) } (K(s, \cdot)) \quad (2.32)$$

by the reproducing property.

Lemma 2.16 Let $K$ be p.d. on $S \times S$ with the cylinder $\sigma$-algebra $\mathcal{B}(S, K)$. Let $\mu$ be a positive measure on $\mathcal{B}(S, K)$ such that $\int K(s, s) \mu(ds) < \infty$, then $L^2(\mu) \hookrightarrow \mathcal{H}(K)$ is a bounded embedding, i.e., $f d\mu \in \mathcal{M}_2(K)$, for all $f \in L^2(\mu)$.

Proof Given $f \in L^2(\mu)$, then

$$\left\| \int f(s) K(s, \cdot) \mu(ds) \right\|_{\mathcal{H}(K)} \leq \int |f(s)| \|K(s, \cdot)\|_{\mathcal{H}(K)} \mu(ds) \leq \left(\text{Schwarz}\right) \|f\|_{L^2(\mu)} \left(\int K(s, s) \mu(ds)\right)^{1/2} = C_{\mu}^{1/2} \|f\|_{L^2(\mu)}.$$ 

Hence, $\int K(s, \cdot) f(s) \mu(ds) = T_K(f d\mu) \in \mathcal{H}(K)$ and

$$\|T_K(f d\mu)\|_{\mathcal{H}(K)}^2 = \iint f(s) K(s, t) f(t) \mu(ds) \mu(dt) = \|f d\mu\|_{\mathcal{M}_2(K)}^2.$$

Lemma 2.17 If $\mu \in \mathcal{M}_2(K)$, then

$$(T_K \mu)(t) = \int \mu(ds) K(s, t)$$

is well defined, and $(T_K \mu)(\cdot) \in \mathcal{H}(K)$. Moreover, $T_K : \mathcal{M}_2(K) \to \mathcal{H}(K)$ is isometric, where

$$\|T_K \mu\|_{\mathcal{H}(K)}^2 = \|\mu\|_{\mathcal{M}_2(K)}^2 = \iint \mu(ds) K(s, t) \mu(dt). \quad (2.33)$$

Proof With the assumption $\mu \in \mathcal{M}_2(K)$, the exchange of $(\cdot, \cdot)_{\mathcal{H}(K)}$ and integral with respect to $\mu$ can be justified. Thus,
\[ \text{LHS}_{(2.33)} = \langle T_K \mu, T_K \mu \rangle_{\mathcal{H}(K)} \]
\[ = \int (T_K \mu)(t) \mu(dt) \]
\[ = \int \int \mu(ds) K(s, t) \mu(dt) \]
\[ = \mu K \mu = \|\mu\|^2_{\mathbb{M}_2(K)} = \text{RHS}_{(2.33)}. \]

\[ \square \]

**Definition 2.18** By a partition \( \{E_i\} \) of \( S \), we mean \( E_i \in \mathcal{B}(S, K) \) of finite measure, \( E_i \cap E_j = \emptyset \) if \( i \neq j \), and \( \cup E_i = S \).

**Lemma 2.19** Let \( \mu \) be a signed measure, then \( \mu \in \mathbb{M}_2(K) \) if and only if
\[ \left\| \sum_{i} \mu(E_i) K(s_i, \cdot) \right\|^2_{\mathcal{H}(K)} = \sup_{\text{all partitions}} \sum_{i} \sum_{j} \mu(E_i) K(s_i, s_j) \mu(E_j) < \infty \]
with \( s_i \in E_i \). In this case, we have the following norm limit
\[ \lim \left\| T_K \mu - \sum_{i} \mu(E_i) K(s_i, \cdot) \right\|_{\mathcal{H}(K)} = 0, \]
where the limit is taken over filters of partitions.

**Proof** For \( \mu \in \mathbb{M}_2(K) \), we must make precise \( \int G(s) \mu(ds) \) as a well defined integral. Again, we take limits over all partitions \( \mathcal{P} \) of \( S \):
\[ \sum_{i} G(s_i) \mu(E_i) = \sum_{i} \mu(E_i) \langle K(s_i, \cdot), G(\cdot) \rangle_{\mathcal{H}(K)} \]
\[ = \left\langle \sum_{i} \mu(E_i) K(s_i, \cdot), G(\cdot) \right\rangle_{\mathcal{H}(K)} \rightarrow \langle T_K \mu, G \rangle_{\mathcal{H}(K)}, \]
and so \( T_K \mu \) is the \( \|\cdot\|_{\mathcal{H}(K)} \)-norm limit of \( \sum \mu(E_i) K(s_i, \cdot) \).

