Canonical Correlation for Stochastic Processes†

by
R. L. Eubank\textsuperscript{a}, and Tailen Hsing\textsuperscript{b,*}

\textsuperscript{a}Department of Mathematics and Statistics, Arizona State University, Tempe, AZ 85287-1804

\textsuperscript{b}Department of Statistics, University of Michigan, Ann Arbor, MI, 48109

Abstract

A general notion of canonical correlation is developed that extends the classical multivariate concept to include function-valued random elements $X$ and $Y$. The approach is based on the polar representation of a particular linear operator defined on reproducing kernel Hilbert spaces corresponding to the random functions $X$ and $Y$. In this context, canonical correlations and variables are limits of finite-dimensional subproblems thereby providing a seamless transition between Hotelling's original development and infinite-dimensional settings. Several infinite dimensional treatments of canonical correlations that have been proposed for specific problems are shown to be special cases of this general formulation. We also examine our notion of canonical correlation from a large sample perspective and show that the asymptotic behavior of estimators can be tied to that of estimators from standard, finite-dimensional, multivariate analysis.

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* E-mail address: thsing@umich.edu

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1. Introduction

Canonical correlation analysis (Hotelling [17]) is one of the principal tools of multivariate statistics for studying the relationship between a pair of vector random variables. Extensions of this notion to areas such as time series (cf. Tsay and Tiao [33], Tiao and Tsay [32], Jewell and Bloomfield [19]) and functional data analysis (cf. Ramsay and Silverman [27,28] and He, Müller and Wang [13,14] have demonstrated the utility of conceptual expansions that allow for random vectors of infinite length or, more generally, random functions corresponding to indexed collections of random variables. In this paper we develop a broad, unifying framework for canonical correlation analysis that allows for both finite dimensional and function-valued random elements.

Throughout this paper the (univariate) covariances (Cov) and correlations (Corr) between real-valued random variables are defined in the usual, second moment, sense. Accordingly, the standard, multivariate analysis, canonical correlation concept involves the study of univariate correlations between linear functions of random vectors $X \in \mathbb{R}^k$ and $Y \in \mathbb{R}^l$, for finite integers $k$ and $l$. Specifically, the first canonical correlation $\rho_1$ and associated weight vectors $a_1$ and $b_1$ are defined as

$$\rho_1^2 = \sup_{a \in \mathbb{R}^k, b \in \mathbb{R}^l} \text{Cov}^2(\langle a, X \rangle_{\mathbb{R}^k}, \langle b, Y \rangle_{\mathbb{R}^l}) = \text{Cov}^2(\langle a_1, X \rangle_{\mathbb{R}^k}, \langle b_1, Y \rangle_{\mathbb{R}^l}),$$  

where $a$ and $b$ are subject to

$$\text{Var}(\langle a, X \rangle_{\mathbb{R}^k}) = \text{Var}(\langle b, Y \rangle_{\mathbb{R}^l}) = 1,$$

with, e.g., $\langle \cdot, \cdot \rangle_{\mathbb{R}^k}$ the standard Euclidean inner product on $\mathbb{R}^k$; for $i > 1$, the $i$th canonical correlation $\rho_i$ and the associated weight vectors $a_i$ and $b_i$ are defined as

$$\rho_i^2 = \sup_{a \in \mathbb{R}^k, b \in \mathbb{R}^l} \text{Cov}^2(\langle a_1, X \rangle_{\mathbb{R}^k}, \langle b, Y \rangle_{\mathbb{R}^l}) = \text{Cov}^2(\langle a_i, X \rangle_{\mathbb{R}^k}, \langle b_i, Y \rangle_{\mathbb{R}^l}),$$

where $a$ and $b$ are subject to (2) and

$$\text{Cov}(\langle a_i, X \rangle_{\mathbb{R}^k}, \langle a_j, X \rangle_{\mathbb{R}^k}) = \text{Cov}(\langle b_i, Y \rangle_{\mathbb{R}^l}, \langle b_j, Y \rangle_{\mathbb{R}^l}) = 0, \ j < i.$$
It is well known that the solutions to (1)–(4) can be characterized through the singular-value decomposition of a particular matrix. In this regard, let $K_X$, $K_Y$ and $K_{XY} = K_{YX}$ be the auto covariance and cross covariance matrices for $X$, $Y$ and let $\lambda_i$ be the $i$th largest eigenvalue of $K_Y^{-1/2}K_{YX}K_X^{-1}K_{XY}K_Y^{-1/2}$ corresponding to the eigenvector $v_i$ in $\mathbb{R}^d$ (with inverse matrices being of the Moore-Penrose variety if necessary). Then $\rho^2_i = \lambda_i$, $b_i = K_Y^{-1/2}v_i$, and $a_i = (1/\sqrt{\lambda_i})K_X^{-1}K_{XY}K_Y^{-1/2}v_i$.

We wish to generalize (1)–(4) and the ensuing computations to allow for situations where one or both of $X$ and $Y$ is function-valued. One way to accomplish this is to replace the Euclidean inner products in (1) and (3) by other inner products in specific Hilbert function spaces of interest such as $L^2[0,1]$, the space of square-integrable functions on $[0,1]$. Work by He, Müller and Wang [13,14] in the context of functional data analysis has demonstrated that such an approach can be effective. An alternative tactic, that allows for a general treatment, is to formulate the problem in the Hilbert space spanned by a second-order stochastic process: i.e., a stochastic process that possesses a well-defined covariance function. Solutions can then be formulated using functional analysis methods in conjunction with the Lévy-Parzen classical isometry between the Hilbert space spanned by a process and the reproducing kernel Hilbert space (RKHS) generated by its covariance kernel. A thorough development of this latter paradigm is the goal of the present paper.

The organization of the remainder of the paper is as follows. Section 2 summarizes the relevant RKHS theory and mathematical results that are needed for the sequel. Section 3 then defines canonical correlations from a general perspective using a RKHS framework. Not surprisingly, the resulting canonical correlations and variables are derived from a “singular-value” decomposition or polar representation of a particular linear operator whose properties we explore in some detail. Section 4 then focuses on important special cases of the general theory that have been studied in the literature. In Section 5, we discuss some of the inferential implications of our work while providing
a connection between the large sample theory for estimators of canonical correlations for the finite-dimensional and infinite-dimensional settings. Finally, in Section 6, we explore the practical feasibility of our work through development of a prototype estimation algorithm for analysis of functional data. All of the proofs and technical results are collected in the Appendix.

2. Reproducing kernel Hilbert spaces and stochastic processes

We devote this section to developing the mathematical tools that will be required in our analysis. In particular, we will state, without proof, some basic facts about RKHSs. Verification of these results as well as more detailed discussions of RKHS theory can be found in Aronszajn [2], Parzen [24], Weinert [35] and Berlinet and Thomas-Agnan [6].

Let \( H \) be a Hilbert space of functions on some set \( E \) and denote by \( \langle \cdot, \cdot \rangle_H \) the inner product in \( H \). A bivariate function \( K \) on \( E \times E \) is said to be a reproducing kernel for \( H \) if

(i) for every \( t \in E \), \( K(\cdot, t) \in H \), and

(ii) for every \( t \in E \) and \( f \in H \), \( f(t) = \langle f, K(\cdot, t) \rangle_H \).

When (i)–(ii) hold, \( H \) is said to be a reproducing kernel Hilbert space (RKHS) with reproducing kernel \( K \). We will refer to (ii) as the reproducing property. It can then be shown that

(iii) \( K \) is the unique reproducing kernel,

(iv) \( K \) is symmetric and nonnegative definite and

(v) functions of the form \( \sum_{i=1}^{m} a_i K(\cdot, t_i), a_i \in \mathbb{R}, t_i \in E, m = 1, 2, \ldots \), are dense in \( H \).

On the other hand, in view of (v), if \( K \) is a symmetric and non-negative definite function on \( E \times E \), one can construct a Hilbert space \( H(K) \) via completion of the
space of all functions on \( E \) of the form \( \sum_{i=1}^{m} a_i K(\cdot, t_i), a_i \in \mathbb{R}, t_i \in E, m = 1, 2, \ldots, \)
under the inner product
\[
\langle \sum_{i=1}^{m} a_i K(\cdot, s_i), \sum_{j=1}^{m'} b_j K(\cdot, t_j) \rangle_{\mathcal{H}(K)} := \sum_{i=1}^{m} \sum_{j=1}^{m'} a_i b_j K(s_i, t_j).
\] (5)

Then, \( \mathcal{H}(K) \) is a RKHS with reproducing kernel \( K \).

Explicit formulae for the RKHS norm and inner product corresponding to a kernel can often be obtained via an application of Parzen’s “integral representation theorem” (Parzen [24], Theorem 4D). In this regard let \( (Q, \mathcal{B}, \mu) \) be a measure space and let \( L^2(Q) \) be the corresponding Hilbert space of functions on \( Q \) that are square-integrable with respect to \( \mu \). Suppose that there is a set of functions \( \{ \phi(t, \cdot) : t \in E \} \) in \( L^2(Q) \) such that
\[
K(s, t) = \int_{Q} \phi(s, q) \phi(t, q) d\mu(q),
\] (6)

for all \( s, t \in E \). Then, the RKHS generated by \( K \) consists of functions of the form
\[
f(t) = \int_{Q} g(q) \phi(t, q) d\mu(q),
\] (7)

for some (a.e. \( \mu \)) unique function \( g \in \overline{\text{span}} \{ \phi(t, \cdot) : t \in E \} \): i.e., for \( g \) in the closure of the linear span of \( \{ \phi(t, \cdot) : t \in E \} \) in \( L^2(Q) \). The inner product for \( f_1, f_2 \in \mathcal{H}(K) \) with corresponding \( L^2(Q) \) functions \( g_1, g_2 \) is then found to be
\[
\langle f_1, f_2 \rangle_{\mathcal{H}(K)} = \langle g_1, g_2 \rangle_{L^2(Q)}.
\] (8)

As shown by Parzen [24], RKHSs provide a fundamental tool for inference concerning second-order stochastic processes. This stems from the isometry or congruence between the Hilbert space spanned by a process and the RKHS generated by its covariance kernel that we will now describe.

Let \( \{ X(t) : t \in E \} \) be a stochastic process on \( E \), where each \( X(t) \) is a map from some probability space into \( \mathbb{R} \). Assume that \( \mathbb{E}[X(t)] = 0 \) for all \( t \in E \) and that the
covariance function $K(s, t) = \mathbb{E}[X(s)X(t)]$, $s, t \in E$, is well-defined. Let $L^2_X$ be the completion of the set of all random variables of the form

$$
\sum_{i=1}^{m} a_i X(t_i), \ a_i \in \mathbb{R}, t_i \in E, m = 1, 2, \ldots,
$$

under the inner product $\langle U, V \rangle_{L^2_X} = \mathbb{E}(UV)$. The elements of $L^2_X$ are linear combinations, in an extended limiting sense (see Chapter 1 of Ash and Gardner [3]), of the random variables that make up the process and therefore represent a natural extension of the finite dimensional linear manifolds of random variables that are the focus of standard multivariate analysis.

Since $K$ is symmetric and nonnegative definite, it generates a RKHS $\mathcal{H}(K)$ as described above and, by the reproducing property,

$$
\| \sum_i a_i X(t_i) \|_{L^2_X}^2 = \sum_{i,j} a_i a_j K(t_i, t_j) = \| \sum_i a_i K(\cdot, t_i) \|_{\mathcal{H}(K)}^2.
$$

Hence the mapping from $\mathcal{H}(K)$ onto $L^2_X$ induced by

$$
\Psi : \sum_i a_i K(\cdot, t_i) \mapsto \sum_i a_i X(t_i)
$$

is isometrically isomorphic, or congruent, i.e., one-to-one and inner product preserving.

It is generally difficult to obtain closed-form expressions for $\Psi$ or $\Psi^{-1}$ since the isometries are explicitly defined only on dense, finite-dimensional, subsets of $\mathcal{H}(K)$ and $L^2_X$. A case where a complete characterization of $\Psi$ is possible corresponds to processes that can be represented by the $L^2$-stochastic integral (see, e.g., Chapter 2 of Ash and Gardner [3])

$$
X(t) = \int_Q \phi(t, q)dZ(q), \ t \in E,
$$

where $Z$ is a complex-valued stochastic process on $Q$ with uncorrelated increments and, for each $t \in E$, $\phi(t, \cdot) \in L^2(Q)$ with $d\mu(q) = \mathbb{E}|dZ(q)|^2$. In this instance (6)
and (7) both hold, and it is easy to show (see Proposition A2) that for any \( f(\cdot) = \int_Q g(q) \phi(\cdot, q) d\mu(q) \) with \( g \in L^2(Q) \),

\[
\Psi(f) = \int_Q g(q) dZ(q).
\] (11)

We conclude this section with some examples of RKHSs that illustrate the use of the integral representation theorem (6)–(8) as well as the implications of (11). These examples will play a further role in the developments in Section 4.

