

# Functional partial canonical correlation

QING HUANG\* and ROSEMARY RENAUT\*\*

School of Mathematics and Statistics, Arizonas State University, Tempe, AZ 85287, USA.  
E-mail: \*qing.huang@asu.edu; \*\*Rosie.Renaut@asu.edu

A rigorous derivation is provided for canonical correlations and partial canonical correlations for certain Hilbert space indexed stochastic processes. The formulation relies on a key congruence mapping between the space spanned by a second order,  $\mathcal{H}$ -valued, process and a particular Hilbert function space deriving from the process' covariance operator. The main results are obtained via an application of methodology for constructing orthogonal direct sums from algebraic direct sums of closed subspaces.

*Keywords:* congruent Hilbert space; covariance operator; Hilbert space indexed process; orthogonal direct sum

## 1. Introduction

Canonical correlation analysis (CCA) is one of the principal tools for studying the relationship between two random vectors in multivariate analysis. There have now been several attempts to widen the definition of CCA to include vectors of infinite length and, more generally, stochastic processes (see, e.g., Eubank and Hsing [8] and references therein). Functional canonical correlation falls into this latter category wherein one obtains data that represent the sample paths of continuous time processes. In this paper we provide a framework for canonical correlation and partial canonical correlation analysis for a class of stochastic processes that includes those arising in functional data.

A somewhat general formulation assumes that we have a probability space  $(\Omega, \mathcal{A}, P)$ , a real, separable Hilbert space  $\mathcal{H}$ , with norm and inner product  $\|\cdot\|$  and  $\langle \cdot, \cdot \rangle$  and an  $\mathcal{H}$ -valued random variable  $X$  in the sense of Laha and Rohatgi [15]; that is,  $X : \Omega \rightarrow \mathcal{H}$  is a measurable function relative to the Borel  $\sigma$ -field generated by the class of all open subsets of  $\mathcal{H}$ . Our attention will be restricted to random variables with  $E\|X\|^2 < \infty$  with expectation being relative to  $P$ . Associated with such a random variable we can define the Hilbert space indexed process

$$Z(f) = \langle X, f \rangle \tag{1.1}$$

for  $f \in \mathcal{H}$ . Then, from Vakhania *et al.* [20] there exists a mean element  $h \in \mathcal{H}$  and a covariance operator  $S$  such that  $E[\langle X, f \rangle] = \langle h, f \rangle$  and  $E[\langle X - h, f \rangle \langle X - h, f' \rangle] = \langle f, S f' \rangle$  for all  $f, f' \in \mathcal{H}$ . For simplicity, we assume that  $\|h\| = 0$ . In that case, the covariance operator is determined by

$$E[\langle X, f \rangle \langle X, f' \rangle] = \langle f, S f' \rangle. \tag{1.2}$$

It is well known that  $S$  in (1.2) is a trace class operator and therefore admits the eigenvalue–eigenvector decomposition

$$S = \sum_{j=1}^{\infty} \lambda_j \phi_j \otimes \phi_j, \tag{1.3}$$

where  $\lambda_1 \geq \lambda_2 \geq \dots > 0$  are the eigenvalues,  $\phi_j$  is the eigenvector associated with  $\lambda_j$  and  $(f \otimes g)h = \langle f, h \rangle g$  for  $f, g, h \in \mathcal{H}$ . A suitably normed version of the range of  $S$  gives us the reproducing kernel Hilbert space

$$\mathcal{H}(S) = \left\{ f: f = \sum_{j=1}^{\infty} \lambda_j f_j \phi_j, \|f\|_{\mathcal{H}(S)}^2 = \sum_{j=1}^{\infty} \lambda_j f_j^2 = \|S^{-1/2} f\|^2 < \infty \right\} \tag{1.4}$$

that includes  $\mathcal{H}$  as a proper subset when  $S$  is not finite dimensional which we hereafter assume to be the case. The reproducing kernel Hilbert space recasts the range of  $S$  under a weaker norm where  $S$  is invertible, since the Picard condition (Engl *et al.* [7])

$$\sum_{j=1}^{\infty} \frac{\langle f, \phi_j \rangle^2}{\lambda_j} = \sum_{j=1}^{\infty} \lambda_j f_j^2 < \infty$$

is satisfied for  $f \in \mathcal{H}(S)$ . For each  $f \in \mathcal{H}(S)$  there corresponds a random variable

$$Z(f) = \sum_{j=1}^{\infty} f_j \langle X, \phi_j \rangle.$$

These types of random variables are well defined and include those in the process (1.1) as a special case. Thus, for inferential purposes we can focus on the Hilbert space

$$L_Z^2 = \left\{ Z(f) = \sum_{j=1}^{\infty} f_j \langle X, \phi_j \rangle: \|Z(f)\|_{L_Z^2}^2 := \text{Var}(Z(f)) = \sum_{j=1}^{\infty} \lambda_j f_j^2 < \infty \right\} \tag{1.5}$$

which consists of all the linear combinations of the  $\langle X, \phi_j \rangle$  that have finite variance. Note that in addition to serving as an index set,  $\mathcal{H}(S)$  is isometrically isomorphic or congruent to  $L_Z^2$ : a relationship that will be exploited in the sequel. Parzen [16] calls  $\mathcal{H}(S)$  a congruent reproducing kernel Hilbert space.

For functional data,  $X$  and the  $\phi_j$  are typically functions on some continuous index set  $E$ . In that instance it follows from Kupresanin *et al.* [14] that working with  $L_Z^2$  is equivalent to working with the space spanned by the  $X$  process: that is,

$$L_X^2 = \overline{\left\{ a: a = \sum_{j=1}^n a_j X(t_j), t_j \in E, a_j \in \mathbb{R}, n = 1, 2, \dots \right\}} \tag{1.6}$$

under the inner product  $E[ab]$  for  $a, b \in L_X^2$ . In fact, functional canonical correlation can be treated directly from this latter perspective using reproducing kernel Hilbert space techniques

along the lines of those employed in Eubank and Hsing [8]. However, our present formulation in terms of  $L^2_Z$  has certain advantages (both mathematical and computational) and appears to generalize more readily to deal with partial canonical correlation and related ideas.

Assume now that we have two  $\mathcal{H}$ -valued random variables  $X_i, i = 1, 2$ , whose associated covariance operators  $S_i, i = 1, 2$ , have the eigenvalue–eigenvector sequences  $\{(\lambda_{ij}, \phi_{ij})\}_{j=1}^\infty$  from (1.3). These, in turn, produce Hilbert spaces  $L^2_{Z_i}, i = 1, 2$ , defined analogous to (1.5) for processes  $Z_i(f_i), i = 1, 2$ , that are indexed by Hilbert spaces  $\mathcal{H}(S_i)$  defined as in (1.4). Then, the (first) canonical correlation between  $Z_1$  and  $Z_2$  is defined to be

$$\rho^2 = \sup_{\|f_i\|_{\mathcal{H}(S_i)}=1, i=1,2} \text{Cov}^2(Z_1(f_1), Z_2(f_2)). \tag{1.7}$$

One can deduce from Eubank and Hsing [8] that (1.7) is well defined with the supremum being attained. We provide an independent verification of this fact in the next section. If  $\tilde{f}_1, \tilde{f}_2$  are maximizing functions, then  $Z_1(\tilde{f}_1), Z_2(\tilde{f}_2)$  are the first canonical variables of the  $Z_1$  and  $Z_2$  processes, respectively. Subsequent canonical correlations and variables can be obtained similar to the first in an iterative process that parallels the one employed in the standard multivariate analysis case; see, for example, Eubank and Hsing [8].

A number of articles dealing with functional canonical correlation and related concepts have focused on the case where the  $Z_i(f_i)$  are restricted to have

$$\sum_{j=1}^\infty f_{ij}^2 < \infty, \quad i = 1, 2, \tag{1.8}$$

which has the consequence that  $\sum_{j=1}^\infty f_{ij}\phi_{ij} \in \mathcal{H}$ . In such instances the supremum (1.7) need not be attained as demonstrated in Cupidon *et al.* [2] and Cupidon *et al.* [1]. Dauxois and Pousse [6], Dauxois *et al.* [4], Dauxois and Nkiet [3] and Dauxois *et al.* [5] largely ignore this issue with the consequence that their statistical applications become relevant only for finite dimensional covariance operators whose ranges are necessarily closed. Such results are, of course, already subsumed by the original Hotelling [12] work. In contrast, He *et al.* [11] impose restrictions on the cross-covariances of coefficients in the two processes' Karhunen–Loève expansions to insure that (1.8) is satisfied. Such restrictions are unnecessary as will be seen in the next section.