More specifically, given a partition \( P = \{E_i\} \in \mathcal{P}, \) let
\[ T(P) := \sum_{i} \mu(E_i) K(s_i, \cdot) \in \mathcal{H}(K), \]
then we have
\[ \|T(P)\|^2_{\mathcal{H}(K)} = \sum_{i} \sum_{j} \mu(E_i) K(s_i, s_j) \mu(E_j) \]
and \( T(P) \rightarrow T_K(\mu) \), as a filter in partitions.

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In the following two lemmas by a standard application of Fubini’s theorem, one can justify the exchange of the integrals and summations inside and outside the inner product.

\textbf{Lemma 2.20} For all \( G \in \mathcal{H}(K) \) and \( \mu \in \mathcal{M}_2(K) \), we have:

\[
\int G(t) \mu \, (dt) = \langle G, T_K \mu \rangle_{\mathcal{H}(K)}.
\]  

(2.34)

**Proof**

\[
\text{LHS}_{(2.34)} = \int \langle G(\cdot), K(\cdot, t) \rangle_{\mathcal{H}(K)} \mu \, (dt)
\]

\[
= \left\{ G, \int \mu \,(dt) \, K(\cdot, t) \right\}_{\mathcal{H}(K)}
\]

\[
= \langle G, T_K \mu \rangle_{\mathcal{H}(K)}.
\]

We conclude that \( \int G(t) \mu \, (dt) = \langle T_K \mu, G \rangle_{\mathcal{H}(K)} \in \mathbb{R} \). Note that since \( \mu \in \mathcal{M}_2(K) \), we may exchange integral with \( \langle \cdot, \cdot \rangle_{\mathcal{H}(K)} \).

\textbf{Lemma 2.21} Let \((S, \mathcal{B}_{(S,K)}, K)\) be as above, and consider signed measures \( \mu \) on \((S, \mathcal{B}_{(S,K)})\). Then

\[
\mu \in \mathcal{M}_2(K) \iff \left| \int G \, d\mu \right| \leq C_\mu \| G \|_{\mathcal{H}(K)}, \forall G \in \mathcal{H}(K).
\]

**Proof** Given \( \mu \in \mathcal{M}_2(K) \), then

\[
\left| \int G(t) \mu \,(dt) \right| = \left| \int \langle K(\cdot, t), G(\cdot) \rangle_{\mathcal{H}(K)} \mu \,(dt) \right|
\]

\[
\leq \left| \int K(\cdot, t) \mu \,(dt), G \right|_{\mathcal{H}(K)}
\]

\[
= \left| \langle T_K \mu, G \rangle_{\mathcal{H}(K)} \right|
\]

\[
\leq \| T_K \mu \|_{\mathcal{H}(K)} \| G \|_{\mathcal{H}(K)},
\]

and so \( C_\mu = \| T_K \mu \|_{\mathcal{H}(K)} < \infty \).

Conversely, suppose \( \left| \int G \, d\mu \right| \leq C_\mu \| G \|_{\mathcal{H}(K)} \) for all \( G \in \mathcal{H}(K) \). Then there exists a unique \( F \in \mathcal{H}(K) \) such that

\[
\int G \, d\mu = \langle G, F \rangle_{\mathcal{H}(K)}, \forall G \in \mathcal{H}(K).
\]
Now take $G = K (\cdot, t)$, and by the reproducing property, we get

$$\int \mu (ds) K (s, t) = \langle K (\cdot, t), F \rangle_{\mathcal{H}(K)} = F (t),$$

where $T_K \mu = F \in \mathcal{H} (K)$ by Riesz, and $\mu = T_K^* F$. We conclude that $\mu \in \mathcal{M}_2 (K)$.