**Example 1.** A simple, but fundamentally important, example of an RKHS can be obtained when \( E \) is finite-dimensional. Thus, let \( E = \{t_1, \ldots, t_m\} \) in which case the kernel \( K \) is equivalent to the matrix \( K = \{K(t_i, t_j)\}_{i,j=1,m} \).

The RKHS is now found to be the set of functions on \( E \) defined by

\[
\mathcal{H}(K) = \left\{ f(\cdot) = \sum_{i=1}^m a_i K(\cdot, t_i) : a = (a_1, \ldots, a_m)' \in \text{Ker}(K)^\perp \right\}
\] (12)

with \( \text{Ker}(K) = \{a \in \mathbb{R}^m : Ka = 0\} \). The inner product between \( f_1, f_2 \in \mathcal{H}(K) \) is

\[
\langle f_1, f_2 \rangle_{\mathcal{H}(K)} = f_1' K^- f_2
\] (13)

with \( f_i = (f_i(t_1), \ldots, f_i(t_m))' \), \( i = 1, 2 \), and \( K^- \) the Moore-Penrose generalized inverse of \( K \). Given a random vector \( X = (X(t_1), \ldots, X(t_m))' \) with mean zero and covariance matrix \( K \) and a function \( f(\cdot) = \sum_{i=1}^m a_i K(\cdot, t_i) \) in \( \mathcal{H}(K) \), we see that

\[
\Psi(f) = \sum_{i=1}^m a_i X(t_i) = X' K^- f.
\] (14)

**Example 2.** Here and hereafter, \( L^2[0, 1] \) and \( L^2([0, 1] \times [0, 1]) \) denote square-integrable functions on \([0, 1]\) and \([0, 1] \times [0, 1]\) with respect to Lebesgue measures. Suppose now that \( X \) is a zero-mean stochastic process on \([0, 1]\) with covariance function \( K \) as described above. Then, the Karhunen-Loève representation (see Section 1.4 of Ash and Gardner [3])

\[
X(t) = \sum_{q=1}^N \langle X, \phi_q \rangle_{L^2[0,1]} \phi_q(t)
\]
holds for each \( t \in [0,1] \), where the series converges in \( L^2_X \). Then, we have \( dZ(q) = \langle X, \phi_q \rangle_{L^2[0,1]} \), which are uncorrelated and \( \lambda_q = \mathbb{E}[dZ(q)]^2 = d\mu(q) \). Now (11) has the consequence that \( \Psi(f) = \sum_{q=1}^{N} f_q \langle X, \phi_q \rangle_{L^2[0,1]} \) for any function \( f = \sum_{q=1}^{N} \lambda_q f_q \phi_q \) with \( \sum_{q=1}^{N} \lambda_q f_q^2 < \infty \). In the special case that \( \sum_{q=1}^{N} f_q^2 < \infty \), the function \( \sum_{q=1}^{N} f_q \phi_q \) is a member of \( L^2[0,1] \). This produces the “computable” formula

\[
\Psi(f) = \left\langle X, \sum_{q=1}^{N} f_q \phi_q \right\rangle_{L^2[0,1]}.
\]

However, if \( N = \infty \) then \( \{ f = \sum_{q=1}^{N} \lambda_q f_q \phi_q : \sum_{q=1}^{N} f_q^2 < \infty \} \) is not dense in \( \mathcal{H}(K) \) (cf. (61)). Thus, (15) is generally only a partial characterization of \( \Psi \).

**Example 3.** In Section 4.3 we deal with a case where the \( X \) process is indexed by a Hilbert function space. This situation has been considered in, e.g., Parzen [25] and more generally in Baxendale [5] for instances where \( E \) is a Banach space. For our developments it suffices to assume that \( E \) is a separable Hilbert space with norm and inner product \( \| \cdot \|_E \) and \( \langle \cdot, \cdot \rangle_E \), respectively, and that

\[
K(t_1,t_2) = \langle t_1, t_2 \rangle_E.
\]

The RKHS is then equal to the dual space \( E^* \) of bounded linear functionals on \( E \). More precisely,

\[
\mathcal{H}(K) = \{ l \in E^* : l(\cdot) = \langle t_l, \cdot \rangle_E \text{ for some } t_l \in E \}
\]

with \( \| l \|_{\mathcal{H}(K)} := \| t_l \|_E \). Thus, all of the three spaces \( \mathcal{H}(K) \), \( E \) and \( L^2_X \) are isometrically isomorphic and, in particular, \( l \in \mathcal{H}(K), t_l \in E \) and \( X(t_l) \in L^2_X \) are the generic elements that correspond to one another in the three spaces.

### 3. Canonical correlations

In this section, let \( E_1, E_2 \) be two index sets and let \( \{ X(s) : s \in E_1 \} \) and \( \{ Y(t) : t \in E_2 \} \) be two real-valued stochastic processes with \( \mathbb{E}[X(s)] = \mathbb{E}[Y(t)] = 0 \) for all \( s, t \),
and auto and cross covariance functions

\[ K_X(s_1, s_2) = \mathbb{E}[X(s_1)X(s_2)], \quad K_Y(t_1, t_2) = \mathbb{E}[Y(t_1)Y(t_2)], \]

and

\[ K_{XY}(s, t) = \mathbb{E}[X(s)Y(t)] = \text{Cov}(X(s), Y(t)). \]

Denote by \( L^2_X \) and \( L^2_Y \) the Hilbert spaces spanned by the \( X \) and \( Y \) processes as defined in §2 and, similarly, let \( \mathcal{H}_X := \mathcal{H}(K_X), \mathcal{H}_Y := \mathcal{H}(K_Y) \) be the congruent RKHSs with reproducing kernels \( K_X, K_Y \) having associated inner products and norms \( \langle \cdot, \cdot \rangle_{\mathcal{H}_X}, \parallel \cdot \parallel_{\mathcal{H}_X}, \langle \cdot, \cdot \rangle_{\mathcal{H}_Y}, \parallel \cdot \parallel_{\mathcal{H}_Y} \).

We now proceed to apply the results from the previous section to the problem of canonical analysis. The basic formulation of canonical correlations in terms of elements in \( L^2_X \) and \( L^2_Y \) is developed in Section 3.1. There we introduce the key linear mapping, \( T \), from \( \mathcal{H}_Y \) to \( \mathcal{H}_X \) that we employ to resolve analytic issues that arise from this formulation. Then, in Section 3.2, we discuss the polar representation for a non-self adjoint operator and investigate its relevance to the operator \( T \) and the canonical correlation problem. Finally, in Section 3.3, we consider the case where \( T \) is Hilbert-Schmidt: a favorable scenario in which our formulation can be implemented quite effectively.

### 3.1. Basic formulation

Provided the following optimization problem can be solved, we define the first canonical correlation \( \rho_1 \) and the associated canonical variables \( \xi_1 \) and \( \zeta_1 \) by

\[ \rho_1^2 = \sup_{\xi \in L^2_X, \zeta \in L^2_Y} \text{Cov}^2(\xi, \zeta) = \text{Cov}^2(\xi_1, \zeta_1), \quad (17) \]

where \( \xi \) and \( \zeta \) are subject to

\[ \text{Var}(\xi) = \text{Var}(\zeta) = 1. \quad (18) \]
Analogous to the finite-dimensional case, for \( i > 1 \), we define the \( i \)-th canonical correlation \( \rho_i \) and associated variables \( \xi_i \) and \( \zeta_i \) by

\[
\rho_i^2 = \sup_{\xi \in L^2_X, \zeta \in L^2_Y} \text{Cov}^2(\xi, \zeta) = \text{Cov}^2(\xi_i, \zeta_i),
\]

where \( \xi \) and \( \zeta \) are subject to (18) and

\[
\text{Cov}(\xi, \xi_j) = \text{Cov}(\zeta, \zeta_j) = 0, \quad j < i.
\]

A notion of canonical correlation similar to (17)–(20) was proposed by Hannan [15]. His approach requires optimization over all square-integrable functions relative to the joint probability measure associated with the \( X \) and \( Y \) processes. In contrast, our consideration of only linear functionals of the processes would seem to provide the more natural extension of the finite-dimensional setting. Indeed, if we assume for the moment that \( \xi_1 \) and \( \zeta_1 \) are well defined in (17), then since \( \xi_1 \in L^2_X \) and \( \zeta_1 \in L^2_Y \), there are sequences \( \xi_{1m} = \sum_{i=1}^{m} a_{im} X(s_i) \) and \( \zeta_{1m'} = \sum_{i=1}^{m'} b_{im'} Y(s_{im'}) \) such that

\[
\rho_1^2 = \lim_{m,m' \to \infty} \text{Corr}^2(\xi_{1m}, \zeta_{1m'}).
\]

Consequently, our infinite-dimensional definition of canonical variables is actually built up from the finite-dimensional multivariate case and clearly reduces to that definition when both the \( X \) and \( Y \) processes have finite-dimensional index sets.

Next we turn to the question of whether the canonical correlations described above are well-defined: namely, whether the optimization problems in (17)–(20) can be solved. As explained in §2, \( L^2_X \) and \( \mathcal{H}_X \) are congruent and \( L^2_Y \) and \( \mathcal{H}_Y \) are congruent. Thus, let \( \Psi_X \) and \( \Psi_Y \) be the isometric isomorphisms from \( \mathcal{H}_X \) to \( L^2_X \) and \( \mathcal{H}_Y \) to \( L^2_Y \), respectively, that satisfy

\[
\Psi_X : \sum_i a_i K_X(\cdot, s_i) \to \sum_i a_i X(s_i),
\]

\[
\Psi_Y : \sum_j b_j K_Y(\cdot, t_j) \to \sum_j b_j Y(t_j).
\]

We can now restate the above definition of canonical correlations in terms of optimization problems in \( \mathcal{H}_X \) and \( \mathcal{H}_Y \), as follows: Provided the following optimization
problem can be solved, define the first canonical correlation $\rho_1$ and the associated RKHS functions $g_1$ and $f_1$ by

$$\rho_1^2 = \sup_{f \in \mathcal{H}_X, g \in \mathcal{H}_Y} \text{Cov}^2(\Psi_X(f), \Psi_Y(g)) = \text{Cov}^2(\Psi_X(f_1), \Psi_Y(g_1)), \tag{21}$$

where $f$ and $g$ are subject to

$$\|f\|^2_{\mathcal{H}_X} = \text{Var}(\Psi_X(f)) = 1 = \text{Var}(\Psi_Y(g)) = \|g\|^2_{\mathcal{H}_Y}; \tag{22}$$

for $i > 1$, the $i$-th canonical correlation $\rho_i$ and associated RKHS functions $f_i$ and $g_i$ are defined by

$$\rho_i^2 = \sup_{f \in \mathcal{H}_X, g \in \mathcal{H}_Y} \text{Cov}^2(\Psi_X(f), \Psi_Y(g)) = \text{Cov}^2(\Psi_X(f_i), \Psi_Y(g_i)), \tag{23}$$

where $f$ and $g$ are subject to (22) and

$$\text{Cov}(\Psi_X(f), \Psi_X(f_j)) = \text{Cov}(\Psi_Y(g), \Psi_Y(g_j)) = 0, \quad j < i. \tag{24}$$

The formulation (21)–(24) serves the purpose of changing the optimization domain from $(L^2_X, L^2_Y)$ to $(\mathcal{H}_X, \mathcal{H}_Y)$, but seemingly brings us no closer to answering questions about the existence, etc., of solutions. The final step in resolving such issues requires us to connect canonical correlations to “singular values” of the mapping defined by

$$(Tg)(s) = \langle K_{XY}(s, \cdot), g(\cdot) \rangle_{\mathcal{H}_Y}, \quad g \in \mathcal{H}_Y. \tag{25}$$

Proposition A3 in the appendix shows that $K_{XY}(s, \cdot)$ is in $\mathcal{H}_Y$, and also establishes that

$$\langle f, Tg \rangle_{\mathcal{H}_X} = \text{Cov}(\Psi_X(f), \Psi_Y(g)) \tag{26}$$

for any two functions $f \in \mathcal{H}_X$ and $g \in \mathcal{H}_Y$. Consequently, finding elements of $L^2_X$ and $L^2_Y$ with maximum absolute correlation is equivalent to finding functions $f \in \mathcal{H}_X$ and $g \in \mathcal{H}_Y$ with $\|f\|_{\mathcal{H}_X} = \|g\|_{\mathcal{H}_Y} = 1$ such that $f$ and $Tg$ have maximum absolute inner product with one another. The Cauchy-Schwarz inequality suggests that potential
maximizers $f, g$ of $|\langle f, Tg \rangle_{\mathcal{H}_X}|$ should have the form $f = c(Tg)$ for some constant $c$. Thus,

$$|\langle f, Tg \rangle_{\mathcal{H}_X}| = |c| |\langle Tg, Tg \rangle_{\mathcal{H}_X}| = |c| \|Tg\|_{\mathcal{H}_X}^2 = \|Tg\|_{\mathcal{H}_X},$$

since $\|c(Tg)\|_{\mathcal{H}_X} = \|f\|_{\mathcal{H}_X} = 1$. From this it is clear that

$$\|Tg\|_{\mathcal{H}_X} = \sqrt{\langle Tg, Tg \rangle_{\mathcal{H}_X}} = \sqrt{\langle g, T^*Tg \rangle_{\mathcal{H}_X}},$$

and, hence, the expression $\|Tg\|_{\mathcal{H}_X}$ subject to $\|g\|_{\mathcal{H}_Y} = 1$ is maximized by the eigenfunction $g$ that corresponds to the largest eigenvalue $\lambda$ of $T^*T$, assuming that such quantities exist, with $f = (1/\sqrt{\lambda})Tg$. The functions $f$ and $g$ are called the first pair of singular functions of $T$ and they determine the first pair of canonical variables. We will expand on this derivation while providing extensions and existence conditions in the next section.