In the present paper, we are interested not only in functional CCA but functional partial canonical correlation, as well. In the case of finite dimensional covariance operators, the idea was proposed by Roy [17]. Given three random vectors  $X_1, X_2$  and  $X_3$ , the partial canonical correlation of  $X_2$  and  $X_3$  relative to  $X_1$  was defined as the ordinary canonical correlation between  $\tilde{X}_2 = X_2 - P_{X_1}X_2$  and  $\tilde{X}_3 = X_3 - P_{X_1}X_3$ , where  $P_{X_1}$  denotes projection onto the linear space spanned by  $X_1$ . Related work by Dauxois and Nkiet [3] and Dauxois *et al.* [5] comes with the restriction of a closed range for covariance operators which, again, confines statistical applications to the finite dimensional setting that was already treated in Roy's original work. In Section 3, we show how the partial canonical correlation concept can be rigorously extended to infinite dimensions and functional data.

In the next section, we set out the main ideas that are needed for rigorous treatment of canonical correlation and related concepts in the context of Hilbert space indexed processes of the basic

form (1.5). The driving force behind our approach is the isometry that exists between the  $L^2_Z$  and  $\mathcal{H}(S)$  spaces. To demonstrate the utility of this analytic framework, we illustrate the idea with two processes in the next section and extend this to three processes and partial canonical correlation in Section 3.

## 2. CCA

In this section, we begin with the case of two processes and establish the properties of canonical correlations and variables as defined in (1.7). Most of the basic techniques that are needed for the three process setting of the next section are illustrated in this somewhat simpler scenario thereby making it the natural starting point for our exposition.

As in Section 1, assume that we have two  $\mathcal{H}$ -valued random variables with associated covariance operators  $S_i, i = 1, 2$ , having eigenvalue–eigenvector sequences  $\{(\lambda_{ij}, \phi_{ij})\}_{j=1}^\infty$ . From Vakhania *et al.* [20], it may be concluded that there are also cross-covariance operators  $S_{12}$  and  $S_{21}$  defined by, for example,

$$E\langle X_1, f_1 \rangle \langle X_2, f_2 \rangle = \langle f_1, S_{12} f_2 \rangle$$

with  $S_{21} = S_{12}^*$  for  $S_{12}^*$  the adjoint of  $S_{12}$ .

Now we construct a new Hilbert space

$$\mathcal{H}_0 = \left\{ h = (f_1, f_2): f_i \in \mathcal{H}(S_i), i = 1, 2, \|h\|_0^2 = \sum_{i=1}^2 \|f_i\|_{\mathcal{H}(S_i)}^2 < \infty \right\}$$

from which we obtain the  $\mathcal{H}_0$  indexed process

$$Z(h) = Z_1(f_1) + Z_2(f_2)$$

with covariance function

$$\begin{aligned} \text{Cov}(Z(h), Z(h')) &= \text{Cov}(Z_1(f_1), Z_1(f'_1)) + \text{Cov}(Z_2(f_2), Z_2(f'_2)) \\ &\quad + \text{Cov}(Z_1(f_1), Z_2(f'_2)) + \text{Cov}(Z_1(f'_1), Z_2(f_2)) \\ &= \langle f_1, f'_1 \rangle_{\mathcal{H}(S_1)} + \langle f_2, f'_2 \rangle_{\mathcal{H}(S_2)} \\ &\quad + \text{Cov}(Z_1(f_1), Z_2(f'_2)) + \text{Cov}(Z_1(f'_1), Z_2(f_2)). \end{aligned} \tag{2.1}$$

In order to avoid the degenerate setting where perfect prediction is possible, we impose the following condition.

**Assumption 2.1.** *There exist no  $(f_1, f_2) \in \mathcal{H}_0$  such that  $|\text{Corr}(Z_1(f_1), Z_2(f_2))| = 1$ .*

The cross-covariance terms in (2.1) can be characterized as deriving from operators between  $\mathcal{H}(S_1)$  and  $\mathcal{H}(S_2)$ . To see this, define the functional

$$l_{f_2}(f_1) = \text{Cov}(Z_1(f_1), Z_2(f_2))$$

on  $\mathcal{H}(S_1)$ . Clearly,  $l_{f_2}$  is linear since covariance is bilinear and, e.g.,  $Z_1(\alpha f_1 + \alpha' f'_1) = \alpha Z_1(f_1) + \alpha' Z_1(f'_1)$  for any scalars  $\alpha, \alpha'$  and any  $f_1, f'_1 \in \mathcal{H}(S_1)$ . Also, by the Cauchy–Schwarz inequality,

$$|l_{f_2}(f_1)| \leq \sqrt{\text{Var } Z_1(f_1) \text{Var } Z_2(f_2)} = \|f_1\|_{\mathcal{H}(S_1)} \|f_2\|_{\mathcal{H}(S_2)}.$$

Thus,  $l_{f_2}$  is a bounded linear functional on  $\mathcal{H}(S_1)$  and by the Riesz representation theorem there is a bounded operator  $C_{12}: \mathcal{H}(S_2) \rightarrow \mathcal{H}(S_1)$  satisfying

$$\text{Cov}(Z_1(f_1), Z_2(f_2)) = \langle f_1, C_{12} f_2 \rangle_{\mathcal{H}(S_1)}. \tag{2.2}$$

There is also a bounded operator  $C_{21}: \mathcal{H}(S_1) \rightarrow \mathcal{H}(S_2)$  with  $C_{21} = C_{12}^*$ , which satisfies  $\text{Cov}(Z_1(f_1), Z_2(f_2)) = \langle C_{21} f_1, f_2 \rangle_{\mathcal{H}(S_2)}$ .

**Proposition 2.1.** *Under Assumption 2.1,  $\|C_{12}\| = \|C_{21}\| < 1$ .*

**Proof.** By the definition of the operator norm, we have

$$\|C_{12}\|^2 = \sup_{f_2 \in \mathcal{H}(S_2), \|f_2\|_{\mathcal{H}(S_2)}=1} \|C_{12} f_2\|_{\mathcal{H}(S_1)}^2.$$

An application of the Cauchy–Schwarz inequality produces

$$\begin{aligned} |\text{Cov}(Z_1(f_1), Z_2(f_2))| &= |\langle f_1, C_{12} f_2 \rangle_{\mathcal{H}(S_1)}| \\ &< \sqrt{\text{Var } Z_1(f_1) \text{Var } Z_2(f_2)} \\ &= \|f_1\|_{\mathcal{H}(S_1)} \|f_2\|_{\mathcal{H}(S_2)} \end{aligned}$$

with the strict inequality coming from Assumption 2.1. Now take  $f_1 = C_{12} f_2$ . □

The operators  $C_{12}$  and  $S_{12}$  are, of course, related as we now explain. For this purpose, define

$$\tilde{\mathcal{H}}(S_i) = \left\{ \tilde{f}_i: \tilde{f}_i = \sum_{j=1}^{\infty} \tilde{f}_{ji} \phi_{ij}, \|\tilde{f}_i\|_{\tilde{\mathcal{H}}(S_i)}^2 = \sum_{j=1}^{\infty} \lambda_{ij} \tilde{f}_{ij}^2 = \|S_i^{1/2} \tilde{f}_i\|^2 < \infty \right\}, \quad i = 1, 2.$$

Then,  $S_i$  is an isometric mapping from  $\tilde{\mathcal{H}}(S_i)$  onto  $\mathcal{H}(S_i)$ ; that is,  $\tilde{\mathcal{H}}(S_i) = S_i^{-1} \mathcal{H}(S_i)$ . This leads us to the following lemma.

**Lemma 2.1.**  *$S_{12}$  is an operator from  $\tilde{\mathcal{H}}(S_2)$  into  $\mathcal{H}(S_1)$  with  $\|S_{12}\| < 1$ .*

**Proof.** For any  $\tilde{f}_2 \in \tilde{\mathcal{H}}(S_2)$  and  $f_1 \in \mathcal{H}(S_1)$

$$\begin{aligned} \text{Cov}(Z_1(f_1), Z_2(S_2 \tilde{f}_2)) &= \sum_{i,j} f_{1i} \tilde{f}_{2j} \langle \phi_{1i}, S_{12} \phi_{2j} \rangle \\ &= \sum_{i,j} f_{1i} \tilde{f}_{2j} \langle S_1^{1/2} \phi_{1i}, S_1^{1/2} S_{12} \phi_{2j} \rangle_{\mathcal{H}(S_1)} \end{aligned}$$

$$\begin{aligned}
 &= \sum_{i,j} \lambda_{1i} f_{1i} \tilde{f}_{2j} \langle \phi_{1i}, S_{12} \phi_{2j} \rangle_{\mathcal{H}(S_1)} \\
 &= \langle f_1, S_{12} \tilde{f}_2 \rangle_{\mathcal{H}(S_1)}.
 \end{aligned}$$

Now use the Cauchy–Schwarz inequality and  $\|S_2 \tilde{f}_2\|_{\mathcal{H}(S_2)} = \|\tilde{f}_2\|_{\tilde{\mathcal{H}}(S_2)}$ . □

Lemma 2.1 provides the means to characterize  $C_{12}$ . Specifically, observe that

$$\begin{aligned}
 \text{Cov}(Z_1(f_1), Z_2(S_2 \tilde{f}_2)) &= \langle f_1, S_{12} \tilde{f}_2 \rangle_{\mathcal{H}(S_1)} \\
 &= \langle f_1, S_{12} S_2^{-1} S_2 \tilde{f}_2 \rangle_{\mathcal{H}(S_1)} \\
 &= \langle f_1, C_{12} S_2 \tilde{f}_2 \rangle_{\mathcal{H}(S_1)}.
 \end{aligned}$$

In addition, the fact that  $S_{12}$  is compact on  $\mathcal{H}$  along with an argument similar to that of Lemma 2.1 reveals that  $C_{12}$  is the limit of a sequence of finite dimensional operators. We summarize these findings as follows.