In summary, the goal is to pass from (1) atomic measures to (2) $\sigma$-finite signed measures, and then to (3) linear functionals on $\mathcal{H} (K)$, continues with respect to the $\| \cdot \|_{\mathcal{H}(K)}$ norm. The respective mappings are specified as follows:

$$T_K : \sum_i c_i \delta_{s_i} \mapsto \sum_i c_i K (s_i, \cdot) \in \mathcal{H} (K); \quad (2.35)$$

$$(T_K \mu) (t) = \int \mu (ds) K (s, \cdot) \in \mathcal{H} (K), \quad \mu \in \mathcal{M}_2 (K); \quad (2.36)$$

$$(T_K l) (t) = l (K (\cdot, t)) \in \mathcal{H} (K), \quad l \in L_2 (K). \quad (2.37)$$

In all cases ($l$ as atomic measures, signed measures, or the general case of linear functionals), the mapping $T_K : L_2 (K) \to \mathcal{H} (K)$ is an isometry, i.e., $\| T_K l \|_{\mathcal{H}(K)} = \| l \|_{L_2 (K)}$. In general, we have

$$T_K (\mathcal{M}_2 (K)) \subseteq T_K (L_2 (K)) = \mathcal{H} (K), \quad (2.38)$$

where $T_K (\mathcal{M}_2 (K))$ is dense in $\mathcal{H} (K)$ in the $\| \cdot \|_{\mathcal{H}(K)}$ norm. In some cases,

$$T_K (\mathcal{M}_2 (K)) = \mathcal{H} (K); \quad (2.39)$$

but not always.

**Remark 2.22** $\mathcal{M}_2 (K)$ and factorizations on $K$ specified by a positive measure $M$ on $X$. Let

$$K (s, t) = \int \psi (s, x) \psi (t, x) M (dx),$$

where $\psi (s, \cdot) \in L^2 (M)$. Let $\mu$ be a signed measure on $S$. Then

$$\mu \in \mathcal{M}_2 (K) \iff T_\mu \psi \in L^2 (M)$$

where $(T_\mu \psi) (x) = \int \mu (ds) \psi (s, x)$. Indeed, using Fubini, one has

$$\iint \mu (ds) K (s, t) \mu (dt) = \int \left( \int \mu (ds) \psi (s, x) \int \mu (dt) \psi (t, x) \right) M (dx)$$

$$= \int \left( (T_\mu \psi) (x) \right)^2 M (dx) = \| T_K (\mu) \|^2_{\mathcal{H}(K)}.$$

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Lemma 2.23 If $K$ is p.d. on $S$ and if the induced metric $d_K (s, t) = \|K_s - K_t\|_{\mathcal{H}(K)}$ is bounded, then $\mathcal{M}_2 (K)$ is complete, and so $T_K (\mathcal{M}_2 (K)) = \mathcal{H} (K)$.

Proof Please see the general discussion in section 2 and Lemma 2.1 in [28] for details. Sketch: With the metric $d_K$, we can complete, and then use Stone-Weierstrass. Indeed, if $l$ is continuous in the $\|\cdot\|_{\mathcal{H}(K)}$ norm, then there exists a signed measure $\mu$ such that $l (G) = \int G (t) \mu (dt)$.

An overview of the relation between $\mathcal{M}_2 (K)$ and $\mathcal{L}_2 (K)$. Let $K : S \times S \to \mathbb{R}$ be a given p.d. kernel on $S$, and consider the RKHS $\mathcal{H} (K)$, as well as the isometry $T_K$ introduced above. We have:

$$T_K (\mathcal{M}_2 (K)) \subseteq T_K (\mathcal{L}_2 (K)) = \mathcal{H} (K)$$

and $T_K (\mathcal{M}_2 (K))$ is dense in $\mathcal{H} (K)$ in the $\|\cdot\|_{\mathcal{H}(K)}$ norm.

We see that $T_K (\mathcal{M}_2 (K))$ may not be closed in $\mathcal{H} (K)$, and so $\mathcal{M}_2 (K)$ may not be complete. However, the $\mathcal{L}_2 (K)$ will be complete since it is a Hilbert space, and $T_K (\mathcal{L}_2 (K)) = \mathcal{H} (K)$. See Lemma 2.24 and Theorem 2.25.

Lemma 2.24 $T_K (\mathcal{L}_2 (K))$ is complete.

Proof Suppose $\{\mu_n\}$ is Cauchy in $\mathcal{L}_2 (K)$, $\|\mu_n - \mu_m\|_{\mathcal{L}_2 (K)} \to 0$, then $F_n = T_K \mu_n$ satisfy $\|F_n - F_m\|_{\mathcal{H}(K)} \to 0$, and so there exists $F \in \mathcal{H} (K)$ such that $\|F_n - F\|_{\mathcal{H}(K)} \to 0$. Define $l (G) := \langle F, G \rangle_{\mathcal{H}(K)}$, for all $G \in \mathcal{H} (K)$. Then, $l \in \mathcal{L}_2 (K)$ and $\|\mu_n - l\|_{\mathcal{L}_2 (K)} \to 0$.