### 3.2. Polar representation

We would now like to parallel the usual finite-dimensional development and characterize the canonical correlations in (23) as “singular values” for the operator (25). To accomplish this we first need to obtain a representation for $T$ that provides an extension of the finite-dimensional, singular-value decomposition of a matrix into our setting. For this purpose we may use the polar representation for a non-self adjoint operator (e.g., §4.21 of Naimark [23]) along with the standard spectral decomposition for a positive, self adjoint linear operator (e.g., Chapter 12 of Rudin [29]). The result is that

$$T = W \int_{\sigma(T^*T)} \lambda^{1/2} dP(\lambda),$$

(27)

where $W$ is a unique partial isometry (i.e., a norm preserving mapping on $\text{Ker}(W)^\perp$ that maps the range of $(T^*T)^{1/2}$ onto the range of $T$ in $\mathcal{H}_X$), $\sigma(T^*T)$ is the spectrum of $T^*T$ and $\{P(\lambda) : \lambda \in \sigma(T^*T)\}$ is the unique resolution of the identity corresponding to $T^*T$. The set $\sigma(T^*T)$ is necessarily a closed subset of $[0, 1]$. 

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An important special case of the previous development is the case where $T^*T$ is compact: i.e., the case where for any bounded sequence $\{g_n\}$ in $\mathcal{H}_Y$ the sequence $(T^*T)g_n$ contains a convergent subsequence in $\mathcal{H}_X$. In that event $\sigma(T^*T)$ is found to be a countable collection of eigenvalues each occurring with finite multiplicity and having at most one accumulation point at zero. If we let $r(T)$ represent the cardinality of $\sigma(T^*T)$, then the spectral representation of $(T^*T)^{1/2}$ has the form

$$T^*T = \sum_{j=1}^{r(T)} \lambda_j \beta_j \otimes \mathcal{H}_Y \beta_j$$

with the $\lambda_j$ and $\beta_j$ being the eigenvalues and eigenfunctions for $T^*T$ and the tensor product notation $g \otimes \mathcal{H}_Y f$ for functions $f \in \mathcal{H}_X, g \in \mathcal{H}_Y$ is defined by

$$(g \otimes \mathcal{H}_Y f) h = \langle g, h \rangle_{\mathcal{H}_Y} f.$$ (28)

Since the mapping $W$ associates $T g$ with $g \in \text{Im}(T^*T) :=$ the range of $T^*T$, this entails that $\alpha_j := W \beta_j = W(T^*T)^{1/2} \beta_j / \sqrt{\lambda_j} = T \beta_j / \sqrt{\lambda_j}$. Thus, we obtain

$$T = \sum_{j=1}^{r(T)} \sqrt{\lambda_j} \beta_j \otimes \mathcal{H}_Y \alpha_j$$ (29)

as the polar representation for $T$. In this context the $\sqrt{\lambda_j}$ are usually referred to as $s$-numbers (e.g., Chapter II of Gohberg and Krein [11]). To emphasize the connection with the ordinary multivariate analysis case we will continue to refer to them as singular values in what follows.

When (29) holds, the squared canonical correlations are precisely the eigenvalues of $T^*T$. To see this, assume for notational simplicity that the $\lambda_j$ are distinct. Then, from (26) and (29) we have

$$\text{Cov}(\Psi_X(f), \Psi_Y(g)) = \langle f, T g \rangle_{\mathcal{H}_X} = \sum_{j=1}^{r(T)} \sqrt{\lambda_j} \langle f, \alpha_j \rangle_{\mathcal{H}_X} \langle g, \beta_j \rangle_{\mathcal{H}_Y},$$

and, by the Cauchy-Schwarz inequality,

$$\text{Cov}^2(\Psi_X(f), \Psi_Y(g)) \leq \lambda_1 \sum_{i=1}^{r(T)} \langle f, \alpha_i \rangle_{\mathcal{H}_X}^2 \sum_{j=1}^{r(T)} \langle g, \beta_j \rangle_{\mathcal{H}_Y}^2 \leq \lambda_1 \|f\|_{\mathcal{H}_X}^2 \|g\|_{\mathcal{H}_Y}^2,$$
where the equality holds if and only if \( f = \alpha_1 \) and \( g = \beta_1 \). For the general case we have \( f \perp \alpha_i, 1 \leq i \leq j-1, g \perp \beta_i, 1 \leq i \leq j-1 \) and \( \text{Cov}^2(\Psi_X(f), \Psi_Y(g)) \leq \lambda_j \|f\|_{\mathcal{H}_X}^2 \|g\|_{\mathcal{H}_Y}^2 \), with equality if and only if \( f = \alpha_j, g = \beta_j \).

Note that we have actually done more than just characterizing the canonical correlation. Specifically, we have established the following.

**Theorem 1.** Assume that \( T \) has polar representation (29). Then, \( \rho_j, f_j, g_j \) in (21) and (23) are given by \( \rho_j = \sqrt{\lambda_j}, f_j = \alpha_j, g_j = \beta_j \) and the corresponding canonical variables of the \( X \) and \( Y \) spaces are \( \xi_j = \Psi_X(f_j) \) and \( \zeta_j = \Psi_Y(g_j) \).

Let us now revisit the finite-dimensional case of Section 1 and Example 1 where \( X \) and \( Y \) are random vectors in \( \mathbb{R}^k \) and \( \mathbb{R}^l \), respectively, and \( K_X, K_Y \) and \( K_{XY} = K'_{YX} \) are the associated auto and cross covariance matrices. Theorem 1 can be applied with \( \mathcal{H}_X, \mathcal{H}_Y \) being equivalent to the linear subspaces \( \text{Ker}(K_X)^\perp, \text{Ker}(K_Y)^\perp \) of \( \mathbb{R}^k \) and \( \mathbb{R}^l \), respectively. The operator \( T \) is then determined by the matrix \( K_{XY}K_X^{-} \) while \( T^* \) and \( T^*T \) are similarly characterized by \( K_{YY}K_X^{-}, K_{XX}K_{YY}K_Y^{-} \). The spectral decomposition produces \( (T^*T)^{1/2} = \sum_{j=1}^{r(T^*T)} \lambda_j^{1/2} v_j \lambda_j^{1/2} v_j' K_Y^{-} \), where the \( \lambda_j \) and \( v_j \) are solutions of the equation

\[
K_Y^{-} K_{YY} K_X^{-} K_{XY} K_Y^{-} v = \lambda v
\]

subject to the condition \( v_j' K_Y^{-} v_r = \delta_{jr} \). Consequently, the \( \lambda_j \) coincide with the usual definition of squared canonical correlations between two random vectors. The RKHS variates in (21)–(23) correspond to the vectors \( g_j = v_j \) and \( f_j = T v_j / \sqrt{\lambda_j} \). In view of (14), this translates into the canonical variables \( \xi_j = f_j' K_X^{-} X \) and \( \zeta_j = g_j' K_Y^{-} Y \), which also agree precisely with Hotelling’s formulation described in Section 1.

Finally, we consider what can be said about canonical correlations and variables when \( T \) is not compact. In this latter instance, singular values and, hence, canonical correlations, can be defined corresponding to eigenvalues of \( T^*T \) under certain conditions. Specifically, assume that the largest point in \( \sigma(T^*T) \) is an eigenvalue \( \lambda_1 \) of
finite multiplicity with an associated eigenvector $g_1$. Then,

$$\text{Cov}^2(\Psi_X(f), \Psi_Y(g)) = \langle W^* f, (T^* T) g \rangle^2_{\mathcal{H}_X}$$

which is clearly maximized by taking $g = g_1$ and $f = W g_1$. Thus, $\Psi_X(W g_1)$ and $\Psi_Y(g_1)$ are the elements in $L^2_X$ and $L^2_Y$ with maximum squared correlation $\lambda_1$. The optimization process can be continued by looking for the next largest point in the spectrum, subject to orthogonality relative to the eigenspace corresponding to $\lambda_1$. Provided this is an eigenvalue of finite multiplicity, it represents the next canonical correlation, etc. The resulting sequence of squared canonical correlations is non-decreasing and therefore has a limit that must either be an eigenvalue of infinite multiplicity or the largest accumulation point of the spectrum. At this final juncture it is no longer possible to define canonical correlations and variables in any meaningful sense.

### 3.3. When $T$ is Hilbert-Schmidt

Given the simplicity of our formulation in the case of compactness explained in Section 3.2, it is worthwhile to investigate when $T$ will possess this property. For this purpose assume that both $\mathcal{H}_X$ and $\mathcal{H}_Y$ are separable and let $\{f_i\}$ and $\{g_j\}$ be CONSs for $\mathcal{H}_X$ and $\mathcal{H}_Y$, respectively. Then, by (25) and (58),

$$K_{XY}(s, t) = \sum_{i=1}^{\infty} \langle T^* f_i(t), f_i(s) \rangle = \sum_{j=1}^{\infty} \langle T g_j(s), g_j(t) \rangle = \sum_{i=1}^{\infty} \phi_{ij} f_i(s) g_j(t),$$

where $\phi_{ij} = \langle T^* f_i, g_j \rangle_{\mathcal{H}_Y} = \langle T g_j, f_i \rangle_{\mathcal{H}_X}$. Thus,

$$T = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \phi_{ij} g_j \otimes_{\mathcal{H}_Y} f_i$$

and we may conclude (Corollary 6.10 and Theorem 6.12 of Rynne and Youngson [30]) that $T$ is compact if and only if $\|T - T_m\| \to 0$ as $n \to \infty$, where

$$T_m = \sum_{i=1}^{m} \sum_{j=1}^{\infty} \phi_{ij} g_j \otimes_{\mathcal{H}_Y} f_i$$
and \( \| T - T_m \| \) is the operator norm of \( T - T_m \); hence, \( T \) is compact if and only if

\[
\lim_{m \to \infty} \sup_{\sum w_j^2 \leq 1} \left( \sum_{j=1}^{\infty} \phi_{ij} w_j \right)^2 = 0. \tag{31}
\]

A sufficient condition for (31) to hold is that

\[
\sum_{i,j=1}^{\infty} \phi_{ij}^2 < \infty \tag{32}
\]

which can be shown to be equivalent to \( T \) being a Hilbert-Schmidt operator in the sense that \( \sum_{i=1}^{\infty} \| T g_i \|_{\mathcal{H}_X} < \infty \). (See, e.g., Theorem 6.16 of Rynne and Youngson [30]). The various loose pieces in our development can be tied together rather nicely in this latter instance to provide a simple, intuitive condition that assures the compactness of \( T \). To formulate this result we need to work with a new RKHS obtained from the direct product of \( \mathcal{H}_X \) and \( \mathcal{H}_Y \).