**Theorem 2.1.**  $C_{12} = S_{12} S_2^{-1}$  is a compact operator from  $\mathcal{H}(S_2)$  into  $\mathcal{H}(S_1)$ .

For  $h \in \mathcal{H}_0$ , define  $Qh = (f_1 + C_{12} f_2, f_2 + C_{21} f_1)$ . It will be convenient to write this in matrix form as

$$Qh = \begin{bmatrix} I & C_{12} \\ C_{21} & I \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} \tag{2.3}$$

with the convention that the resulting vector is viewed as an element of  $\mathcal{H}_0$ . Observe that

$$\text{Cov}(Z(h), Z(h')) = \langle h, Qh' \rangle_0.$$

This leads to the following proposition.

**Proposition 2.2.**  $Q : \mathcal{H}_0 \rightarrow \mathcal{H}_0$  is invertible with inverse defined by

$$Q^{-1}(h) = (C_{11.2}^{-1} f_1 - C_{12} C_{22.1}^{-1} f_2, C_{22.1}^{-1} f_2 - C_{21} C_{11.2}^{-1} f_1), \tag{2.4}$$

where  $h = (f_1, f_2) \in \mathcal{H}_0$  and  $C_{ii.k} = I - C_{ik} C_{ki} = (I - C_{ik} C_{ki})^*$  for  $i, k = 1, 2, i \neq k$ .

Analogous to (2.3), (2.4) will also be expressed as

$$Q^{-1}h = \begin{bmatrix} C_{11.2}^{-1} & -C_{12} C_{22.1}^{-1} \\ -C_{21} C_{11.2}^{-1} & C_{22.1}^{-1} \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}.$$

**Proof.** The form of the inverse as stated in (2.4) follows directly once we have shown all the relevant inverse operators exist. Thus, let us concentrate on the latter task.

We can write  $Q = I - T$  with

$$Th = (-C_{12}f_2, -C_{21}f_1) = - \begin{bmatrix} 0 & C_{12} \\ C_{21} & 0 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}.$$

Then

$$\begin{aligned} \|Th\|_0^2 &= \|C_{12}f_2\|_{\mathcal{H}(S_1)}^2 + \|C_{21}f_1\|_{\mathcal{H}(S_2)}^2 \\ &\leq \|C_{12}\|^2 \|f_2\|_{\mathcal{H}(S_2)}^2 + \|C_{21}\|^2 \|f_1\|_{\mathcal{H}(S_1)}^2 \\ &= \|C_{12}\|^2 [\|f_1\|_{\mathcal{H}(S_1)}^2 + \|f_2\|_{\mathcal{H}(S_2)}^2] \\ &= \|C_{12}\|^2 \|h\|_0^2 \\ &< \|h\|_0^2 \end{aligned}$$

by Proposition 2.1. Theorem 4.40 of Rynne and Youngson [18] now has the consequence that  $I - T = Q$  is invertible.

To complete the proof, we need to show that  $C_{11.2}$  and  $C_{22.1}$  are invertible. This again follows from Theorem 4.40 of Rynne and Youngson [18] because  $C_{11.2} = I - C_{12}C_{21}$  with  $\|C_{21}\| = \|C_{12}\| < 1$  from Proposition 2.1. □

Now define

$$\mathcal{H}(Q) = \left\{ h: h = Q \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}, f_i \in \mathcal{H}(S_i), i = 1, 2, \|h\|_{\mathcal{H}(Q)}^2 = \|Q^{-1/2}h\|_0^2 < \infty \right\}.$$

The next proposition follows immediately from this definition.

**Proposition 2.3.**  $\mathcal{H}(Q)$  is congruent to

$$L_Z^2 = \{ Z(h): h \in \mathcal{H}_0, \|Z(h)\|_{L_Z^2}^2 := \text{Var}(Z(h)) < \infty \}$$

under the mapping  $\Psi(h) = Z(Q^{-1}h)$ .

With Proposition 2.3 in hand we can now give our formulation of CCA. Specially, we seek elements  $f_i \in \mathcal{H}(S_i)$  of unit norm that maximize  $|\text{Cov}(Z_1(f_1), Z_2(f_2))|$ . But

$$\text{Cov}(Z_1(f_1), Z_2(f_2)) = \text{Cov}(Z(f_1, 0), Z(0, f_2)) = \left\langle Q \begin{bmatrix} f_1 \\ 0 \end{bmatrix}, Q \begin{bmatrix} 0 \\ f_2 \end{bmatrix} \right\rangle_{\mathcal{H}(Q)}$$

which leads to the conclusion that it is equivalent to find  $f_i \in \mathcal{H}(S_i)$  to maximize the right-hand side of this last expression.

The analysis from this point is driven by the results of Sunder [19] as described in Section 4. For that purpose, we decompose  $\mathcal{H}(Q)$  into a sum of the closed subspaces  $M_1$  and  $M_2$  with

$$M_1 = \left\{ h \in \mathcal{H}(Q) : h = Q \begin{bmatrix} f_1 \\ 0 \end{bmatrix} := (f_1, C_{21} f_1), f_1 \in \mathcal{H}(S_1) \right\},$$

$$M_2 = \left\{ h \in \mathcal{H}(Q) : h = Q \begin{bmatrix} 0 \\ f_2 \end{bmatrix} := (C_{12} f_2, f_2), f_2 \in \mathcal{H}(S_2) \right\}.$$

Regarding  $M_1$  and  $M_2$ , we have the following result.

**Proposition 2.4.**  $\mathcal{H}(Q) = M_1 + M_2$  with “+” indicating an algebraic direct sum.

**Proof.** Clearly any element of  $\mathcal{H}_0$  can be written as the sum of elements in  $M_1$  and  $M_2$ . We therefore need only show that  $M_1 \cap M_2 = \{0\}$ . Thus, suppose there exist  $f_i \in \mathcal{H}(S_i), i = 1, 2$ , such that  $(f_1, C_{21} f_1) = (C_{12} f_2, f_2)$ . Then

$$\text{Var}(Z_1(f_1)) = \langle f_1, f_1 \rangle_{\mathcal{H}(S_1)} = \langle f_1, C_{12} f_2 \rangle_{\mathcal{H}(S_1)}$$

and

$$\text{Var}(Z_2(f_2)) = \langle f_2, f_2 \rangle_{\mathcal{H}(S_2)} = \langle f_2, C_{21} f_1 \rangle_{\mathcal{H}(S_2)} = \langle C_{12} f_2, f_1 \rangle_{\mathcal{H}(S_1)}.$$

But, these relations have the consequence that  $|\text{Corr}(Z_1(f_1), Z_2(f_2))| = 1$  which contradicts Assumption 2.1. □

To relate Proposition 2.4 to Sunder’s scheme in the Appendix, let  $L_1 = M_1$  and  $L_2 = M_2 \cap M_1^\perp$  in Theorem A.1. Then, for  $h_1 = Q \begin{bmatrix} f_1 \\ 0 \end{bmatrix} \in M_1$  and  $h_2 = Q \begin{bmatrix} 0 \\ f_2 \end{bmatrix} \in M_2$ , the first canonical correlation satisfies

$$\begin{aligned} \rho &= \sup_{\substack{h_1 \in M_1, h_2 \in M_2 \\ \|h_i\|_{\mathcal{H}(Q)}=1, i=1,2}} |\langle h_1, h_2 \rangle_{\mathcal{H}(Q)}| = \sup_{\substack{h_1 \in L_1, \tilde{h}_2 \in L_2 \\ \|h_1\|_{\mathcal{H}(Q)}=1, \|\tilde{h}_2 + B\tilde{h}_2\|_{\mathcal{H}(Q)}=1}} |\langle h_1, B\tilde{h}_2 \rangle_{\mathcal{H}(Q)}| \\ &\leq \sup_{\substack{\tilde{h}_2 \in L_2 \\ \|\tilde{h}_2 + B\tilde{h}_2\|_{\mathcal{H}(Q)}=1}} \|B\tilde{h}_2\|_{\mathcal{H}(Q)} \end{aligned}$$

for  $B = P_{L_1|M_2}(P_{L_2|M_2})^{-1}$ . Taking  $h_1 = B\tilde{h}_2/\|B\tilde{h}_2\|_{\mathcal{H}(Q)}$ , we see that the bound is attainable and holds with equality. Thus, we have shown that  $\rho$  is obtained by maximizing  $\|B\tilde{h}_2\|_{\mathcal{H}(Q)}$  subject to

$$\|B\tilde{h}_2 + \tilde{h}_2\|_{\mathcal{H}(Q)}^2 = \langle \tilde{h}_2, (I + B^*B)\tilde{h}_2 \rangle_{\mathcal{H}(Q)} = 1.$$