Theorem 2.25 The isometry $T_K$ maps $\mathcal{L}_2 (K)$ onto $\mathcal{H} (K)$.

Proof We shall show that $\ker (T_K^*) = 0$. Suppose $T_K^* (G) = 0$. Then for all $\mu$,

$$0 = \langle \mu, T_K^* G \rangle_{\mathcal{M}_2 (K)} = \langle T_K \mu, G \rangle_{\mathcal{H}(K)}.$$ 

Now take $\mu = \delta_t, t \in S$; then

$$0 = \langle T_K (\delta_t), G \rangle_{\mathcal{H}(K)} = \langle K (\cdot, t), G (\cdot) \rangle_{\mathcal{H}(K)} = G (t).$$

Thus, $G (t) = 0$ for all $t \in S$, and so $G = 0$ in $\mathcal{H} (K)$.

In Sect. 2 above, in the framework of (general) stochastic analysis, we presented a natural isometric transform. A key part of this construction entails an identification of the “right” Hilbert spaces for the purpose. In the next section below, we shall now apply this to a general class of stationary Gaussian processes. Moreover, in this stochastic framework, we then arrive at anew and explicit transform which serves as an infinite-dimensional stochastic analysis-Fourier transform; see Theorem 3.9 and Proposition 3.11.
3 An infinite-dimensional Fourier transform for Gaussian processes via kernel analysis

Our last section below deals with a number of applied transform-results. In more detail, they are infinite-dimensional and stochastic transforms. They are motivated to a large extent by our results (see [23]) on dynamical PCA (DPCA). Moreover, our results below will combine two main themes in our paper, i.e., combining (i) adaptive kernel tricks (positive definite kernels, their Hilbert spaces, and choices of feature spaces) with (ii) a new analysis of corresponding classes of Gaussian processes/fields. This approach also builds on our parallel results on Monte Carlo simulation and use of Karhunen–Loève analysis. These new transforms, and their applications (see especially Corollary 3.5 and the subsequent results in Sect. 3), are motivated directly by DPCA analysis, and they apply directly to design of DPCA algorithms.

In this section we discuss two of the positive definite kernels \( K \) used in [23].

We show that each kernel \( K \) is associated with a certain transform for its reproducing kernel Hilbert space (RKHS) \( \mathcal{H}(K) \). The transform is studied in detail;—it may be viewed as an infinite-dimensional Fourier transform, see Definition 3.3. In detail, this transform \( T \) is defined on an \( L^2 \) path-space \( L^2(\Omega, \mathbb{P}) \) of Brownian motion; and \( T \) is shown to be an isometric isomorphism of \( L^2(\Omega, \mathbb{P}) \) onto the RKHS \( \mathcal{H}(K) \); see Corollary 3.5. For earlier results dealing with the use of RKHSs in PCA, and related areas, see e.g., [6, 9, 33].

Consider the following positive definite (p.d.) kernel on \( \mathbb{R} \times \mathbb{R} \);

\[
K(s, t) := e^{-\frac{1}{2}|s-t|}, \quad s, t \in \mathbb{R}. \tag{3.1}
\]

In order to understand its PCA properties, we consider the top part of the spectrum in sampled versions of (3.1). We show below that \( K \) is the covariance kernel of the complex process \( \{e^{iX_t}\}_{t \in \mathbb{R}} \) where \( \{X_t\}_{t \in \mathbb{R}} \) is the standard Gaussian process.

Let \( X_t \) be the standard Brownian motion indexed by \( t \in \mathbb{R} \); i.e., \( X_0 = 0, X_t \sim N(0, t) \), where \( X_t \) is realized on a probability space \( (\Omega, \mathcal{F}, \mathbb{P}) \), such that, for all \( s, t \in \mathbb{R} \),

\[
\mathbb{E}(X_s X_t) = \begin{cases} 
|s| \wedge |t| & \text{if } s \text{ and } t \text{ have the same sign} \\
0 & \text{if } st \leq 0.
\end{cases} \tag{3.2}
\]

Here \( \mathbb{E}(\cdot) \) denotes the expectation,

\[
\mathbb{E}(\cdots) = \int_{\Omega} (\cdots) \, d\mathbb{P}. \tag{3.3}
\]

Remark 3.1 The process \( \{X_t\}_{t \in \mathbb{R}} \) can be realized in many different but equivalent ways.