The direct product space \( \mathcal{H}_X \otimes \mathcal{H}_Y \) is defined to be the completion of the set of functions on \( E_1 \times E_2 \) of the form \( h(s,t) = \sum_i u_i(s)v_i(t) \) with \( u_i \in \mathcal{H}_X, v_i \in \mathcal{H}_Y \); equivalently, if \( \{ f_i \} \) and \( \{ g_j \} \) are CONSs for \( \mathcal{H}_X, \mathcal{H}_Y \), respectively, then \( \mathcal{H}_X \otimes \mathcal{H}_Y \) consists of all functions of the form \( h(s,t) = \sum_{i,j} c_{ij} f_i(s)g_j(t) \) with \( \sum_{i,j} c_{ij}^2 < \infty \). If we define an inner product on \( \mathcal{H}_X \otimes \mathcal{H}_Y \) by

\[
\langle h_1, h_2 \rangle_{\mathcal{H}_X \otimes \mathcal{H}_Y} = \sum_{i,j} c_{ij}^{(1)} c_{ij}^{(2)}, \text{ for } h_i(s,t) = \sum_{i,j} c_{ij}^{(i)} f_i(s)g_j(t),
\]

\( \mathcal{H}_X \otimes \mathcal{H}_Y \) is also a RKHS with reproducing kernel

\[
K((s_1, t_1), (s_2, t_2)) = K_X(s_1, s_2)K_Y(t_1, t_2), \; (s_i, t_i) \in E_1 \times E_2.
\]

Note from this definition that if \( f \in \mathcal{H}_X \), \( g \in \mathcal{H}_Y \), \( h \in \mathcal{H}_X \otimes \mathcal{H}_Y \), then

\[
\langle h, fg \rangle_{\mathcal{H}_X \otimes \mathcal{H}_Y} = \langle \langle h, f \rangle_{\mathcal{H}_X}, g \rangle_{\mathcal{H}_Y} = \langle \langle h, g \rangle_{\mathcal{H}_Y}, f \rangle_{\mathcal{H}_X}. \tag{33}
\]

The following result is now straightforward.
Theorem 2. Assume that both $\mathcal{H}_X$ and $\mathcal{H}_Y$ are separable. Then, the cross covariance function $K_{XY}$ is in $\mathcal{H}_X \otimes \mathcal{H}_Y$ if and only if $T$ is a Hilbert-Schmidt operator.

In summary, the developments in this section have led to a general notion of canonical correlations that directly parallels and extends Hotelling’s original, finite dimensional, formulation. The most immediate and intuitive extension of Hotelling’s method corresponds to the case where $T$ is compact and a sufficient condition for this to occur is that $\mathcal{H}_X, \mathcal{H}_Y$ be separable and $K_{XY} \in \mathcal{H}_X \otimes \mathcal{H}_Y$. This latter condition has more than just theoretical merit. It also provides the impetus for a prototype data analysis methodology based on our RKHS formulation that is the subject of Section 6.

4. Examples.

The purpose of this section is to examine several infinite-dimensional definitions of canonical correlations that have appeared in the literature from the perspective of the work in the previous section. We will treat three situations corresponding to developments in functional data analysis, time series model identification and statistical learning algorithms. Specifically, we will address the issue of canonical correlation analysis for functional data and demonstrate some technical difficulties with some proposals that have been advanced for the solution of this problem. Then, we show that (i) the definition of canonical correlation for stationary processes due to Jewell and Bloomfield [19], (ii) the correlation coefficient that arises in the ACE algorithm of Breiman and Friedman [8] and (iii) the classical canonical correlation concept for bivariate distributions of Lancaster [20] are all special cases of our definition of canonical correlations.

4.1. Functional data analysis

To simplify the presentation we will focus here on the case where $E_1 = E_2 = [0, 1]$,
and $K_X$ and $K_Y$ are continuous covariance kernels. By Mercer’s Theorem, write

$$K_X(s, t) = \sum_i \lambda_i \phi_i(s) \phi_i(t), \quad K_Y(s, t) = \sum_j \nu_j \theta_j(s) \theta_j(t),$$

where $\{\phi_i\}$ and $\{\theta_j\}$ are each CONSs for $L^2[0, 1]$. Then, the Karhunen-Loève representations are

$$X(\cdot) = \sum_i U_i \phi_i(\cdot) \quad \text{and} \quad Y(\cdot) = \sum_j V_j \theta_j(\cdot),$$

(34)

where the $\{U_i\}$ and $\{V_j\}$ are sequences of zero mean, uncorrelated random variables with

$$\mathbb{E}(U^2_i) = \lambda_i, \quad \mathbb{E}(V^2_j) = \nu_j, \quad \mathbb{E}(U_i V_j) = \gamma_{ij}. \quad \text{(35)}$$

By (34) and (35), $K_{XY}(s, t) = \sum_{i,j} \gamma_{ij} \phi_i(s) \theta_j(t)$, and the forms of the RKHSs $\mathcal{H}_X$ and $\mathcal{H}_Y$ can be determined as in Example 2 of Section 2. From this we see that the operator $T$ in (25) satisfies

$$(Tg)(s) = \langle K_{XY}(s, \cdot), g(\cdot) \rangle_{\mathcal{H}_Y} = \langle \sum_{i,j} \gamma_{ij} \phi_i(\cdot) \theta_j(\cdot), g(\cdot) \rangle_{\mathcal{H}_Y}$$

$$= \sum_{i,j} \rho_{ij} \langle g, \tilde{\theta}_j \rangle_{\mathcal{H}_Y} \tilde{\phi}_i(s), \quad g \in \mathcal{H}_Y,$$

where $\rho_{ij} = \gamma_{ij}/(\lambda_i \nu_j)^{1/2}$ is the correlation between $U_i$ and $V_j$ and, by Proposition A4, $\{\tilde{\phi}_i = \sqrt{\lambda_i} \phi_i\}$ and $\{\tilde{\theta}_j = \sqrt{\nu_j} \theta_j\}$ are CONSs for the RKHSs $\mathcal{H}_X$ and $\mathcal{H}_Y$, respectively. As a result,

$$T = \sum_{i,j} \rho_{ij} \tilde{\theta}_j \otimes_{\mathcal{H}_Y} \tilde{\phi}_i,$$

(36)

and, by Theorem 2, $T$ is Hilbert-Schmidt if and only if $\sum_{i,j} \rho_{ij}^2 < \infty$. In this case $T$ admits a polar representation of the form (29) and the canonical correlations and variables for the $X$ and $Y$ process can be determined as in Theorem 1.

He, Müller and Wang [13] (denoted by HMW hereafter) developed a notion of canonical correlation for processes of the form (34) through a direct extension of
finite-dimensional matrix formulations with integral operators being used in the place of matrices. Specifically, define the $L^2[0,1]$ operators

$$R_{XX} = \sum_i \lambda_i \phi_i \otimes L^2[0,1] \phi_i, \quad R_{YY} = \sum_j \nu_j \theta_j \otimes L^2[0,1] \theta_j \quad \text{and} \quad R_{XY} = \sum_{i,j} \gamma_{ij} \theta_j \otimes L^2[0,1] \phi_i.$$ 

Then, HMW obtain canonical correlations as singular values of the operator $R$ defined by

$$R = R_{XX}^{-1/2} R_{XY} R_{YY}^{-1/2}.$$ 

One of the difficulties with this development is that the $L^2[0,1]$ operators $R_{XX}$ and $R_{YY}$ are not generally invertible. To circumvent this problem HMW impose conditions (Condition 4.5 in HMW) on the $\rho_{ij}$ which insure that the domain and range of $R$ are subsets of $F_{YY}$ and $F_{XX}$, respectively, where

$$F_{XX} := \left\{ f \in L^2[0,1] : \sum_i \lambda_i^{-1} |\langle f, \phi_i \rangle |^2 < \infty \quad \text{and} \quad f \perp \text{Ker}(R_{XX}) \right\}$$

$$= \left\{ f = \sum_{i=1}^{\infty} f_i \phi_i : \sum_i \lambda_i^{-1} f_i^2 < \infty \right\},$$

with $F_{YY}$ defined similarly. With these restrictions, it can be seen that

$$R = \sum_{i,j} \rho_{ij} \theta_j \otimes L^2[0,1] \phi_i. \quad (37)$$

A question of interest here is how the canonical correlations and variables produced by $R$ in (37) differ from those provided by $T$. To address this issue let $\Gamma_X$ and $\Gamma_Y$ be parallels of the isometry $\Gamma$ in (60) between the closed linear spans of \{\phi_i\} and $\mathcal{H}_X$, and that of \{\theta_j\} and $\mathcal{H}_Y$, respectively. Then, under the conditions in HMW mentioned above, $R = \Gamma_X^{-1} T \Gamma_Y$. Comparing (36) and (37), it can be concluded that, in this case, the singular-value decompositions of $R$ and $T$ are completely equivalent in the sense that the singular values of $R$ and $T$ are the same and the singular functions of the two operators can be mapped back and forth by the isometries. However, this implies that the singular functions of $T$ are in $\Gamma_X(F_{XX})$ and $\Gamma_Y(F_{YY})$. It is easy to verify
that $\Gamma_X(F_{XX}) = \{ \sum_i \lambda_i f_i \phi_i, \sum_i f_i^2 < \infty \}$ and $\Gamma_Y(F_{YY}) = \{ \sum_j \nu_j g_j \theta_j, \sum_j g_j^2 < \infty \}$. In view of (61), $\Gamma_Y(F_{YY})$ and $\Gamma_X(F_{XX})$ are, in general, proper subspaces of $\mathcal{H}_Y$ and $\mathcal{H}_X$. The HMW range and domain restrictions therefore have the effect of restricting optimization to elements of $\mathcal{H}_Y$ and $\mathcal{H}_X$ having congruent members in $L^2_Y$ and $L^2_X$ that can be recovered by the computable formula (15). It follows from this that the HMW canonical correlations and variables will, in general, not agree with those defined via relations (17)–(20). An example of this is provided by Example 4.4 of HMW, which assumes (34) and (35) with

$$\lambda_i = \frac{1}{i^2}, \quad \nu_j = \frac{1}{j^2}, \quad \gamma_{ij} = \frac{1}{(i+1)^2(j+1)^2}, \quad i, j \geq 1.$$

The derivations there show that the pair of random variables

$$\frac{1}{c} \sum_{i=1}^{\infty} \frac{i^2}{(i+1)^2} U_i \quad \text{and} \quad \frac{1}{c} \sum_{j=1}^{\infty} \frac{j^2}{(j+1)^2} V_j,$$

where $c = \sum_{i=1}^{\infty} i^2/(i+1)^4$, constitute the canonical variables based on our definition, but not under the HMW approach.

### 4.2. Time series analysis

Another application of our work is to the development of canonical correlations for time series settings such as those considered in §3 of Hannan [15] and by Jewell and Bloomfield [19]. We focus primarily on developments in Jewell and Bloomfield [19] that concern the canonical correlations between the past and future of a stationary time series.

Let $\{Z(t) : t = 0, \pm 1, \ldots \}$ represent a second-order stationary process with mean zero and take $X(t) = Z(t)$ and $Y(t) = Z(1-t)$ for $t = 1, 2, \ldots$. The canonical correlations between the $X$ and $Y$ processes in this case have been studied by Jewell and Bloomfield [19] when $Z$ is Gaussian. Their results provide a theoretical cornerstone for time series model identification methodology such as that developed in Tiao and Tsay [32] and Tsay and Tiao [33]. Our definition of canonical correlations coincides
with theirs. But, our development circumvents the need for complex analysis and also dispenses with the normality condition.

For simplicity, let \( Z(\cdot) \) be a real-valued, covariance stationary process having a spectral measure that is absolutely continuous with respect to Lebesgue measure. If we denote the corresponding spectral density by \( p \), then the \( Z \) covariance function can be expressed as

\[
R(t) = \mathbb{E}[Z(0)Z(t)] = \int_{-\pi}^{\pi} e^{itq}p(q)dq,
\]

where \( i = \sqrt{-1} \). Accordingly, the auto covariance functions for \( X \) and \( Y \) are

\[
K_X(s, t) = K_Y(s, t) = R(t - s), \ s, t = 1, 2, \ldots
\]

In this case, \( \mathcal{H}_X = \mathcal{H}_Y \) consist of functions of the form \( g(t) = \int_{-\pi}^{\pi} h(q)e^{-itq}p(q)dq \) with \( h(q) = \sum_{j=1}^{\infty} h_j e^{ijq} \) for some sequence of real numbers \( \{h_j\} \) in the set of square-summable sequences on the positive integers. See (6) and (7) of \( \S 2 \).

Now observe that the cross covariance function is

\[
K_{XY}(s, t) = R(s + t - 1), \ s, t = 1, 2, \ldots
\]

and use (8) to see that

\[
(Tg)(s) = \sum_{j=1}^{\infty} h_j R(t + j - 1) = (T^*g)(t).
\]

This shows that \( T \) can be viewed as a self adjoint Hankel operator corresponding to the Hankel matrix \( A = \{a_{i+j} = R(j + k - 1)\}_{i,j,k=1}^{\infty} \). As noted by Jewell and Bloomfield [19], a number of properties of \( T \) can be deduced immediately by exploiting this representation for the operator. Specifically, it follows from Hartman [16] that \( T \) is compact if and only if there exists a continuous choice for the spectral density \( p \) and a classical result due to Kronecker (see, e.g., \( \S 4 \) of Peller [26]) has the consequence that \( T \) has finite rank if and only if \( p \) is a rational function: i.e., if and only if \( Z \) is an ARMA process.
The RKHS framework makes it possible to provide a relatively simple development of the relationship between the compactness of $T$ and the dependence structure for the $Z$ process. Specifically, if

$$\alpha_n = \sup \{ \text{Corr}(U, V) : U \in L^2_{\{Z(s), s \leq 0\}}, V \in (L^2_{\{Z(t), t \leq n\}})^{\perp} \},$$

then we will say that $Z$ is strong-mixing if $\alpha_n \to 0$ as $n \to \infty$. The proof of the following result is given in the appendix.