The operator  $B^*B$  is compact as a result of Theorem 2.1 and Theorem 2.2 below. In addition,  $I + B^*B$  is self-adjoint, positive, invertible and has a self-adjoint square-root  $(I + B^*B)^{1/2}$ . We

can therefore work with  $\tilde{h}'_2 = (I + B^*B)^{1/2}\tilde{h}_2$  and maximize

$$\|B\tilde{h}_2\|_{\mathcal{H}(Q)} = \|B(I + B^*B)^{-1/2}\tilde{h}'_2\|_{\mathcal{H}(Q)}$$

subject to  $\tilde{h}'_2 \in L_2$  and  $\|\tilde{h}'_2\|_{\mathcal{H}(Q)}^2 = 1$ . The maximizer is the eigenvector for the largest eigenvalue of  $(I + B^*B)^{-1/2}B^*B(I + B^*B)^{-1/2}$ . Some algebra reveals that the resulting eigenvalue problem is equivalent to finding a vector  $\tilde{h}_2 \in L_2$  with  $\|\tilde{h}_2\|_{\mathcal{H}(Q)}^2 = 1$  such that

$$B^*B\tilde{h}_2 = \alpha^2\tilde{h}_2 \tag{2.5}$$

in which case  $\rho = \alpha/\sqrt{1 + \alpha^2}$ .

Now suppose that  $\tilde{h}_2 \in L_2$  is any vector that satisfies (2.5). Its  $M_1$  component is  $B\tilde{h}_2$  and its  $M_2$  component is  $B\tilde{h}_2 + \tilde{h}_2$ . These correspond to the canonical variables  $\Psi(B\tilde{h}_2/\alpha)$  and  $\Psi((\tilde{h}_2 + B\tilde{h}_2)/\sqrt{1 + \alpha^2})$  of the  $Z_1$  and  $Z_2$  spaces, respectively.

In combination Corollaries A.2 and A.4 from the Appendix give us the desired characterization for  $B^*B$ : namely,

**Theorem 2.2.** For  $h = (0, \tilde{f}_2) \in L_2$ ,  $B^*B(0, \tilde{f}_2) = (0, C_{21}C_{12}C_{22.1}^{-1}\tilde{f}_2)$ .

An application of Proposition A.1 from the Appendix now reveals that the conclusion of Theorem 2.2 can be restated as  $B^*B(0, \tilde{f}_2) = (0, C_{21}C_{12}f_2)$  for some  $f_2 \in \mathcal{H}(S_2)$  and the eigenvalue problem (2.5) is equivalent to  $C_{21}C_{12}f_2 = \alpha^2C_{22.1}f_2$  or

$$C_{21}C_{12}f_2 = \rho^2 f_2.$$

By interchanging the roles of  $M_1$  and  $M_2$  it follows that the optimal choice for  $f_1$  is the eigenvector corresponding to the same eigenvalue  $\rho^2$  of  $C_{12}C_{21}$ . Thus,  $\rho$  is the largest singular value of  $C_{21}$ ,  $f_1, f_2$  are its right and left hand singular functions and  $Z_1(f_1), Z_2(f_2)$  are the corresponding canonical variables. More generally, a similar analysis reveals that the collection of all such singular values gives rise to a sequence of canonical correlations that correspond to canonical variable pairs with maximum possible correlation subject to being uncorrelated with previous pairs in the sequence.

We conclude this section with examples that illustrate some of the features of our CCA formulation.

**Example 2.1.** Suppose that  $S_1$  and  $S_2$  are full-rank, finite-dimensional matrices. Then,  $C_{12} = S_{12}S_2^{-1}$  and  $C_{21} = S_{21}S_1^{-1}$  so that finding eigenvalues and eigenvectors for  $C_{21}C_{12}$  is equivalent to the singular value decomposition of  $S_1^{-1/2}S_{12}S_2^{-1/2}$  which, in turn, is equivalent to Hotelling's classic solution for the finite dimensional case as established in Kshirsagar [13].

**Example 2.2.** Functional data analysis generally focuses on the case where the  $X_i$  are random element of  $L^2[0, 1]$ ; that is, the set of square integrable function on the interval  $[0, 1]$ . One assumes the  $X_i$  admit point-wise representations as the continuous time stochastic processes

$\{X_i(t, \omega): t \in [0, 1], \omega \in \Omega\}, i = 1, 2$ . Inference is then based on the linear combinations described in (1.6).

The (assumed continuous) process covariance kernels are

$$K_i(t, t') = \text{Cov}(X_i(t), X_i(t')) = \sum_{j=1}^{\infty} \lambda_{ij} \phi_{ij}(t) \phi_{ij}(t')$$

with the  $(\lambda_{ij}, \phi_{ij}), j = 1, \dots, i = 1, 2$ , being the eigenvalues and eigenvectors of the  $L^2[0, 1]$  integral operators defined by

$$(S_i f)(t) = \int_0^1 f(s) K_i(t, s) ds.$$

The RKHS that is congruent to  $L^2_{X_i}$  is  $\mathcal{H}(S_i)$ .

In the case of two processes, we also have the cross-covariance kernels

$$\begin{aligned} K_{12}(t_1, t_2) &= \text{Cov}(X_1(t_1), X_2(t_2)) \\ &= \text{Cov}(X_2(t_2), X_1(t_1)) \\ &= K_{21}(t_2, t_1). \end{aligned}$$

From Eubank and Hsing [8], we know that  $K_{12}(\cdot, t_2) \in \mathcal{H}(S_1)$ , and  $K_{12}(t_1, \cdot) \in \mathcal{H}(S_2)$ ; so, if  $f_i = \sum_{j=1}^{\infty} \lambda_{ij} f_{ij} \phi_{ij} \in \mathcal{H}(S_i)$ ,

$$(R_{12} f_2)(t) = \langle K_{12}(t, \cdot), f_2(\cdot) \rangle_{\mathcal{H}(S_2)}$$

defines a bounded operator from  $\mathcal{H}(S_2)$  into  $\mathcal{H}(S_1)$  with the property that

$$\begin{aligned} \text{Cov}(Z_1(f_1), Z_2(f_2)) &= \sum_k \sum_j f_{1j} f_{2k} \int_0^1 K_{12}(s, t) \phi_{1j}(s) \phi_{2k}(t) ds dt \\ &= \langle f_1, R_{12} f_2 \rangle_{\mathcal{H}(S_1)}. \end{aligned}$$

Therefore,  $R_{12} = C_{12}$  and our CCA formulation coincides with that in Eubank and Hsing [8].

**Example 2.3.** The developments in this section suggest a new approach to estimation in the functional CCA setting of the previous example. The idea stems from (2.2) which has the consequence that

$$\text{Cov}(Z_1(\phi_{1i}), Z_2(\phi_{2j})) = \langle \phi_{1i}, C_{12} \phi_{2j} \rangle_{\mathcal{H}(S_1)}. \tag{2.6}$$

It follows from Hansen [10] that a singular value decomposition of

$$A_m = \{ \langle \phi_{1i}, C_{12} \phi_{2j} \rangle_{\mathcal{H}(S_1)} \}_{i,j=1:m} \tag{2.7}$$

for some finite integer  $m$  will produce singular values that approximate the singular values for the operator  $C_{12}$  and that the singular vectors provide coefficients for linear combinations of the

$\phi_{ij}$  that approximate its singular functions. The only question is how to estimate the inner products in (2.7). The answer is revealed by examining the left hand of (2.6). The realized values of the  $Z_i(\phi_{ij})$ ,  $j = 1, \dots, m$  can be estimated directly using the scores one obtains from a principal components analysis of functional data. Thus, their sample covariance matrix provides an obvious choice for an estimator of (2.7).