Note that

\[
\mathbb{E}\left(|X_s - X_t|^2\right) = |s - t|, \tag{3.4}
\]
so the process $X_t$ has stationary and independent increments. In particular, if $s, t > 0$, then $|s - t| = s + t - 2 s \wedge t$, and

$$s \wedge t = \frac{s + t - |s - t|}{2}. \quad (3.5)$$

**Proposition 3.2** The kernel $K$ from (3.1) is positive definite.

**Proof** Let $\{X_t\}_{t \in \mathbb{R}}$ be the standard Brownian motion and let $e^{iX_t}$ be the corresponding complex process, then by direct calculation,

$$e^{-\frac{1}{2}|t|} = \mathbb{E} \left( e^{iX_t} \right), \quad \forall t \in \mathbb{R}; \quad (3.6)$$

and

$$e^{-\frac{1}{2}|s-t|} = \mathbb{E} \left( e^{iX_s} e^{-iX_t} \right) = \left\langle e^{iX_s}, e^{iX_t} \right\rangle_{L^2(\mathbb{P})}, \quad \forall s, t \in \mathbb{R}. \quad (3.7)$$

The derivation of (3.6) and (3.7) is based on power series expansion of $e^{iX_t}$, and the fact that

$$\mathbb{E} \left( X_t^{2n} \right) = (2n-1)!! |t|^n, \quad \text{and} \quad (3.8)$$

$$\mathbb{E} \left( |X_t - X_s|^{2n} \right) = (2n-1)!! |t-s|^n, \quad (3.9)$$

where

$$(2n-1)!! = (2n-1)(2n-3)\cdots 5 \cdot 3 = \frac{(2n)!}{2^n n!}. \quad (3.10)$$

Now the positive definite property of $K$ follows from (3.7), since the RHS of (3.7) is p.d. In details: for all $\left( c_j \right)_{j=1}^N, c_j \in \mathbb{R}$:

$$\sum_j \sum_k c_j c_k e^{-\frac{1}{2} |t_j-t_k|} = \sum_j \sum_k c_j c_k \mathbb{E} \left( e^{iX_{t_j}} e^{-iX_{t_k}} \right) = \mathbb{E} \left( \left| \sum_j c_j e^{iX_{t_j}} \right|^2 \right) \geq 0. \quad \Box$$

### 3.1 An Infinite-dimensional Fourier transform

**Definition 3.3** Let $\mathcal{H}(K)$ be the RKHS from the kernel $K$ in (3.1); and define the following transform $T : L^2(\mathbb{P}) \longrightarrow \mathcal{H}(K)$,

$$T(F)(t) := \mathbb{E} \left( e^{-iX_t} F \right) = \int_{\Omega} e^{-iX_t(\omega)} F(\omega) \, d\mathbb{P}(\omega) \quad (3.11)$$
for all \( F \in L^2(\mathbb{P}) \). Here, \( \{X_t\} \) is the Brownian motion.

Our new Fourier transforms have properties in common with its classical counterparts. It is isometric between the respective Hilbert spaces but the Hilbert spaces are different in the infinite dimensional framework.

It is known that the standard Brownian motion, indexed by \( \mathbb{R} \), has a continuous realization (see e.g., [16], page 46, Theorem 2.1.) Hence the transform \( \mathcal{T} \) defined by (3.11) maps \( L^2(\Omega, \mathbb{P}) \) into the bounded continuous functions on \( \mathbb{R} \). Corollary 3.5, below, is the stronger assertion that \( \mathcal{T} \) maps \( L^2(\Omega, \mathbb{P}) \) isometrically onto the RKHS \( \mathcal{H}(K) \) where \( K \) is the kernel in (3.1).