**Theorem 3.** The process $Z$ is strong-mixing if and only if $T$ is compact.

A more general scenario occurs when $X$ and $Y$ represent two covariance stationary processes with respective covariance functions $R_X, R_Y$ and spectral densities $p_X, p_Y$. In this case if $K_{XY}(t, s) = \sum_{j,k} a_{ij} R_X(t - k) R_Y(s - j)$ we find that $(Tg)(t) = \sum_{j,k,l} a_{jk} h_l R_X(l + k) R_Y(t + j)$ which represents the product of two bi-infinite Hankel operators on the set of square-summable sequences. The spectral theory is more complicated than the previous case and we will explore this further in future work.

### 4.3. Bivariate distributions, ACE and ICA

Let $U$ and $V$ be random variables with probability distributions that are absolutely continuous with respect to measures $\mu_U, \mu_V$ on sets $Q_U$ and $Q_V$. Denote the corresponding densities by $p_U, p_V$ and assume that $p_U > 0, p_V > 0$ a.e. $\mu_U, \mu_V$. Then a problem that arises in several contexts concerns finding functions $s_1, t_1$ in function spaces $E_1, E_2$ so that the transformed variables $s_1(U)$ and $t_1(V)$ have maximum correlation: i.e.,

$$\rho^2 = \sup_{s \in E_1, t \in E_2} \text{Corr}^2(s(U), t(V)) = \text{Corr}^2(s_1(U), t_1(U)).$$  \hspace{1cm} (38)

When $E_1 = L^2(Q_U)$ and $E_2 = L^2(Q_V)$, $s_1$ and $t_1$ are the optimal transformations obtained from the ACE (Alternating Conditional Expectation) and ALS (Alternating Least Squares) algorithms of Breiman and Friedman [8] and van der Burg and
De Leeuw [34], respectively. (See, e.g., Buja [9].) A similar formulation has been employed by Bach and Jordan [4] for Independent Component Analysis (ICA) where the optimization is conducted only on closed subspaces of \( L^2(Q_U) \) and \( L^2(Q_V) \). As observed by Buja [9], the problem is also related in a fundamental way to the classical work by Lancaster [20] on the structure of bivariate distributions. Lancaster’s approach to the decomposition of bivariate densities has applications that include the development of methodology for tests of independence. (See, e.g., Eubank, LaRiccia and Rosenstein [10].) On the surface, Lancaster’s use of the term “canonical correlation” in his setting seems to have no connection to the traditional use of the phrase in standard multivariate analysis. We will see, however, that Lancaster’s notion of canonical correlations is another special case of the general theory in §3.

To begin, let us define the \( X \) and \( Y \) processes by \( \{ X(s) = s(U) : s \in E_1 \} \) and \( \{ Y(t) = t(V) : t \in E_2 \} \) with

\[
E_1 = \{ s \in L^2(Q_U) : \mathbb{E}[s(U)] = 0 \}, \quad E_2 = \{ t \in L^2(Q_V) : \mathbb{E}[t(V)] = 0 \},
\]

where

\[
\langle s_1, s_2 \rangle_{E_1} = \mathbb{E}[s_1(U)s_2(U)] = K_X(s_1, s_2), \quad \langle t_1, t_2 \rangle_{E_2} = \mathbb{E}[t_1(V)t_2(V)] = K_Y(t_1, t_2).
\]

By Example 3 of §2, \( \mathcal{H}_X, E_1, L^2_X \) are congruent and so are \( \mathcal{H}_Y, E_2, L^2_Y \). In accordance with the notation of that example, let \( f \in \mathcal{H}_X, s_f \in E_1, s_f(U) \in L^2_X \) be the elements that correspond to one another under the isometric mappings for \( \mathcal{H}_X, E_1, L^2_X \), and similarly, let \( g \in \mathcal{H}_Y, t_g \in E_2 \) and \( t_g(U) \in L^2_Y \) be the elements that correspond to one another in \( \mathcal{H}_Y, E_2, L^2_Y \).

If we now allow \((U, V)\) to have bivariate density \( p \) with respect to the product measure \( \mu = \mu_U \times \mu_V \) on \( Q = Q_U \times Q_V \), then

\[
K_{XY}(s,t) = \int_Q s(u)t(v)p(u,v)d\mu(u,v) = K_Y(\mathbb{E}^V s, t) = K_X(\mathbb{E}^U t, s) \quad (39)
\]

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for conditional expectation operators

\[
\begin{align*}
E^V s &= E[s(U)|V = \cdot] : E_1 \to E_2, \\
E^U t &= E[t(V)|U = \cdot] : E_2 \to E_1.
\end{align*}
\]

Since \( g = K_Y(\cdot, t_g), g \in \mathcal{H}_Y \), it follows from the reproducing property that

\[
(Tg)(s) = \langle K_{XY}(s, \cdot), K_Y(\cdot, t_g) \rangle_{\mathcal{H}_Y} = K_{XY}(s, t_g) = K_X(E^Ut_g, s). 
\tag{40}
\]

Similarly,

\[
(T^*f)(t) = \langle K_{XY}(\cdot, t), K_X(\cdot, s_f) \rangle_{\mathcal{H}_X} = K_{XY}(s_f, t) = K_Y(E^Vs_f, t). 
\tag{41}
\]

Thus, by isometry, \( E^V \) is compact if and only if the same is true for \( E^U \) which, in turn, is equivalent to the compactness of \( T \) or \( T^* \).

If \( T^*T \) is compact then we may write \( T = \sum \rho_j f_j \otimes g_j \), where the \( f_j \) and \( g_j \) are the eigenvectors of \( T T^* \) and \( T^*T \) corresponding to the eigenvalue \( \rho_j^2 \). Using (40)–(41), we find

\[
\begin{align*}
& s_{Tg} = E^Ut_g, \quad t_{T^*f} = E^Vs_f, 
\end{align*}
\tag{42}
\]

and hence that

\[
(T^*Tg)(t) = K_Y(E^V E^Ut_g, t) 
\tag{43}
\]

and

\[
(TT^*f)(s) = K_X(E^U E^Vs_f, s). 
\tag{44}
\]

A direct calculation using (43)–(44) reveals that the functions \( s_{f_j} \) and \( t_{g_j} \) that correspond to the linear functionals \( f_j \) and \( g_j \) in the polar representation of \( T \) are, respectively, eigenvectors of the \( L^2(Q_U \times Q_U) \) and \( L^2(Q_V \times Q_V) \) integral operator kernels

\[
K_U(u_1, u_2) = \int_{Q_V} \frac{p(u_1, v)p(u_2, v)}{p_V(v)} d\mu_V(v) 
\tag{45}
\]
and

$$K_V(v_1, v_2) = \int_{Q_U} \frac{p(u, v_1)p(u, v_2)}{pU(u)} d\mu_U(u).$$

(46)

The canonical variables of the $X$ and $Y$ space that correspond to $\rho_j$ are then $s_{f_j}(U)$ and $t_{g_j}(V)$.

The functions $s_{f_j}$ and $t_{g_j}$ have interpretations in terms of the conditional expectation operators as a result of (40)–(41). Specifically, since $T g_j = \rho_j f_j$ and $T^* f_j = \rho_j g_j$ we see from (42) that

$$\mathbb{E}^U t_{g_j} = \rho_j s_{f_j} \quad \text{and} \quad \mathbb{E}^V s_{f_j} = \rho_j t_{g_j}.$$  

(47)

This last result is the motivation for the ACE algorithm in Breiman and Friedman [8] for computing the first set of canonical variables. In this regard, ACE can now be seen as representing the $L^2_X$ and $L^2_Y$ image of the power method for computing singular values of an operator (e.g., Householder [9], §7.4) being applied to $T$ to obtain $f_1$ and $g_1$ in $\mathcal{H}_X$ and $\mathcal{H}_Y$. In view of (45)–(46) an alternative approach would be to numerically solve for $s_{f_1}$ and $t_{g_1}$ directly via their corresponding integral operators. Like ACE, the latter approach can also be implemented with data through the use of nonparametric smoothers.

Now let us consider conditions under which $T$ is compact. For this purpose let $\{\phi_i\}, \{\theta_i\}$ be CONSs in $\mathcal{H}_X, \mathcal{H}_Y$ and $a_{ij} = \langle \phi_i, (\theta_j, K_{XY})_{\mathcal{H}_Y}\rangle_{\mathcal{H}_X}$, where, by the congruence of $\mathcal{H}_X$ and $E_1$ and (42),

$$a_{ij} = \langle \phi_i, T\theta_j \rangle_{\mathcal{H}_X} = \langle s_{\phi_i}, s_{T\theta_j} \rangle_{E_1} = \langle s_{\phi_i}, \mathbb{E}^U t_{\theta_j} \rangle_{E_1} = K_{XY}(s_{\phi_i}, t_{\theta_j}).$$

(48)

Theorem 2 then has the implication that $T^*T$ is Hilbert-Schmidt if and only if

$$\|K_{XY}\|_{\mathcal{H}_X \otimes \mathcal{H}_Y}^2 = \sum_{i,j} a_{ij}^2 < \infty.$$  

Using the fact that $\langle 1, s_{\phi_i} \rangle_{E_1} = \langle 1, t_{\theta_j} \rangle_{E_2} = 0$, it is easy to verify that

$$\langle s_{\phi_i}(\cdot), (t_{\theta_j}(\cdot), \frac{p(\cdot, \cdot)}{pU(\cdot)pV(\cdot)} - 1 \rangle_{E_2} \rangle_{E_1} = K_{XY}(s_{\phi_i}, t_{\theta_j}) = a_{ij}. $$
By (33) and the fact that \( \{ \phi_i \theta_j \} \) is a CONS for \( \mathcal{H}_X \otimes \mathcal{H}_Y \), we then conclude that

\[
\frac{p}{p_U p_V} - 1 = \sum_{i,j} a_{ij} s_{\phi_i} t_{\theta_j} \quad \text{a.e. } \mu. \tag{49}
\]

Hence, \( \sum_{i,j} a_{ij}^2 = \int_Q (p_U p_V - 1)^2 p_U p_V d\mu \) which is Pearson’s classical \( \phi^2 \) dependence measure. Consequently, when \( T^* T \) is Hilbert-Schmidt \( U \) and \( V \) are independent if and only if \( \phi^2 = 0 \).

The polar representation of \( T \) in conjunction with the Hilbert-Schmidt condition and (49) allow us to write \( p = p_U p_V + \sum_{j=1}^{\infty} \rho_j s_{f_j} t_{g_j} \) a.e. \( \mu \) which is Lancaster’s canonical decomposition of a bivariate density (e.g., Lancaster [20], p. 95). He termed the \( \rho_j \) “canonical correlations” and we see that the name is indeed justified as they represent maximal correlations between linear combinations and limits of linear combinations of elements of the sets of square-integrable functions of the random variables \( U \) and \( V \). In particular, this has the implication that when \( T \) is Hilbert-Schmidt \( U \) and \( V \) are independent if and only if every linear combination of square-integrable functions of \( U \) is uncorrelated with every linear combination of square-integrable functions of \( V \).

Similar developments to those in this section are possible for other choices of \( E_1 \) and \( E_2 \) that restrict optimization to function spaces with properties that are of interest for other applications. A specific instance of this is provided by the work of Bach and Jordan [4] who assume that the functions of interest lie in RKHSs such as those in Example 2. The calculations for this case are conceptually the same as before and, for example, we can again show that \( T \) is Hilbert-Schmidt if and only if \( p/\sqrt{p_U p_V} \in E_1 \otimes E_2 \) under the the Bach and Jordan choices for \( E_1 \) and \( E_2 \). However, the details are somewhat involved and will be treated more thoroughly elsewhere.

5. Statistical inference

Our major goal in this section is to show that, under a quite general sampling scheme, consistent estimation of the various quantities in the RKHS-based canonical
correlation analysis can be achieved as sample size tends to infinity. To accomplish this we will employ sets of \( m \) grid points \( E_{1m} = \{s_1, \ldots, s_m\} \subset E_1, E_{2m} = \{t_1, \ldots, t_m\} \subset E_2 \). Then, the idea is that we will either observe sample paths from the \( X \) and \( Y \) processes over \( E_{1m}, E_{2m} \) or project more densely observed readings onto these grids. Similar developments are possible with sets \( E_{1m_1}, E_{2m_2} \) of different size and the grid elements are actually allowed to depend on sample size considerations subsequently subject only to a denseness condition. One can argue on this latter basis that our results should extend to cases where all sample paths are observed at different grid points provided that such grids eventually share a dense set of ordinates. From a practical perspective, the most restrictive assumption is that we observe the \( X \) and \( Y \) processes without error. Both the theoretical results of this section and our estimation algorithm will need modification to effectively deal with signal plus noise scenarios.