Suppose we have observed sample path pairs  $(x_{1j}(\cdot), x_{2j}(\cdot))$ ,  $j = 1, \dots, n$ . The resulting estimation algorithm can then be summarized as follows.

1. Carry out a principal components analysis of the  $x_{ij}$ ,  $j = 1, \dots, n$  to obtain the estimated eigenfunctions  $\hat{\phi}_{ij}$ ,  $j = 1, \dots, m$  and  $n \times m$  score matrices

$$W_i = \{ \{ \hat{\phi}_{ij}, x_{ik}(\cdot) \} \}_{k=1:n, j=1:m}$$

for  $i = 1, 2$ . Let  $\hat{A}_m$  be the  $m \times m$  sample cross covariance matrix obtained from  $W_1$  and  $W_2$ .

2. If  $\hat{A}_m = UDV^T$  for  $U = [u_1, \dots, u_m]$ ,  $V = [v_1, \dots, v_m]$  and  $D = \text{diag}(d_1, \dots, d_m)$  is the singular value decomposition of  $\hat{A}_m$ , the  $i$ th canonical correlation is estimated by  $d_i$  and the corresponding canonical weight functions by  $u_i^T[\hat{\phi}_{21}, \dots, \hat{\phi}_{2m}]$  and  $v_i^T[\hat{\phi}_{11}, \dots, \hat{\phi}_{1m}]$ .

A simple numerical example will be used to illustrate this estimation scheme. The setting is that of Eubank and Hsing [8] where the two processes are

$$X_1(t) = \sum_{j=1}^{20} j^{-1/2} Z_{1j} \sqrt{2} \sin(j\pi t),$$

$$X_2(t) = (Z_{11} + Z_{21}) \sin(\pi t) + \sum_{j=2}^{20} j^{-1/2} Z_{2j} \sqrt{2} \sin(j\pi s),$$

for  $t \in [0, 1]$  and the  $Z_{ij}$  i.i.d. standard normal random variables. In this instance, there is only one nonzero canonical correlation: namely,  $\rho_1 = 1/\sqrt{2} \doteq 0.707$ .

We sampled  $n$  process pairs at 100 equally spaced points and conducted principal components analysis on the resulting data using the function `pca.fd` from the `fda` package in R retaining 9 components (or harmonics) for both processes. This basic experiment was then replicated 100 times. For samples of size  $n = 250$ , the observed means (standard deviations) of the first two sample canonical correlations were 0.7248 (0.0818) and 0.0777 (0.0122), respectively. For samples of size  $n = 500$ , the means (standard deviations) were 0.7147 (0.0591) and 0.055 (0.0095).

This rather crude implementation suffices for the present expository purposes. However, for use in practice one should at least employ consistent estimators for the eigenfunctions such as those studied in Yao *et al.* [21] and Hall *et al.* [9].

### 3. PCCA

A similar approach to that of the previous section can be used to address the PCCA setting. There are now three  $\mathcal{H}$ -valued random variables  $X_i$ ,  $i = 1, 2, 3$ , with associated covariance operators

$S_i, i = 1, 2, 3$ . As in Section 2, we can also define the cross-covariance operators  $S_{12}, S_{13}, S_{23}$  and their adjoints.

For  $i = 1, 2, 3$ , the Hilbert spaces  $L^2_{Z_i}$  spanned by the process  $Z_i(f_i)$  indexed by their congruent Hilbert spaces  $\mathcal{H}(S_i)$  are defined as in (1.5) and (1.4). Hence, by the Riesz representation theorem, there are bounded operators  $C_{ij} : \mathcal{H}(S_j) \rightarrow \mathcal{H}(S_i)$  satisfying

$$\text{Cov}(Z_i(f_i), Z_j(f_j)) = \langle f_i, C_{ij} f_j \rangle_{\mathcal{H}(S_i)}$$

for  $i, j = 1, 2, 3$  and  $i \neq j$ . Also, we have that  $C_{ij} = C_{ji}^*$ .

We now construct the new Hilbert space

$$\mathcal{H}_0 = \left\{ h = (f_1, f_2, f_3) : f_i \in \mathcal{H}(S_i), i = 1, 2, 3, \|h\|_0^2 = \sum_{i=1}^3 \|f_i\|_{\mathcal{H}(S_i)}^2 < \infty \right\}.$$

Then, our corresponding  $\mathcal{H}_0$  indexed process is  $Z(h) = \sum_{i=1}^3 Z_i(f_i)$ .

As in the previous section we need to rule out the case where perfect prediction is possible. For this purpose, we require that Assumption 2.1 holds for both of the process pairs  $Z_1, Z_2$  and  $Z_1, Z_3$  as well as the following.

**Assumption 3.1.** *There exist no  $f_2 \in \mathcal{H}(S_2)$  or  $f_3 \in \mathcal{H}(S_3)$  such that*

$$|\text{Corr}(Z_2(f_2) - P_{Z_1} Z_2(f_2), Z_3(f_3) - P_{Z_1} Z_3(f_3))| = 1.$$

For  $h \in \mathcal{H}_0$ , define

$$Qh = (f_1 + C_{12}f_2 + C_{13}f_3, C_{21}f_1 + f_2 + C_{23}f_3, C_{31}f_1 + C_{32}f_2 + f_3)$$

which we will express in the matrix form

$$Qh = \begin{bmatrix} I & C_{12} & C_{13} \\ C_{21} & I & C_{23} \\ C_{31} & C_{32} & I \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}.$$

We then see that

$$\text{Cov}(Z(h), Z(h')) = \langle h, Qh' \rangle_0.$$

Our next result gives the three process parallel of Proposition 2.2.

**Proposition 3.1.** *Let  $E = [C_{12} \ C_{13}]$ ,  $F = \begin{bmatrix} C_{21} \\ C_{31} \end{bmatrix}$ ,  $D = \begin{bmatrix} I & C_{32} \\ C_{23} & I \end{bmatrix}$  and  $G = D^{1/2}(I - V)D^{1/2}$  with*

$$V = \begin{bmatrix} 0 & -C_{22.1}^{-1/2}(C_{23} - C_{21}C_{13})C_{33.1}^{-1/2} \\ -C_{33.1}^{-1/2}(C_{32} - C_{31}C_{12})C_{22.1}^{-1/2} & 0 \end{bmatrix}. \tag{3.1}$$

Then,

$$Q^{-1} = \begin{bmatrix} I + EG^{-1}F & -EG^{-1} \\ G^{-1}F & G^{-1} \end{bmatrix}. \tag{3.2}$$

From Proposition 2.2, we know that  $C_{22,1}$  and  $C_{33,1}$  are invertible. The result will therefore follow if we can show that the norm of  $V$  in (3.1) is strictly less than unity. This is a consequence of the next two lemmas and Theorem 4.40 of Rynne and Youngson [18].

**Lemma 3.1.** *The projection of  $Z_2(f_2)$  onto  $L^2_{Z_1}$  is  $Z_1(C_{12}f_2)$  and the projection of  $Z_3(f_3)$  onto  $L^2_{Z_1}$  is  $Z_1(C_{13}f_3)$ .*

**Proof.** If  $P_{Z_1}Z_2(f_2)$  denotes the projection, it must satisfy

$$\text{Cov}(Z_1(f_1), P_{Z_1}Z_2(f_2)) = \text{Cov}(Z_1(f_1), Z_2(f_2))$$

for every  $f_1 \in \mathcal{H}(S_1)$ . Since there is some  $\check{f}_1 \in \mathcal{H}(S_1)$  such that  $P_{Z_1}Z_2(f_2) = Z_1(\check{f}_1)$ ,

$$\begin{aligned} \text{Cov}(Z_1(f_1), Z_2(f_2)) &= \langle f_1, C_{12}f_2 \rangle_{\mathcal{H}(S_1)} \\ &= \text{Cov}(Z_1(f_1), Z_1(\check{f}_1)) \\ &= \langle f_1, \check{f}_1 \rangle_{\mathcal{H}(S_1)}. \end{aligned}$$

Therefore,  $\check{f}_1 = C_{12}f_2$ . The second half of the lemma is proved similarly. □

**Lemma 3.2.**  $\|C_{22,1}^{-1/2}(C_{23} - C_{21}C_{13})C_{33,1}^{-1/2}\|_{\mathcal{H}(S_2)} < 1$ .

**Proof.** First, observe that by Lemma 3.1 and Assumption 3.1

$$\begin{aligned} &|\text{Cov}(Z_2(f_2) - Z_1(C_{12}f_2), Z_3(f_3) - Z_1(C_{13}f_3))| \\ &= |\langle f_2, C_{23}f_3 \rangle_{\mathcal{H}(S_2)} - \langle f_2, C_{21}C_{13}f_3 \rangle_{\mathcal{H}(S_2)}| \\ &< (\text{Var}(Z_2(f_2) - Z_1(C_{12}f_2)))^{1/2} (\text{Var}(Z_3(f_3) - Z_1(C_{13}f_3)))^{1/2} \\ &= \langle f_2, C_{22,1}f_2 \rangle_{\mathcal{H}(S_2)}^{1/2} \langle f_3, C_{33,1}f_3 \rangle_{\mathcal{H}(S_3)}^{1/2} \\ &= \|C_{22,1}^{1/2}f_2\|_{\mathcal{H}(S_2)} \|C_{33,1}^{1/2}f_3\|_{\mathcal{H}(S_3)}. \end{aligned}$$