Set

\[
K_t (\cdot) = e^{-\frac{1}{2}|t-\cdot|} \in \mathcal{H}(K),
\]

then by the reproducing property in \( \mathcal{H}(K) \), we have

\[
\langle K_t, \psi \rangle_{\mathcal{H}(K)} = \psi (t), \quad \forall \psi \in \mathcal{H}(K).
\]

**Lemma 3.4** Let \( \mathcal{T} \) be the generalized Fourier transform in (3.11), and \( \mathcal{T}^* \) be the adjoint operator; see the diagram below.

\[
\begin{align*}
L^2(\mathbb{P}) & \xrightarrow{\mathcal{T}} \mathcal{H}(K) \\
\mathcal{H}(K) & \xleftarrow{\mathcal{T}^*}
\end{align*}
\]

Then, we have

\[
\mathcal{T} (e^{iX_t}) = K_t, \quad \text{and}
\]

\[
\mathcal{T}^* (K_t) = e^{iX_t}.
\]

**Proof** Recall the definition \( \mathcal{T} (F) (s) := \mathbb{E} (e^{-iX_s} F) \).

**Proof of (3.15).** Setting \( F = e^{iX_t} \), then

\[
\mathcal{T} (e^{iX_t}) (s) = \mathbb{E} (e^{-iX_s} e^{iX_t}) = \mathbb{E} (e^{i(X_t-X_s)}) = e^{-\frac{1}{2}|t-s|} = K_t (s).
\]

**Proof of (3.16).** Let \( F \in L^2(\mathbb{P}) \), then

\[
\langle \mathcal{T}^* (K_t), F \rangle_{L^2(\mathbb{P})} = \langle K_t, \mathcal{T} (F) \rangle_{\mathcal{H}(K)} = \mathcal{T} (F) (t) = \mathbb{E} (e^{-iX_t} F) = \left\langle e^{iX_t}, F \right\rangle_{L^2(\mathbb{P})}.
\]

\[ \square \]
Corollary 3.5 The generalized Fourier transform in (3.14) is an isometric isomorphism from $L^2(\mathbb{P})$ onto $\mathcal{H}(K)$, with $T(e^{iX_t}) = K_t$, see (3.15). Here, $\mathcal{H}(K)$ is a Hilbert space that allows generalized spectral decompositions.

Proof This is a direct application of (3.15) and (3.16). Also note that span $\{e^{iX_t}\}$ is dense in $L^2(\mathbb{P})$, and span $\{K_t\}$ is dense in $\mathcal{H}(K)$. For the density of span $\{e^{iX_t}\}$, see e.g., [21], Lemma 2.7. \qed

Conclusion 3.6 $\mathcal{H}(K)$ is naturally isometrically isomorphic to $L^2(\mathbb{P})$.

Remark 3.7 To understand this isometric isomorphism $L^2(\mathbb{P}) \xrightarrow{\sim} \mathcal{H}(K)$, we must treat $L^2(\mathbb{P})$ as a complex Hilbert space, while $\mathcal{H}(K)$ is defined as a real Hilbert space; i.e., the generating functions $e^{iX_t} \in L^2(\mathbb{P})$ are complex, where the inner product in $L^2(\mathbb{P})$ is $\langle u, v \rangle_{L^2(\mathbb{P})} = \int_{\Omega} uv d\mathbb{P}$; but the functions $K_t, t \in \mathbb{R}$, in $\mathcal{H}(K)$ are real valued.

Remark 3.8 Assume the normalization $X_0 = 0$, and $0 < s < t$. The two processes $X_t-s$, and $X_t - X_s$ are different, but they have the same distribution $N(0, t-s)$. Indeed, we have

\[
\mathbb{E}\left(e^{iX_t} e^{-iX_s}\right) = \mathbb{E}\left(e^{i(X_t-X_s)}\right) = \sum_{n=0}^{\infty} \frac{i^n}{n!} \mathbb{E}\left((X_t - X_s)^n\right) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \mathbb{E}\left((X_t - X_s)^{2n}\right) \quad \text{(since the odd terms cancel)}
\]

by (3.8)

= \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} (2n - 1)!! (t-s)^n

by (3.9)

\[
= \frac{1}{n!} \sum_{n=0}^{\infty} \left(-\frac{1}{2}(t-s)\right)^n \leq \frac{1}{n!} \sum_{n=0}^{\infty} \frac{1}{n} \left(-\frac{1}{2}(t-s)\right)^n = e^{-\frac{1}{2}(t-s)} = \mathbb{E}\left(e^{iX_t-s}\right).
\]