Corresponding to \( E_{1m}, E_{2m} \) let \( \hat{\mathcal{H}}^m_Y \) and \( \hat{\mathcal{H}}^m_X \) be the RKHSs generated to the restrictions of \( K_X \) and \( K_Y \) to \( E_{1m} \times E_{1m} \) and \( E_{2m} \times E_{2m} \), respectively. Then, we define

\[
\hat{\mathcal{H}}^m_X = \text{span}\{K_X(\cdot, s_1), \ldots, K_X(\cdot, s_m)\} \quad \text{and} \quad \hat{\mathcal{H}}^m_Y = \text{span}\{K_Y(\cdot, t_1), \ldots, K_Y(\cdot, t_m)\},
\]

which are subspaces of \( \mathcal{H}_X \) and \( \mathcal{H}_Y \).

Assume for the rest of this section that \( K_{XY} \in \mathcal{H}_X \otimes \mathcal{H}_Y \) (cf. Theorem 2) and let \( \tilde{K}^m_{XY} \) to be the minimum \( \mathcal{H}_X \otimes \mathcal{H}_Y \) norm interpolant to \( K_{XY} \) on \( E_1 \times E_2 \). If we define the matrices \( K_X(m) = \{K_X(s_i, s_j)\}, K_Y(m) = \{K_Y(t_i, t_j)\}, K_{XY}(m) = \{K_{XY}(s_i, t_j)\} \), then

\[
\tilde{K}^m_{XY}(s, t) = \sum_{i,j} a_{ij} K_X(s, s_i) K_Y(t, t_j),
\]

with \( A = \{a_{ij}\} \) the solution of \( K_X(m) A K_Y(m) = K_{XY}(m) \): i.e.,

\[
A = K_X^{-1}(m) K_{XY}(m) K_Y^{-1}(m).
\] (50)
It follows that if $E_{1m}, E_{2m}$ grow dense in $E_1, E_2$, then
\[
\|\tilde{K}_{XY}^m - K_{XY}\|_{\mathcal{H}_X \otimes \mathcal{H}_Y} \to 0.
\] (51)

Using $\tilde{K}_{XY}^m$ we approximate $T$ in (25) with
\[
(T_m g)(s) = \langle \tilde{K}_{XY}^m(s, \cdot), g \rangle_{\mathcal{H}_Y} = \sum_{i,j} a_{ij} K_X(s, s_i) (K_Y(\cdot, t_j), g)_{\mathcal{H}_Y} = \sum_{i,j} a_{ij} K_X(s, s_i) g(t_j).
\]

The singular values of $T_m$ have a direct connection to those from standard multivariate analysis, as revealed by the following result.

**Lemma 4.** The set of singular values of $T_m$ are equal to the set of canonical correlations between the vectors $X(m) = (X(s_1), \ldots, X(s_m))'$ and $Y(m) = (Y(t_1), \ldots, Y(t_m))'$.

The random variables $\sum_{i=1}^m a_i X(s_i)$ and $\sum_{i=1}^m b_i Y(t_i)$ form a pair of canonical variables of $X(m), Y(m)$ if and only if $\sum_{i=1}^m a_i K_X(\cdot, s_i)$ and $\sum_{i=1}^m b_i K_Y(\cdot, t_i)$ form the corresponding pair of polar representation functions for $T_m$.

The next result concerns the approximation of $T$ by $T_m$ as $m \to \infty$. In order for $T_m$ to completely reflect $T$ in the limit we need for the subspaces $\tilde{\mathcal{H}}_X^m$ and $\tilde{\mathcal{H}}_Y^m$ to become dense in $\mathcal{H}_X$ and $\mathcal{H}_Y$, respectively. Although more general developments are possible, it will simplify the presentation if we accomplish this by simply assuming that $\{E_{1m}\}, \{E_{2m}\}$ are nondecreasing sequences of sets.

**Lemma 5.** Let $E_{1m}, E_{2m}$ be nondecreasing set sequences such that $\text{span}\{K_X(\cdot, s) : s \in \cup_n E_{1m}\}$ and $\text{span}\{K_Y(\cdot, t) : t \in \cup_n E_{2m}\}$ are dense in $\mathcal{H}_X$ and $\mathcal{H}_Y$, respectively. Assume that the singular values of $T$ are distinct, and denote by $\rho_k$ the $k$th largest singular value with corresponding polar functions $f_k \in \mathcal{H}_X$ and $g_k \in \mathcal{H}_Y$. Also, let $\rho_{km}$ be the $k$th largest canonical correlation between the vectors $X(m) = (X(s_1), \ldots, X(s_m))'$ and $Y(m) = (Y(t_1), \ldots, Y(t_m))'$ with $\sum_{i=1}^m a_{ikm} X(s_i)$ and $\sum_{i=1}^m b_{ikm} Y(t_i)$ the corresponding canonical variables for $k = 1, \ldots, m$. Then, for each fixed $k$, as $n \to \infty$ we have $\rho_{km} \to \rho_k$.

\[
f_{km} := \sum_{i=1}^m a_{ikm} K_X(\cdot, s_i) \to f_k(\cdot) \text{ in } \mathcal{H}_X \text{ and } g_{km} := \sum_{i=1}^m b_{ikm} K_Y(\cdot, t_i) \to g_k(\cdot) \text{ in } \mathcal{H}_Y.
\]
Note that if \((f_k, g_k)\) is a pair of polar functions then so is \((-f_k, -g_k)\). Thus, the convergence of \((f_{km}, g_{km})\) refers to convergence to one of the two possible pairs.

By the congruence of \(L^2_X\) and \(\mathcal{H}_X\) and that of \(L^2_Y\) and \(\mathcal{H}_Y\), the convergence of \(\|f_{km} - f_k\|_{\mathcal{H}_X}\) and \(\|g_{km} - g_k\|_{\mathcal{H}_Y}\) to 0 is equivalent to
\[
\sum_{i=1}^{m} a_{ikm} X(s_i) \xrightarrow{L^2_X} \Psi_X(f_k) \quad \text{and} \quad \sum_{i=1}^{m} b_{ikm} Y(t_i) \xrightarrow{L^2_Y} \Psi_Y(g_k).
\]

Thus, fix \(m\) and suppose that we observe \(n\) iid copies of \(X(m)\) and \(Y(m)\). Based on this sample, for each \(k\) let \(\hat{\rho}_{km}^{n}\) be an estimate of \(\rho_{km}\) and \(\sum_{i=1}^{m} \hat{a}_{ikm} X(t_i)\) and \(\sum_{i=1}^{m} \hat{b}_{ikm} Y(s_i)\) be estimates of \(\sum_{i=1}^{m} a_{ikm} X(t_i)\) and \(\sum_{i=1}^{m} b_{ikm} Y(s_i)\). An obvious example of such estimates are the sample canonical correlations and variables that can be obtained using ordinary multivariate canonical correlation analysis on the \(X(m), Y(m)\) data. The following result now follows simply from Lemma 5.

**Theorem 6.** For fixed \(k, m\) suppose that \(\hat{\rho}_{km}^{n} \xrightarrow{p} \rho_{km}\), \(\sum_{i=1}^{m} \hat{a}_{ikm} X(s_i) \xrightarrow{L^2_X} \sum_{i=1}^{m} a_{ikm} X(s_i)\), and \(\sum_{i=1}^{m} \hat{b}_{ikm} Y(t_i) \xrightarrow{L^2_Y} \sum_{i=1}^{m} b_{ikm} Y(t_i)\) as \(n \to \infty\). Then, under the conditions of Lemma 5,

\[
\lim_{m \to \infty} \limsup_{n \to \infty} \mathbb{P}(|\hat{\rho}_{km}^{n} - \rho_{km}| > \varepsilon) = 0, \quad \varepsilon > 0,
\]
\[
\lim_{m \to \infty} \limsup_{n \to \infty} \| \sum_{i=1}^{m} \hat{a}_{ikm} X(s_i) - \Psi_X(f_k) \|_{L^2_X} = 0,
\]
\[
\lim_{m \to \infty} \limsup_{n \to \infty} \| \sum_{i=1}^{m} \hat{b}_{ikm} Y(t_i) - \Psi_Y(g_k) \|_{L^2_Y} = 0.
\]

Procedures that satisfy the assumptions of Theorem 6 do exist; the most common one is the finite-dimensional sample canonical correlations and variables. (See, e.g., Muirhead and Wateraux [22] and Anderson [1].) For such a procedure, the interpretation of the theorem is that provided \(m\) tends to \(\infty\) at a slow enough rate with sample size \(n\), it is consistent under the RKHS framework. The derivation of the suitable rate of \(m\) differs from case to case, and typically requires a subtle analysis using perturbation theory. In general, one will need \(m\) to be much smaller than \(n\) to
establish such a result. Indeed, work by Bickel and Levina [7] in a related setting can be regarded as a testament to the dangers of letting \( m \) grow too rapidly.

One can view \( m \) in Theorem 6 as playing the role of a crude regularization parameter. From this perspective, it seems natural to replace interpolation on subspaces of restricted size with standard methods from nonparametric smoothing with the hopes of realizing better finite sample performance. Indeed, Leurgans, Moyeed and Silverman [21] state that smoothing is “absolutely essential” for functional canonical correlation. Accordingly, we explore one approach that has ties to their work in the next section.

6. Algorithm and numerical example

This section introduces a prototype smoothing based method that can be employed to implement the inferential concepts presented in §5. The discussion here is aimed at demonstrating that practical implementation of our approach is feasible rather than providing a thoroughly refined treatment of computational issues. Indeed, development and extension of the methodology that follows are topics of ongoing research.

To illustrate the idea, we will focus on the case of \( E_1 = E_2 = [0, 1] \) with \( K_X, K_Y \) and \( K_{XY} \) smooth theoretical covariance functions of the \( X, Y \) processes. Also let \( K_X = \{K_X(s_i, s_j)\}, K_Y = \{K_Y(t_i, t_j)\}, K_{XY} = \{K_{XY}(s_i, t_j)\}. \) Then, given readings \( x_i, y_i, i = 1, \ldots, n, \) from \( n \) copies of \( X \) and \( Y \) sample path pairs at indices corresponding to the grid points \( s_1, \ldots, s_m \) and \( t_1, \ldots, t_m, \) respectively, we propose to estimate the various quantities of interest via the following algorithmic steps.

(a) Estimate \( K_X, K_Y \) and \( K_{XY} \) by the sample covariance matrices \( \hat{K}_X, \hat{K}_Y \) and \( \hat{K}_{XY}. \)

(b) Compute a smooth, continuous version \( \tilde{K}_X, \tilde{K}_Y \) of \( \hat{K}_X, \hat{K}_Y \) via some suitable smoothing method. As one possibility we adopt here the approach discussed in
Silverman (1996) that uses cubic smoothing splines along with computation of the eigenvalues and eigenvectors from a generalized eigen equation of the form

$$\hat{K}_X f = \lambda (I + \eta D) f.$$  \hfill (53)

Here $\eta$ is a smoothing parameter and $D$ is a matrix such that $f'Df = \int [f''(x)]^2$ for the natural cubic spline $f$ that interpolates $f = (f(s_1), \ldots, f(s_m))'$ (see, e.g., formula (2.3) of Green and Silverman [12]). The smoothing parameter $\eta$ is chosen as follows. For $\eta \in (0, \infty)$ and $i = 1, \ldots, n$, let $f_i^{[-i]}(\eta), \ldots, f_i^{[-i]}(\eta)$ be the eigenvectors that correspond to the nonzero eigenvalues of the eigen equation

$$\hat{K}_X^{[-i]} f = \lambda (I + \eta D) f,$$  \hfill (54)

where $\hat{K}_X^{[-i]}$ denotes the sample covariance matrix computed without the $i$th observation $x_i$. For each $\ell$ let $\Pi^{[-i]}_\ell(\eta)$ be the projection onto the linear space spanned by $f_j^{[-i]}(\eta), 1 \leq j \leq \ell$, and define the cross-validation (CV) criterion

$$CV(\eta) = \sum_{\ell=1}^M \sum_{i=1}^n \left\| (I - \Pi^{[-i]}_\ell(\eta)) x_i \right\|^2,$$

where $M$ is chosen subjectively to be a relatively small number to save computations. We then pick an $\eta$ that minimizes $CV(\eta)$.

(c) Suppose that the nonzero eigenvalues obtained from Step (b) are $\lambda_1, \ldots, \lambda_L$ with corresponding eigenvectors $f_1, \ldots, f_L$. Let $f_1, \ldots, f_L$ be the interpolating natural cubic splines for $f_1, \ldots, f_L$ and set

$$\tilde{K}_X(s, s') = \sum_{i=1}^L \lambda_i f_i(s) f_i(s') \quad \text{and} \quad \tilde{K}_X = \{ \tilde{K}_X(s_i, s_j) \}$$

with $\tilde{K}_Y$ and $\tilde{K}_Y$ defined similarly.