Now, let  $\tilde{f}_2 = C_{22,1}^{1/2}f_2$  and  $\tilde{f}_3 = C_{33,1}^{1/2}f_3$  to obtain

$$\langle \tilde{f}_2, C_{22,1}^{-1/2}(C_{23} - C_{21}C_{13})C_{33,1}^{-1/2}\tilde{f}_3 \rangle_{\mathcal{H}(S_2)} < \|\tilde{f}_2\|_{\mathcal{H}(S_2)} \|\tilde{f}_3\|_{\mathcal{H}(S_3)}.$$

Finally, taking  $\tilde{f}_2 = C_{22,1}^{-1/2}(C_{23} - C_{21}C_{13})C_{33,1}^{-1/2}\tilde{f}_3$  completes the proof. □

Now define

$$\mathcal{H}(Q) = \left\{ h: h = Q \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}, f_i \in \mathcal{H}(S_i), i = 1, 2, 3, \|h\|_{\mathcal{H}(Q)}^2 = \|Q^{-1/2}h\|_0^2 < \infty \right\}.$$

Then, as in Proposition 2.3, we have

**Proposition 3.2.**  $\mathcal{H}(Q)$  is congruent to

$$L_Z^2 = \{Z(h): h \in \mathcal{H}_0, \|Z(h)\|_{L_Z^2}^2 = \text{Var}(Z(h)) < \infty\}$$

under the mapping  $\Psi(h) = Z(Q^{-1}h)$ .

For the PCCA formulation, we wish to find  $f_2 \in \mathcal{H}(S_2)$  and  $f_3 \in \mathcal{H}(S_3)$  to maximize

$$|\text{Cov}(Z_2(f_2) - Z_1(C_{12}f_2), Z_3(f_3) - Z_1(C_{13}f_3))|.$$

Since

$$\begin{aligned} &\text{Cov}(Z_2(f_2) - Z_1(C_{12}f_2), Z_3(f_3) - Z_1(C_{13}f_3)) \\ &= \text{Cov}(Z(-C_{12}f_2, f_2, 0), Z(-C_{13}f_3, 0, f_3)), \end{aligned}$$

it suffices to find  $f_2 \in \mathcal{H}(S_2)$  and  $f_3 \in \mathcal{H}(S_3)$  to maximize

$$\left| \left\langle Q \begin{bmatrix} -C_{12}f_2 \\ f_2 \\ 0 \end{bmatrix}, Q \begin{bmatrix} -C_{13}f_3 \\ 0 \\ f_3 \end{bmatrix} \right\rangle_{\mathcal{H}(Q)} \right|.$$

Again, we apply the results of Sunder described in Section 4. For this purpose, write  $\mathcal{H}(Q) = M_1 + M_2 + M_3$  with

$$M_1 = \left\{ h \in \mathcal{H}(Q): h = Q \begin{bmatrix} f_1 \\ 0 \\ 0 \end{bmatrix} := (f_1, C_{21}f_1, C_{31}f_1) \right\},$$

$$M_2 = \left\{ h \in \mathcal{H}(Q): h = Q \begin{bmatrix} 0 \\ f_2 \\ 0 \end{bmatrix} := (C_{12}f_2, f_2, C_{32}f_2) \right\}$$

and

$$M_3 = \left\{ h \in \mathcal{H}(Q): h = Q \begin{bmatrix} 0 \\ 0 \\ f_3 \end{bmatrix} := (C_{13}f_3, C_{23}f_3, f_3) \right\}.$$

An argument similar to that for Proposition 2.4 produces the following proposition.

**Proposition 3.3.**  $\mathcal{H}(Q) = M_1 + M_2 + M_3$  with “+” indicating an algebraic direct sum.

Now let  $L_1 = M_1, L_2 = M_2 \cap M_1^\perp, L_3 = M_3 \cap M_2^\perp \cap M_1^\perp$  and take

$$\hat{h}_2 = Q \begin{bmatrix} -C_{12}f_2 \\ f_2 \\ 0 \end{bmatrix} \in M_2 - P_{L_1}M_2 \quad \text{and} \quad \hat{h}_3 = Q \begin{bmatrix} -C_{13}f_3 \\ 0 \\ f_3 \end{bmatrix} \in M_3 - P_{L_1}M_3$$

with  $\|\hat{h}_i\|_{\mathcal{H}(Q)} = 1, i = 2, 3$ . Then, arguing as in the previous section we see that the first partial canonical correlation can be characterized as

$$\begin{aligned} \rho &= \sup_{\substack{\hat{h}_2 \in M_2 - P_{L_1}M_2, \hat{h}_3 \in M_3 - P_{L_1}M_3 \\ \|\hat{h}_i\|_{\mathcal{H}(Q)} = 1, i = 2, 3}} |(\hat{h}_2, \hat{h}_3)_{\mathcal{H}(Q)}| \\ &= \sup_{\tilde{h}_3 \in L_3, \|\tilde{h}_3 + B\tilde{h}_3\|_{\mathcal{H}(Q)} = 1} \|B\tilde{h}_3\|_{\mathcal{H}(Q)} \end{aligned}$$

for  $B = P_{L_2|M_3}(P_{L_3|M_3})^{-1}$ . The bound is attained by taking  $\hat{h}_2 = B\tilde{h}_3/\|B\tilde{h}_3\|_{\mathcal{H}(Q)}$  in which case the first partial canonical correlation is  $\alpha/\sqrt{1 + \alpha^2}$  with  $\alpha^2$  the largest eigenvalue of  $B^*B$ . If  $\tilde{h}_3$  is an eigenvector corresponding to  $\alpha^2$ , the partial canonical variable for the  $Z_2$  space is  $\Psi(B\tilde{h}_3/\alpha)$  and the partial canonical variable for the  $Z_3$  space is  $\Psi((\tilde{h}_3 + B\tilde{h}_3)/\sqrt{1 + \alpha^2})$ .

Now, through Corollaries A.6 and A.7, we finally obtain

**Theorem 3.1.** For  $h = (0, 0, \tilde{f}_3) \in L_3$ ,

$$B^*Bh = (0, 0, (C_{32} - C_{31}C_{12})C_{22,1}^{-1}(C_{23} - C_{21}C_{13})C_0^{-1}\tilde{f}_3).$$

This result in combination with Corollary A.5 reveals that partial canonical correlations are the singular values of the operator  $C_{33,1}^{-1/2}(C_{32} - C_{31}C_{12})C_{22,1}^{-1/2}$ .

**Example 3.1.** The basic computational algorithm from Example 2.3 can be adapted for computing sample partial canonical correlations. One now carries out principal components analysis of the data from all three processes and then regresses the scores for the  $X_2, X_3$  process data onto the scores from the  $X_1$  sample paths. The Example 2.3 computational scheme is then applied to the residuals from the two regression analyses.

To illustrate the idea, consider again the two processes from Example 2.3. Sample paths were generated as before except that in each instance we subtracted a term  $\beta Z \cos(\pi s)$  with  $Z$  a standard normal random variable and  $\beta$  equal to 1 for the  $X_1$  process and 2 for the  $X_2$  process. The only nonzero partial canonical correlation in this case is again  $1/\sqrt{2}$ . The first two partial canonical correlations obtained from an empirical experiment using the same parameters as in Example 2.3 had means (standard deviations) of 0.7107 (0.0875) and 0.0818 (0.0157) for samples of size 250 and 0.7141 (0.0599) and 0.0553 (0.0089) for samples of size 500.

### 4. Summary

We have developed a framework that can be used to study the correlation properties of groups of Hilbert space indexed stochastic processes. Our applications have been restricted to groups of size two or three; however, it is clear that similar analyses are possible with any finite number of processes. For example, the partial canonical correlation work of Section 3 extends in principle to examination of pairs of residual processes after correcting for projections onto several other processes.

We note in passing that it has been assumed that all the  $\mathcal{H}$ -valued random variables take values in the same Hilbert space. The extension to where some or all of the variables produce elements of different Hilbert spaces incurs some additional notational expense but is otherwise straightforward.

### Technical Appendix

In this Appendix, we collect some of the mathematical details that were needed for our main results. In particular, the developments in Sunder [19] play a pivotal role in Sections 2–3. Thus, we first summarize the key aspects of that work that were employed in the paper.