Theorem 3.9 For the Gaussian kernel $K_{\text{Gauss}}(x, y) = e^{\frac{x^2+y^2}{2t}}$, we have

\[
e^{-x^2/2t} = \mathbb{E}\left(e^{ixX_1/\sqrt{t}}\right), \quad \text{and} \quad (3.17)
\]

\[
e^{-(x-y)^2/2t} = \mathbb{E}\left(e^{ixX_1/\sqrt{t}} e^{-iyX_1/\sqrt{t}}\right) = \left\langle e^{ixX_1/\sqrt{t}}, e^{iyX_1/\sqrt{t}} \right\rangle_{L^2(\mathbb{P})}. \quad (3.18)
\]
**Proof** A direct calculation yields

\[
\mathbb{E}\left(e^{ix X_{1/t}}\right) = \sum_{n=0}^{\infty} \frac{(ix)^n}{n!} \mathbb{E}\left(X^n_{1/t}\right)
\]

\[
= \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n}}{(2n)!} \frac{1}{t^n}
\]

\[
= \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n}}{2^n n!} \frac{1}{t^n}
\]

\[
= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{x^2}{2t}\right)^n = e^{-x^2/2t},
\]

which is (3.17); and (3.18) follows from this. \(\square\)

**Lemma 3.10** Assume \(0 < s < t\). If \(F \in L^2(\Omega, B_s, P)\), where \(B_s = \sigma\)-algebra generated by \(\{X_u ; u \leq s\}\), then

\[
T(F)(t) = e^{-\frac{t-s}{2}} T(F)(s).
\] (3.19)

**Proof**

\[
\text{LHS}_{(3.19)} = \mathbb{E}\left(e^{-i X_s} F\right) = \mathbb{E}\left(e^{-i(X_t-X_s)} e^{-i X_s} F\right)
\]

the independence of increment \(= \mathbb{E}\left(e^{-i(X_t-X_s)}\right) \mathbb{E}\left(e^{-i X_s} F\right) = e^{-\frac{t-s}{2}} T(F)(s) = \text{RHS}_{(3.19)}.
\]

\(\square\)

**Proposition 3.11** Let \(0 < s < t\), and let \(H_n(\cdot), n \in \mathbb{N}_0\), be the Hermite polynomials; then

\[
T(X^n_s)(t) = i^n e^{-\frac{t-s}{2}} s^n H_n(\sqrt{s}).
\] (3.20)

**Proof** By Lemma 3.10, we have

\[
T\left(X^n_s\right)(t) = e^{-\frac{t-s}{2}} T\left(X^n_s\right)(s)
\]

\[
= e^{-\frac{t-s}{2}} \mathbb{E}\left(e^{-i X_s} X^n_s\right)
\]

\[
= e^{-\frac{t-s}{2}} i^n \left(\frac{d}{d\lambda}\right)^n |_{\lambda=1} \mathbb{E}\left(e^{-i\lambda X_s}\right)
\]
\[ = e^{-\frac{t-s}{2}} i^n \left( \frac{d}{d\lambda} \right)^n |_{\lambda=1} \left( e^{-\frac{\lambda^2 s}{2}} \right) \]
\[ = i^n e^{-\frac{t-s}{2}} e^{-\frac{s}{2}} H_n \left( \sqrt{s} \right) \]
\[ = i^n e^{-\frac{s}{2}} s^n H_n \left( \sqrt{s} \right) \]

which is the RHS in (3.20). In the calculation above, we have used the following version of the Hermite polynomials \( H_n (\cdot) \), the probabilist’s variant; defined by

\[ \left( \frac{d}{d\xi} \right)^n e^{-\frac{\xi^2}{2}} = H_n (\xi) e^{-\frac{\xi^2}{2}} \]

with the substitution \( \xi = \sqrt{s} \lambda \) for \( s > 0 \) fixed, and \( \lambda \to 1 \Leftrightarrow \xi \to \sqrt{s} \).

Note, the third “=” follows from standard calculation for the generating functions of Gaussian random variables (see e.g., [16]):

\[ i^n \left( \frac{d}{d\lambda} \right)^n E \left( e^{-i\lambda X_s} \right) = E \left( (-i)^n X_s^n e^{-i\lambda X_s} \right) \]

\[ \Leftrightarrow \]

\[ i^n \left( \frac{d}{d\lambda} \right)^n E \left( e^{-i\lambda X_s} \right) = E \left( X_s^n e^{-i\lambda X_s} \right) \]

and so

\[ i^n \left( \frac{d}{d\lambda} \right)^n |_{\lambda=1} E \left( e^{-i\lambda X_s} \right) = E \left( X_s^n e^{-iX_s} \right) . \]

\[ \square \]

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