(d) In accordance with the assumption that $K_{XY} \in \mathcal{H}_X \otimes \mathcal{H}_Y$, we can now compute $\hat{A} = \hat{K}_X \hat{K}_{XY} \hat{K}_Y$. However, we also include a smoothing parameter here:
namely, the number \( r_x, r_y \) of eigenvectors used to construct the generalized inverses \( \hat{K}_X^{-1} \) and \( \hat{K}_Y^{-1} \). For convenience assume that \( r_x = r_y = r \). (The choice of \( r \) can be obtained from a CV procedure explained further below.) The matrix \( \hat{A} \) is then used to produce a smooth cross covariance function via

\[
\hat{K}_{XY}(s, t) = \left[ \hat{K}_X(s, s_1), \ldots, \hat{K}_X(s, s_m) \right] \hat{A} \left[ \hat{K}_Y(t, t_1), \ldots, \hat{K}_Y(t, t_m) \right]',
\]

and thereby obtain \( \hat{K}_{XY} = \{ \hat{K}_{XY}(s_i, t_j) \} \).

(e) Let \( \hat{T} \) and \( \hat{T}^\ast \) be the operators

\[
(\hat{T} g)(s) = \langle \hat{K}_{XY}(s, \cdot), g(\cdot) \rangle_{\mathcal{H}(\hat{K}_Y)}, \quad g \in \mathcal{H}(\hat{K}_Y),
\]

\[
(\hat{T}^\ast f)(t) = \langle \hat{K}_{XY}(\cdot, t), f(\cdot) \rangle_{\mathcal{H}(\hat{K}_X)}, \quad f \in \mathcal{H}(\hat{K}_X)
\]

and let us focus on those \( g \in \mathcal{H}(\hat{K}_Y) \) that are in \( \text{span}(\hat{K}_Y(t_1, \cdot), \ldots, \hat{K}_Y(t_m, \cdot)) \) with \( g = (g(t_1), \ldots, g(t_m))' \). Then,

\[
\langle \hat{T}^\ast \hat{T} g, g \rangle_{\mathcal{H}(\hat{K}_Y)} = g' \hat{K}_Y^{-1} \hat{K}_Y \hat{K}_X^{-1} \hat{K}_{XY} \hat{K}_Y^{-1} g,
\]

\[
\langle g, g \rangle_{\mathcal{H}(\hat{K}_Y)} = g' \hat{K}_Y^{-1} g,
\]

\[
\Psi_{\hat{K}_Y}(g) = g' \hat{K}_Y^{-1} Y
\]

with similar identities holding for \( \langle \hat{T} T^\ast f, f \rangle_{\mathcal{H}(\hat{K}_X)}, \langle f, f \rangle_{\mathcal{H}(\hat{K}_X)} \) and \( \Psi_{\hat{K}_Y}(f) \). A matrix singular-value decomposition of \( \hat{K}_Y^{-1} \hat{K}_Y X \hat{K}_X^{-1} \hat{K}_{XY} \hat{K}_Y^{-1} \) produces eigenvectors \( g_i \) and eigenvalues \( \lambda_i, i = 1, \ldots, r \) with the natural cubic spline interpolant \( g_i \) of \( g_i \) giving \( f_j = (1/\sqrt{\lambda_j}) \hat{T} g_j, j = 1, \ldots, r. \) That is,

\[
f_j(s) = (1/\sqrt{\lambda_j})[\hat{K}_X(s, s_1), \ldots, \hat{K}_X(s, s_m)] \hat{A} g_j,
\]

\[
f_j = (f(s_1), \ldots, f(s_m))' = (1/\sqrt{\lambda_j}) \hat{K}_{XY} \hat{K}_Y g_j.
\]

The estimated canonical variables are then taken to be

\[
\hat{\xi}_j = \Psi_{\hat{K}_X}(f_j) =: (a_j, X)_{\mathbb{R}^m}, \quad \text{and} \quad \hat{\zeta}_j = \Psi_{\hat{K}_Y}(g_j) =: (b_j, Y)_{\mathbb{R}^m}.
\]

(55)
Remark 6.1. An adaptive method for choosing the smoothing parameter $r$ in Step (d) can be patterned after developments in Leurgans, Moyeed, and Silverman [21]. Let the vectors $a_{j}^{[i,r]}$ and $b_{j}^{[i,r]}$ be those obtained in (55) with smoothing parameter $r$ and with the pair $x_i, y_i$ left out in the cross covariance computation. Note, however, that we continue to use the same smoothed principal components for the auto covariances that were computed initially. Now compute

$$d[r] = n^{-1} \sum_{i=1}^{n} \langle a_{1}^{[i,r]}, x_{i} \rangle_{\mathbb{R}^m} \langle b_{1}^{[i,r]}, y_{i} \rangle_{\mathbb{R}^m}$$

and select $\hat{r}$ to be the maximizer of $|d[r]|$. We have found this approach to be effective in some limited numerical work.

Remark 6.2. While our notion of canonical correlations is different from that of Leurgans, Moyeed, and Silverman [21], it is possible to compare the smoothing procedures that are used in the implementation of the two concepts. Perhaps the most substantial difference in this respect is that Leurgans et al. [21] do not estimate the covariance functions in estimating functional canonical correlations. Instead, they work directly with sample covariance matrices and put a roughness penalty on the singular vectors. We have experimented with that approach in our context of canonical correlations, as well. However, the results to date have been disappointing relative to other options that we have considered.

To illustrate the use of our estimation algorithm, consider the case where

$$X(s) = \sum_{j=1}^{20} j^{-1/2} U_j \sqrt{2} \sin(j \pi s),$$

$$Y(t) = (U_3 + V_1) \sqrt{2} \sin(\pi t) + \sum_{j=2}^{20} j^{-1/2} V_j \sqrt{2} \sin(j \pi t),$$

for $s, t \in [0, 1]$ and the $U_j$ and $V_j$ are iid standard normal random variables. A typical $(X, Y)$ process pair obtained from (56)-(57) is shown in panel (a) of Figure 1.
Figure 1: Canonical analysis for simulated data: (a) solid (dashed) curve is $X \ (Y)$ sample path, (b) upper (lower) solid curve is $g_1 \ (f_1)$ and upper (lower) dashed curve is $\hat{g}_1 \ (\hat{f}_1)$, (c) $\hat{\xi}_1$ versus $\xi_1$ and (d) $\hat{\zeta}_1$ versus $\zeta_1$.

In this instance,

\[
K_X(s, s') = \sum_{j=1}^{20} 2^{j-1} \sin(j\pi s) \sin(j\pi s'),
\]

\[
K_Y(t, t') = 4 \sin(\pi t) \sin(\pi t') + \sum_{j=2}^{20} 2^{j-1} \sin(\pi t) \sin(j\pi t'),
\]

\[
K_{XY}(s, t) = \frac{2}{\sqrt{3}} \sin(3\pi s) \sin(\pi t).
\]
The integral representation theorem discussed in §2 then has the consequence that $\mathcal{H}_Y$ consist of functions of the form $g(t) = \sum_{j=1}^{20} \lambda_j g_j \sqrt{2} \sin(j \pi t)$ for real coefficients $g_j$ and $\lambda_1 = 2, \lambda_j = 1/j, j = 2, \ldots, 20$. Similarly, the functions in $\mathcal{H}_X$ can be represented as $f(s) = \sum_{j=1}^{20} \lambda_j f_j \sqrt{2} \sin(j \pi s)$ with $\lambda_j = 1/j, j = 1, \ldots, 20$. Direct calculations then reveal that $(Tg)(s) = g_1 \sqrt{2} \sin(3 \pi s)/\sqrt{3}$ and $(T^* f)(t) = f_3 \sqrt{3} \sin(\pi t)/\sqrt{3}$. As a result, there is only one nonzero canonical correlation $\rho_1 = 1/\sqrt{2} = .707$ for which the corresponding singular functions are $f_1(s) = \sqrt{2} \sin(3 \pi s)/\sqrt{3}$ and $g_1(t) = 2 \sin(\pi t)$.

An application of Proposition A2 then produces the canonical variables $\xi_1 = U_3$ and $\zeta_1 = (U_3 + V_1)/\sqrt{2}$.

We analyzed 100 $(X, Y)$ process pairs (that included the pair in panel (a) of Figure 1) that were simulated from (56)-(57) via our estimation algorithm. Here we took $m = 60$ while selecting $s$ and $t$ as uniformly spaced points on $[0, 1]$. The first three estimated canonical correlations were $\hat{\rho}_1 = .672, \hat{\rho}_2 = .167$ and $\hat{\rho}_3 = .008$. The estimated (and actual) polar representation functions $\hat{f}_1, \hat{g}_1$ corresponding to $\hat{\rho}_1$ are shown in panel (b) of Figure 1 while plots of the estimated and true first canonical variables are provided in panels (c) and (d) for the $X$ and $Y$ spaces, respectively.

We replicated the experiment that produced the results in Figure 1 a total of 100 times. The first quartile, median and third quartiles for the first, second and third estimated canonical correlations were (.6241, .6742, .7137), (.1445, .2012, .2622) and (.0371, .0778, .1334), respectively. The parallel statistics for the cross-validation estimator of $r$ are (3, 3, 4) with a minimum of 2 and a maximum of 12. The value $\hat{r} = 12$ represents a single outlier (both in terms of the value of $\hat{r}$ as well as the corresponding canonical correlation estimates) with the next smallest choice being 8.

At least in terms of this particular type of data, the simulation suggests that our algorithm succeeds in consistently detecting the presence of a single, dominant set of canonical variables. However, the resolution of, e.g., the second, null canonical correlation leaves something to be desired. This type of performance is apparently
not entirely unusual for estimation in this setting.

The definitive empirical study of functional canonical correlation is currently provided by He, Müller and Wang [14]. These authors note the difficulty of estimating higher (than first) order canonical correlations and the poor performance of our estimator for the second canonical correlations in the simulation is undoubtedly a reflection of this same issue. In this regard it is of interest to note that the (empirical) mean squared errors (after removing the case with \( \hat{r} = 12 \)) for estimating the first and second canonical correlations were .0065 and .0532 in our simulation experiment. These are quite comparable to the empirical mean squared error values .0052 and .0770 that were reported by He, Müller and Wang [14] for estimating the first two canonical correlations in a similar setting using their FCA-EB Two-Stage procedure with their \( EC_1 \) estimator being employed for estimation of \( \rho_1 \).

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References.


Appendix

Proposition A1. If $\eta \in L^2_X$, then $\Psi^{-1}(\eta)(\cdot) = \mathbb{E}[\eta X(\cdot)]$.

Proof. Note that this is a result due to Loève. Let $\eta$ be the limit of a sequence $\eta_n = \sum_{i=1}^{n} a_{ni}X(t_{ni})$ in $L^2_X$ and observe that $f_n = \Psi^{-1}(\eta_n)$, $f = \Psi^{-1}(\eta)$ satisfy $\|f_n - f\|_{\mathcal{H}(K)} \to 0$. Since norm convergence implies point-wise convergence in $\mathcal{H}(K)$, for each $t \in E$,

$$f_n(t) = \sum_{i=1}^{n} a_{ni}\Psi^{-1}(X(t_{ni}))(t) = \sum_{i=1}^{n} a_{ni}K(t, t_{ni}) = \sum_{i=1}^{n} a_{ni}\mathbb{E}[X(t)X(t_{ni})] = \mathbb{E}[\eta_n X(t)]$$

converges to $f(t)$ and continuity of the $L^2_X$ inner product insures that $\lim \mathbb{E}[\eta_n X(t)] = \mathbb{E}[\eta X(t)]$. \qed

Proposition A2. Assume that $X$ is a stochastic process satisfying (10), and having a covariance function denoted by $K$. Then each $f \in \mathcal{H}(K)$ can be written as $f(\cdot) = \int_{Q} g(q)\phi(\cdot, q)d\mu(q)$ for some $g \in L^2(Q)$, and (11) holds.

Proof. The conclusion follows from Proposition A1 upon recognizing that

$$\mathbb{E} \left( \int_{Q} g(q)dZ(q)X(t) \right) = \int_{Q} g(q)\phi(t, q)d\mu(q) = f(t).$$

\qed

Proposition A3. The mapping $T$ in (25) is a bounded linear operator from $\mathcal{H}_Y$ to $\mathcal{H}_X$ with adjoint

$$(T^* f)(t) = \langle K_{XY}(\cdot, t), f(\cdot) \rangle_{\mathcal{H}_X}, \quad f \in \mathcal{H}_X, \quad (58)$$

and operator norm at most 1.