Assume that a Hilbert space  $\mathcal{H}$  can be written as the algebraic direct sum of  $n$  closed subspaces  $M_1, \dots, M_n$ . That is,

$$\mathcal{H} = \sum_{i=1}^n M_i,$$

where  $M_i \cap \sum_{j \neq i} M_j = \{0\}$ . Now, for  $1 \leq k \leq n$  define

$$L_k = \left( \sum_{i=1}^k M_i \right) \cap \left( \sum_{i=1}^{k-1} M_i \right)^\perp.$$

Then,  $L_k \perp M_i$ , for  $i = 1, \dots, k - 1$ , and by construction  $\sum_{i=1}^k L_i = \sum_{i=1}^k M_i$  for  $k = 1, \dots, n$ .

Let  $P_{M_k}$  and  $P_{L_k}$  be the orthogonal projection operators onto  $M_k$  and  $L_k$ , respectively. Then, for  $1 \leq k \leq n$  and  $1 \leq j \leq k \leq n$  we define the restriction of  $P_{L_j}$  to  $M_k$  by  $P_{L_j|_{M_k}}x = P_{L_j}x$  for  $x \in M_k$  and use  $P_{M_k|_{L_j}}y = P_{M_k}y$  for  $y \in L_j$  to indicate the restriction of  $P_{M_k}$  to  $L_j$ . Sunder [19] establishes the following relationship between the  $M_k$  and  $L_k$ .

**Theorem A.1.** *For  $x \in M_k$ , we can write  $M_k$  as*

$$\begin{aligned} M_k &= \{(P_{L_1|_{M_k}}x, \dots, P_{L_{k-1}|_{M_k}}x, P_{L_k|_{M_k}}x, 0, \dots, 0)\} \\ &= \{(P_{L_1|_{M_k}}(P_{L_k|_{M_k}})^{-1}P_{L_k|_{M_k}}x, \dots, P_{L_k|_{M_k}}x, 0, \dots, 0)\} \\ &= \{(A_{L_1|_{L_k}}z, \dots, A_{L_{k-1}|_{L_k}}z, z, 0, \dots, 0)\}, \end{aligned}$$

where  $z = P_{L_k|_{M_k}}x \in L_k$  and  $A_{L_j|_{L_k}} = P_{L_j|_{M_k}}(P_{L_k|_{M_k}})^{-1}$  for  $1 \leq j \leq k \leq n$ .

Theorem A.1 has the consequence that problems involving optimization over  $M_k$  can instead be formulated in terms of equivalent problems on  $L_k$  which is how it is applied in Sections 2–3.

We next turn to the proof of Theorem 2.2. This is accomplished via the following proposition and its corollaries.

**Proposition A.1.** *If  $h = (C_{12}f_2, f_2) \in M_2$ , then  $P_{L_1|M_2}h = (C_{12}f_2, C_{21}C_{12}f_2)$  and  $P_{L_2|M_2}h = (I - P_{L_1|M_2})h = (0, C_{22.1}f_2)$ .*

**Proof.** Let  $h_1 = (f_1, C_{21}f_1) \in M_1 = L_1$ . Then,

$$\langle P_{L_1|M_2}h_2, h_1 \rangle_{\mathcal{H}(Q)} = \langle h_2, h_1 \rangle_{\mathcal{H}(Q)}$$

for every  $h_1 \in M_1$ . Writing  $P_{L_1|M_2}h_2 = (f_1^*, C_{21}f_1^*)$  leads to

$$\begin{aligned} \langle P_{L_1|M_2}h_2, h_1 \rangle_{\mathcal{H}(Q)} &= \langle (f_1^*, C_{21}f_1^*), (f_1, 0) \rangle_0 = \langle f_1^*, f_1 \rangle_{\mathcal{H}(S_1)} \\ &= \langle (C_{12}f_2, f_2), h_1 \rangle_{\mathcal{H}(Q)} = \langle (C_{12}f_2, f_2), (f_1, 0) \rangle_0 \\ &= \langle C_{12}f_2, f_1 \rangle_{\mathcal{H}(S_1)} \end{aligned}$$

for every  $f_1 \in \mathcal{H}(S_1)$ . So,  $f_1^* = C_{12}f_2$ . □

**Corollary A.1.** *If  $h = (0, \tilde{f}_2) \in L_2$ ,  $(P_{L_2|M_2})^{-1}h = (C_{12}C_{22.1}^{-1}\tilde{f}_2, C_{22.1}^{-1}\tilde{f}_2)$ .*

**Corollary A.2.** *For  $h = (0, \tilde{f}_2) \in L_2$ , we have*

$$Bh := P_{L_1|M_2}(P_{L_2|M_2})^{-1}h = (C_{12}C_{22.1}^{-1}\tilde{f}_2, C_{21}C_{12}C_{22.1}^{-1}\tilde{f}_2).$$

**Corollary A.3.** *Let  $h = (0, \tilde{f}_2)$ ,  $h' = (0, \tilde{f}'_2) \in L_2$ . Then,*

$$\langle h, h' \rangle_{\mathcal{H}(Q)} = \langle (0, \tilde{f}_2), Q^{-1}(0, \tilde{f}'_2) \rangle_0 = \langle \tilde{f}_2, C_{22.1}^{-1}\tilde{f}'_2 \rangle_{\mathcal{H}(S_2)}.$$

With a little extra effort we also obtain the following corollary.

**Corollary A.4.**  $B^*(f_1, C_{21}f_1) = (0, C_{21}f_1)$ .

**Proof.** For  $h = (f_2, C_{21}f_1) \in M_1 = L_1$  and  $\tilde{h} = (0, \tilde{f}_2) \in L_2$ ,

$$\begin{aligned} \langle h, B\tilde{h} \rangle_{\mathcal{H}(Q)} &= \langle Q^{-1}h, B\tilde{h} \rangle_0 \\ &= \langle (f_1, 0), (C_{12}C_{22.1}^{-1}\tilde{f}_2, C_{21}C_{12}C_{22.1}^{-1}\tilde{f}_2) \rangle_0 \\ &= \langle f_1, C_{12}C_{22.1}^{-1}\tilde{f}_2 \rangle_{\mathcal{H}(S_1)} = \langle C_{22.1}^{-1}C_{21}f_1, \tilde{f}_2 \rangle_{\mathcal{H}(S_2)} \\ &= \langle B^*h, \tilde{h} \rangle_{\mathcal{H}(Q)}. \end{aligned}$$

An application of Corollary A.3 completes the proof. □

Finally, we give the details for proving Theorem 3.1. Analogous to the proof of Theorem 2.2, the steps are broken down into a proposition and its subsequent corollaries.

**Proposition A.2.** *If  $h = (C_{12}f_2, f_2, C_{32}f_2)$ ,  $P_{L_1|M_2}h = (C_{12}f_2, C_{21}C_{12}f_2, C_{31}C_{12}f_2)$  and  $P_{L_2|M_2}h = (I - P_{L_1|M_2})h = (0, C_{22.1}f_2, (C_{32} - C_{31}C_{12})f_2)$ .*

**Proof.** For  $h_1 = (f_1, C_{21}f_1, C_{31}f_1) \in M_1 = L_1$ , we have the relation

$$\langle P_{L_1|M_2}h, h_1 \rangle_{\mathcal{H}(Q)} = \langle h, h_1 \rangle_{\mathcal{H}(Q)}.$$

Writing  $P_{L_1|M_2}h = (f_1^*, C_{21}f_1^*, C_{31}f_1^*)$  leads to

$$\begin{aligned} \langle P_{L_1|M_2}h, h_1 \rangle_{\mathcal{H}(Q)} &= \langle (f_1^*, C_{21}f_1^*, C_{31}f_1^*), (f_1, 0, 0) \rangle_0 \\ &= \langle f_1^*, f_1 \rangle_{\mathcal{H}(S_1)} \\ &= \langle h, h_1 \rangle_{\mathcal{H}(Q)} \\ &= \langle (C_{12}f_2, f_2, C_{32}f_2), (f_1, 0, 0) \rangle_0 \\ &= \langle C_{12}f_2, f_1 \rangle_{\mathcal{H}(S_1)} \end{aligned}$$

for every  $f_i \in \mathcal{H}(S_i)$  with  $i = 1, 2$ . So  $f_1^* = C_{12}f_2$ . □

For subsequent notational convenience, let

$$C_0 = C_{33.1} - (C_{32} - C_{31}C_{12})C_{22.1}^{-1}(C_{23} - C_{21}C_{13}).$$

**Corollary A.5.** *If  $h = (C_{13}f_3, C_{23}f_3, f_3)$ ,  $P_{L_1|M_3}h = (C_{13}f_3, C_{21}C_{13}f_3, C_{31}C_{13}f_3)$ ,  $P_{L_2|M_3}h = (0, (C_{23} - C_{21}C_{13})f_3, (C_{33.1} - C_0)f_3)$  and  $P_{L_3|M_3}h = (0, 0, C_0f_3)$ .*

**Proof.** For  $\tilde{h}_2 = (0, C_{22.1}f_2, (C_{32} - C_{31}C_{12})f_2) \in L_2$  and  $h \in M_3$ , we have the relation  $\langle P_{L_2|M_3}h, \tilde{h}_2 \rangle_{\mathcal{H}(Q)} = \langle h, \tilde{h}_2 \rangle_{\mathcal{H}(Q)}$ . If we write  $P_{L_2|M_3}h = (0, C_{22.1}f_2^*, (C_{32} - C_{31}C_{12})f_2^*)$ , then

$$\begin{aligned} \langle P_{L_2|M_3}h, \tilde{h}_2 \rangle_{\mathcal{H}(Q)} &= \langle (0, C_{22.1}f_2^*, (C_{32} - C_{31}C_{12})f_2^*), (-C_{12}f_2, f_2, 0) \rangle_0 \\ &= \langle C_{22.1}f_2^*, f_2 \rangle_{\mathcal{H}(S_2)} \\ &= \langle h, \tilde{h}_2 \rangle_{\mathcal{H}(Q)} \\ &= \langle (0, 0, f_3), (0, C_{22.1}f_2, (C_{32} - C_{31}C_{12})f_2) \rangle_0 \\ &= \langle f_3, (C_{32} - C_{31}C_{12})f_2 \rangle_{\mathcal{H}(S_3)} \\ &= \langle (C_{23} - C_{21}C_{13})f_3, f_2 \rangle_{\mathcal{H}(S_2)}. \end{aligned}$$

So,  $f_2^* = C_{22.1}^{-1}(C_{23} - C_{21}C_{13})f_3$ . □

**Corollary A.6.** For  $h = (0, 0, \tilde{f}_3) \in L_3$ ,

$$Bh = (0, (C_{23} - C_{21}C_{13})C_0^{-1}\tilde{f}_3, (C_{32} - C_{31}C_{12})C_{22.1}^{-1}(C_{23} - C_{21}C_{13})C_0^{-1}\tilde{f}_3).$$

**Corollary A.7.** If  $h = (0, C_{22.1}f_2, (C_{32} - C_{31}C_{12})f_2) \in L_2$ , then

$$B^*h = (0, 0, (C_{32} - C_{31}C_{12})f_2).$$

**Proof.** For  $h = (0, C_{22.1}f_2, (C_{32} - C_{31}C_{12})f_2) \in L_2$  and  $\tilde{h}_3 = (0, 0, \tilde{f}_3) \in L_3$ ,

$$\begin{aligned} \langle B\tilde{h}_3, h \rangle_{\mathcal{H}(Q)} &= \langle B\tilde{h}_3, Q^{-1}h \rangle_0 \\ &= \langle B\tilde{h}_3, (-C_{12}f_2, f_2, 0) \rangle_0 \\ &= \langle (C_{23} - C_{21}C_{13})C_0^{-1}\tilde{f}_3, f_2 \rangle_{\mathcal{H}(S_2)} \\ &= \langle C_0^{-1}\tilde{f}_3, (C_{32} - C_{31}C_{12})f_2 \rangle_{\mathcal{H}(S_3)} \\ &= \langle \tilde{h}_3, B^*h \rangle_{\mathcal{H}(Q)} \\ &= \langle Q^{-1}\tilde{h}_3, B^*h \rangle_0 \\ &= \langle ([C_{21}C_{22.1}^{-1}(C_{23} - C_{21}C_{13}) - C_{13}]C_0^{-1}\tilde{f}_3, \\ &\quad - C_{22.1}^{-1}(C_{23} - C_{21}C_{13})C_0^{-1}\tilde{f}_3, C_0^{-1}\tilde{f}_3), B^*h \rangle_0. \quad \square \end{aligned}$$

## Acknowledgements

The authors' research was supported by NSF Grant DMS 0652833. Rosemary Renaut acknowledges the support of AFOSR Grant 025717: Development and Analysis of Non-Classical Numerical Approximation Methods, and NSF Grant DMS 1216559: Novel Numerical Approximation Techniques for Non-Standard Sampling Regimes. A helpful consultation with Randy Eubank and Jack Spielberg, and the input of two referees and an associate editor are gratefully acknowledged.

## References

- [1] Cupidon, J., Eubank, R., Gilliam, D. and Ruymgaart, F. (2008). Some properties of canonical correlations and variates in infinite dimensions. *J. Multivariate Anal.* **99** 1083–1104. [MR2419340](#)
- [2] Cupidon, J., Gilliam, D.S., Eubank, R. and Ruymgaart, F. (2007). The delta method for analytic functions of random operators with application to functional data. *Bernoulli* **13** 1179–1194. [MR2364231](#)
- [3] Dauxois, J. and Nkiet, G.M. (2002). Measures of association for Hilbertian subspaces and some applications. *J. Multivariate Anal.* **82** 263–298. [MR1921388](#)
- [4] Dauxois, J., Nkiet, G.M. and Romain, Y. (2004). Canonical analysis relative to a closed subspace. *Linear Algebra Appl.* **388** 119–145. [MR2077855](#)

- [5] Dauxois, J., Nkiet, G.M. and Romain, Y. (2004). Linear relative canonical analysis of Euclidean random variables, asymptotic study and some applications. *Ann. Inst. Statist. Math.* **56** 279–304. [MR2067157](#)
- [6] Dauxois, J. and Pousse, A. (1975). Une extension de l'analyse canonique. Quelques applications. *Ann. Inst. H. Poincaré Sect. B (N.S.)* **11** 355–379. [MR0408118](#)
- [7] Engl, H.W., Hanke, M. and Neubauer, A. (1996). *Regularization of Inverse Problems. Mathematics and Its Applications* **375**. Dordrecht: Kluwer Academic. [MR1408680](#)
- [8] Eubank, R.L. and Hsing, T. (2008). Canonical correlation for stochastic processes. *Stochastic Process. Appl.* **118** 1634–1661. [MR2442373](#)
- [9] Hall, P., Müller, H.-G. and Wang, J.-L. (2006). Properties of principal component methods for functional and longitudinal data analysis. *Ann. Statist.* **34** 1493–1517. [MR2278365](#)
- [10] Hansen, P.C. (1988). Computation of the singular value expansion. *Computing* **40** 185–199. [MR0961122](#)
- [11] He, G., Müller, H.-G. and Wang, J.-L. (2003). Functional canonical analysis for square integrable stochastic processes. *J. Multivariate Anal.* **85** 54–77. [MR1978177](#)
- [12] Hotelling, H. (1936). Relations between two sets of variates. *Biometrika* **28** 321–377.
- [13] Kshirsagar, A.M. (1972). *Multivariate Analysis. Statistics Textbooks and Monographs* **2**. New York: Dekker. [MR0343478](#)
- [14] Kupresanin, A., Shin, H., King, D. and Eubank, R.L. (2010). An RKHS framework for functional data analysis. *J. Statist. Plann. Inference* **140** 3627–3637. [MR2674153](#)
- [15] Laha, R.G. and Rohatgi, V.K. (1979). *Probability Theory*. New York: Wiley. [MR0534143](#)
- [16] Parzen, E. (1970). Statistical inference on time series by RKHS methods. In *Proc. Twelfth Biennial Sem. Canad. Math. Congr. on Time Series and Stochastic Processes; Convexity and Combinatorics (Vancouver, B.C., 1969)* 1–37. Montreal, QC: Canad. Math. Congr. [MR0275616](#)
- [17] Roy, S.N. (1957). *Some Aspects of Multivariate Analysis*. New York: Wiley. [MR0092296](#)
- [18] Rynne, B.P. and Youngson, M.A. (2000). *Linear Functional Analysis. Springer Undergraduate Mathematics Series*. London: Springer. [MR1744871](#)
- [19] Sunder, V.S. (1988).  $N$  subspaces. *Canad. J. Math.* **40** 38–54. [MR0928213](#)
- [20] Vakhania, N.N., Tarieladze, V.I. and Chobanyan, S.A. (1987). *Probability Distributions on Banach Spaces. Mathematics and Its Applications (Soviet Series)* **14**. Dordrecht: Reidel. Translated from the Russian and with a preface by Wojbor A. Woyczynski. [MR1435288](#)
- [21] Yao, F., Müller, H.-G. and Wang, J.-L. (2005). Functional data analysis for sparse longitudinal data. *J. Amer. Statist. Assoc.* **100** 577–590. [MR2160561](#)

Received May 2012 and revised December 2013