Proof. Let $\Pi_Y$ be the projection operator onto $L^2_Y$ from the set of square-integrable functions on the joint probability space for the $X$ and $Y$ process. Then, for any square-integrable $\eta$ in the probability space, Proposition A1 entails that

$$\mathbb{E}[\eta Y(\cdot)] = \mathbb{E}[(\Pi_Y \eta)Y(\cdot)] = \Psi_Y^{-1}(\Pi_Y \eta)(\cdot) \in \mathcal{H}_Y$$
because \( \Pi_Y \eta - \eta \perp L^2_Y \). In particular, taking \( \eta = X(s) \) for any \( s \in E_1 \) we obtain \( K_{XY}(s, \cdot) \in \mathcal{H}_Y \), and, interchanging the roles of \( X \) and \( Y \), we also conclude that \( K_{XY}(\cdot, t) \in \mathcal{H}_X \) for any \( t \in E_2 \). But, \( \langle K_{XY}(*, \cdot), K_Y(t, \cdot) \rangle_Y = K_{XY}(*, t) \in \mathcal{H}_X \) as a result of the reproducing property. Thus, by the RKHS property (v) listed in \( \S 2 \),

\[ \langle K_{XY}(s, \cdot), g(\cdot) \rangle_Y \in H_X \]

for any \( g \in H_Y \).

Now take \( f_m(\cdot) = \sum_{i=1}^{m} a_{im} K_X(\cdot, s_{im}) \in H_X \) and \( g_{m'}(\cdot) = \sum_{i=1}^{m'} b_{im'} K_Y(\cdot, t_{im'}) \in H_Y \), and observe that

\[ \langle T g_{m'}, f_m \rangle_{H_X} = \text{Cov} \left( \sum_{i=1}^{m} a_{im} X(s_{im}), \sum_{i=1}^{m'} b_{im'} Y(t_{im'}) \right) \text{.} \]

(59)

Thus, the Cauchy-Schwarz inequality insures that \( |\langle T g_{m'}, f_m \rangle_{H_X}| / \|g_{m'}\|_{H_Y} \leq \|f_m\|_{H_X} \) and the norm of \( T \) is at most 1. Finally, verification of (58) is straightforward.

\( \Box \)

**Proposition A4.** Consider the integral operator \( U : L^2[0,1] \mapsto L^2[0,1] \) defined by

\[ (Uf)(t) = \int_0^1 K(\cdot, t)f(t)dt, \quad f \in L^2[0,1], \]

where \( K \) is a continuous covariance kernel. Denote by \( \lambda_q \) the nonzero eigenvalues of \( U \) and \( \phi_q \) the corresponding eigenfunctions and let \( \mathcal{H} \) be the closed linear span of \( \{ \phi_q \}_{q=1}^N \) in \( L^2[0,1] \). Then, \( \mathcal{H} \) and \( \mathcal{H}(K) \) are congruent under the mapping \( \Gamma : \mathcal{H} \mapsto \mathcal{H}(K) \) defined by

\[ \Gamma(f) := \sum_{q=1}^{N} \sqrt{\lambda_q} f_q \phi_q \]

(60)

for \( f = \sum_{q=1}^{N} f_q \phi_q \in \mathcal{H} \).

**Proof.** By Mercer’s Theorem (e.g., Riesz and Nagy 1978, page 245), the integral representation theorem (6)–(8) can be applied with \( Q = \{ 1, 2, \ldots \} \), \( \mathcal{B} \) the Borel sets for \( Q \), \( \mu(B) = \sum_{q \in B} \lambda_q \) for \( B \in \mathcal{B} \), and \( \phi(t,q) = \phi_q(t) \). Thus, the RKHS corresponding to \( K \) is

\[ \mathcal{H}(K) = \left\{ f = \sum_{q=1}^{N} \lambda_q g_q \phi_q : \sum_{q=1}^{N} \lambda_q^2 g_q^2 < \infty \right\} \text{.} \]

(61)
and, for \( f_i = \sum_{q=1}^{N} \lambda_q g_{iq} \phi_q, i = 1, 2 \), in \( \mathcal{H}(K) \), and the inner product is given by

\[
\langle f_1, f_2 \rangle_{\mathcal{H}(K)} = \sum_{q=1}^{N} \lambda_q g_{1q} g_{2q}.
\]

Since \( \Gamma(f) = \sum_{q=1}^{N} \lambda_q (f_q / \sqrt{\lambda_q}) \phi_q \), by (62) we have

\[
\|\Gamma(f)\|_{\mathcal{H}(K)}^2 = \sum_{q=1}^{N} \lambda_q (f_q / \sqrt{\lambda_q})^2 = \sum_{q=1}^{N} f_q^2 = \|f\|_{L^2[0,1]}^2.
\]

The inverse mapping can be treated similarly.

\[\square\]

**Proof of Theorem 3.** Define \( \Pi_n \) to be the projection of \( \mathcal{H}_X \) onto the subspace spanned by \( \{K_X(j, \cdot) : j = 1, \ldots, n\} \) and \( T_n = \Pi_n \circ T \). Since \( \text{Im}(T_n) \) is finite-dimensional, \( T_n \) is compact. Let \( g = \sum_{j=1}^{\infty} a_j K_Y(j, \cdot) \in \mathcal{H}_Y \) be such that \( \|g\|_{\mathcal{H}_Y} = 1 \).

Then, by the reproducing property,

\[
(T - T_n)g(t) = (I - \Pi_n)(K_{XY}(t, \cdot), g(\cdot))_Y = (I - \Pi_n) \sum_{j=1}^{\infty} a_j K_{XY}(t, j)
\]

\[
= (I - \Pi_n) \mathbb{E}[X(t)V],
\]

where \( V := \sum_{j=1}^{\infty} a_j Y(j) \). It then follows from Proposition A1 that \( \Psi_X((T - T_n)g) \) is the projection of \( V \) onto \( (L^2_{\{Z(t), t \leq n\}})^\perp \).

Suppose first that \( Z \) is strong-mixing. Then

\[
\|(T - T_n)g\|_{\mathcal{H}_X} = \sup_{U \in (L^2_{\{Z(t), t \leq n\}})^\perp} |\text{Corr}(U, V)| \leq \alpha_n \to 0.
\]

(63)

Thus, \( T_n \) converges to \( T \) in operator norm and so \( T \) is also compact.

Next assume that \( Z \) is not strong-mixing and \( T \) is compact. Then the two conditions combined imply that there exists a sequence of elements \( V_n \in L^2_{\{Z(s), s \leq 0\}}, U_n \in (L^2_{\{Z(t), t \leq n\}})^\perp \) with unit norms such that \( \text{Corr}(U_n, V_n) \to 0 \) and \( T g_n \) with \( g_n = \Psi_Y^{-1} V_n \) converges to some \( g \in \mathcal{H}_X \). Hence,

\[
(T - T_n)g_n = (I - \Pi_n)T g_n = (I - \Pi_n)g + (I - \Pi_n)(T g_n - g).
\]

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Clearly both terms tend to zero and, consequently, \((T - T_n)g_n\) tends to zero. However, as in (63),

\[
\|(T - T_n)g_n\|_{\mathcal{H}_X} = \sup_{U \in (L^2_{\mathbb{Z}(t), \tau \leq n))} |\text{Corr}(U, V_n)| \geq |\text{Corr}(U_n, V_n)| \not\to 0,
\]

and we arrive at a contradiction.

\[\Box\]

**Proof of Lemma 4.** On \(\hat{\mathcal{H}}_Y^m\) define the operator

\[
(\hat{T}_m h)(s) = \langle \hat{K}_{XY}^m(s, \cdot)|_{E_{2m}}, h \rangle_{\hat{\mathcal{H}}_Y^m} = \sum_{i,j} a_{ij} K_X(s, s_i) h(t_j), \quad s \in E_{1m}. \tag{64}
\]

Observe that \(T_m\) and \(\hat{T}_m\) have the same singular values, with the polar functions of the two operators being related by the mappings

\[
\Pi_X : \quad f \to f|_{E_{1m}}, \quad \hat{\mathcal{H}}_X^m \to \hat{\mathcal{H}}_X^m,
\]

\[
\Pi_Y : \quad g \to g|_{E_{2m}}, \quad \hat{\mathcal{H}}_Y^m \to \hat{\mathcal{H}}_Y^m.
\]

Now, if \(h \in \hat{\mathcal{H}}_Y\) we may write \(h(\cdot) = \sum_{i=1}^{m} h_i \hat{K}_Y(t_i, \cdot)\) for \(h_m = (h_1, \ldots, h_m)' \in \mathbb{R}^m\).

We then take

\[
H = K_X^{-1/2}(m) K_{XY}(m) K_Y^{-1/2}(m),
\]

and apply (5), (64) and (50) to obtain

\[
\langle \hat{T}_m \hat{T}_m h, h \rangle_{\hat{\mathcal{H}}_Y^m} = \langle \hat{T}_m h, \hat{T}_m h \rangle_{\hat{\mathcal{H}}_X^m} = h_m' A' K_X(m) A h_m
\]

\[
= h_m' K_Y^{-1/2}(m) K'_{XY}(m) K_X^{-1/2}(m) K_{XY}(m) K_Y^{-1/2}(m) h_m
\]

\[
= \langle \mathbf{K}_Y^{-1/2}(m) h_m, \mathbf{H} \mathbf{H} (\mathbf{K}_Y^{-1/2}(m) h_m) \rangle
\]

and \(\|h\|^2_{\hat{\mathcal{H}}_Y^m} = h_m' K_Y(m) h_m\). Hence, the polar representation of \(T_m\) is equivalent to that of \(H\) in \(\mathbb{R}^m\), where the latter clearly leads to the canonical correlations and variables of the vectors \(X(m)\) and \(Y(m)\).
Proof of Lemma 5. First, the assumption implies that there exist CONSs \( \{f_i, i \geq 1\}, \{g_j, j \geq 1\} \) for \( \mathcal{H}_X, \mathcal{H}_Y \), such that \( \{f_i, 1 \leq i \leq m\}, \{g_j, 1 \leq j \leq m\} \) are orthonormal bases for \( \tilde{\mathcal{H}}_X, \tilde{\mathcal{H}}_Y \). By (33),

\[
\langle (T - T_m)g, f \rangle_{\mathcal{H}_X} = \langle (K_{XY} - \tilde{K}^m_{XY}, g)_{\mathcal{H}_Y}, f \rangle_{\mathcal{H}_X} = \langle K_{XY} - \tilde{K}^m_{XY}, fg \rangle_{\mathcal{H}_X \otimes \mathcal{H}_Y}.
\]

Letting \( f = (T - T_m)g \), we have by the Cauchy-Schwarz inequality that

\[
\| (T - T_m)g \|_{\mathcal{H}_X}^2 \leq \| K_{XY} - \tilde{K}^m_{XY} \|_{\mathcal{H}_X \otimes \mathcal{H}_Y} : \| (T - T_m)g \|_{\mathcal{H}_X} \cdot \| g \|_{\mathcal{H}_Y},
\]

which, by (51), implies that \( \| (T - T_m) \| \to 0 \). It then follows that

\[
\lim_{n \to \infty} \sup_{\| g \|_{\mathcal{H}_Y} = 1} | \langle T^* T g, g \rangle_{\mathcal{H}_Y} - \langle T_m^* T_m g, g \rangle_{\mathcal{H}_Y} | = 0.
\]

(65)

Thus, the largest eigenvalue of \( T_m^* T_m \) converges to that of \( T^* T \). By (65), the largest eigenvalue of \( T_m^* T_m \) is \( \rho^2_{1m} \). Hence \( \rho_{1m} \to \rho_1 \).

Next, using the eigenfunctions \( g_i \) of \( T^* T \) as basis functions for \( \text{Ker}(T^* T)\perp \), we have

\[
T^* T g_{1m} = \sum_{i=1}^{\infty} \langle g_{1m}, g_i \rangle_{\mathcal{H}_Y} T^* T(g_i) = \sum_{i=1}^{\infty} \langle g_{1m}, g_i \rangle_{\mathcal{H}_Y} \rho^2_i g_i.
\]

Thus, \( \| T^* T g_{1m} \|_{\mathcal{H}_Y}^2 = \sum_{i=1}^{\infty} \langle g_{1m}, g_i \rangle_{\mathcal{H}_Y}^2 \rho^4_i \), while it follows from Lemma 5 that

\[
\| T^* T g_{1m} \|_{\mathcal{H}_Y}^2 = \| T_m^* T_m g_{1m} \|_{\mathcal{H}_Y}^2 + o(1) = \rho^4_1 + o(1).
\]

Since the \( \rho_i \) are decreasing we must have \( \langle g_{1m}, g_1 \rangle^2_{\mathcal{H}_Y} \to 1 \) and \( \sum_{i=2}^{\infty} \langle g_{1m}, g_i \rangle^2_{\mathcal{H}_Y} \to 0 \), or equivalently \( g_{1m} \to +g_1 \) or \( -g_1 \) in \( \mathcal{H}_Y \). Similar arguments can be used to establish the remainder of the lemma.

\( \square \)