Functional Inverse Regression in an Enlarged Dimension Reduction Space

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Abstract: We consider an enlarged dimension reduction space in functional inverse regression. Our operator and functional analysis based approach facilitates a compact and rigorous formulation of the functional inverse regression problem. It also enables us to expand the possible space where the dimension reduction functions belong. Our formulation provides a unified framework so that the classical notions, such as covariance standardization, Mahalanobis distance, SIR and linear discriminant analysis, can be naturally and smoothly carried out in our enlarged space. This enlarged dimension reduction space also links to the linear discriminant space of Gaussian measures on a separable Hilbert space.

Key words and phrases: Functional inverse regression, functional dimension reduction, functional linearity condition, sliced inverse regression.

1 Introduction

Traditionally, sufficient dimension reduction problems refer to the estimation of the space spanned by the columns of $\beta$, where $\beta$ satisfies $Y \perp X \mid \beta^T X$. Here, $X$ is a $p$-dimensional covariate vector, which we assume to satisfy $E(X) = 0$ for simplicity, $\beta$ is a $p \times d$ matrix and $Y$ is a univariate response variable. An equivalent form is $Y = f(\beta^T X, \epsilon)$, where $\epsilon$ is a mean zero random variable independent of $X$. By far the most well known procedure of estimation in this problem is sliced inverse regression (SIR, [Li (1991)]), where solving the leading $d$ eigenvectors of the generalized eigenvalue problem $\Gamma_\epsilon v = \lambda \Gamma v$ is all one needs to do to obtain the column
space of $\beta$. Here $\Gamma = \text{cov}(X)$ and $\Gamma_e = \text{cov}\{E(X \mid Y)\}$. SIR is constructed under a linearity condition which requires $E(X \mid \beta^T X) = \Gamma \beta (\beta^T \Gamma \beta)^{-1} \beta^T X$ and is then further developed into a whole class of inverse regression based methods for dimension reduction. To understand the inverse regression based methods from a different angle, we can normalize the covariates through viewing $Z \equiv \Gamma^{-1/2} X$ as new covariates and $\eta \equiv \Gamma^{1/2} \beta$ as new dimension reduction matrix. Considering the dimension reduction problem in terms of $(Z, Y, \eta)$ instead of $(X, Y, \beta)$ enables much simplification and permits clearer exhibition of the critical operations (Li (1991); Ma and Zhu (2012)).

Dimension reduction problems have been extended from the traditional regression domain to the functional data analysis domain. See Jiang et al. (2014) and references therein. The model considered in the functional dimension reduction framework is

$$Y = f(\langle \beta_1, X \rangle_{L^2}, \ldots, \langle \beta_d, X \rangle_{L^2}, \epsilon),$$

where $Y$ is still a univariate response variable, $X$ is now a covariate function, $\beta_1, \ldots, \beta_d$ are parameter functions in $L^2(I)$, and $\langle \cdot, \cdot \rangle_{L^2}$ denotes the inner product of two functions in the $L^2(I)$ space. Since the matrix vector product $\beta^T X$ in the traditional case can be expressed as $(\beta_1^T X, \ldots, \beta_d^T X)^T$ which can also be viewed as a vector of inner products between the vector $\beta_k$ and the covariate $X$, one might think that the extension to the functional data framework is straightforward. However, there are many subtleties when finite dimensional quantities are extended to infinite dimensional ones, such as $\beta_1, \ldots, \beta_d$ and $X$ to $\beta_1(\cdot), \ldots, \beta_d(\cdot)$ and $X(\cdot)$. Some properties we take for granted in finite dimension may not hold automatically, e.g., some vector norm or the inner product between vectors may not be finite. If we want to perform the similar standardization as in the finite dimensional case by forming $Z(\cdot) \equiv \Gamma^{-1/2} X(\cdot)$ as new covariate function, and $\eta_j(\cdot) \equiv \Gamma^{1/2} \beta_j(\cdot)$ as new dimension reduction functions for the functional correspondence of the variance-covariance matrix (operator) $\Gamma$, not only do we need to consider the extensions from vectors to functions and matrices to operators, but also to define a proper normed spaces and their corresponding requirements on these functions. A careful and rigorous consideration of these issues will enable less restrictive models and more flexible estimation. In fact, one of the main messages of this article is to point out that the requirement of the parameter functions $\beta_j(\cdot)$’s being $L^2(I)$ in Jiang et al. (2014) is too strong and can be relaxed to include more interesting examples.

During the process of our investigation, we also realize that it is crucial to formulate the functional dimension reduction problem properly in order to facilitate the subsequent application of the existing mathematical tools from functional analysis involving Reproducing Kernel Hilbert Space (RKHS) and operator theories. To better prepare for such a task, we summarize some preliminary results in Section 2 and provide an outline of either a proof or an understanding for each result. In Section 3 we give a few motivating examples, wherein the dimension reduction functions fall out of the space required in Jiang et al. (2014) and hence cannot be solved under their model. We then present an extension of the functional dimension
reduction model in Section 4 together with some main results. Our extension works on an
enlarged space, so that the classical notion of SIR in standardized scale can be carried out.

2 Preliminary

2.1 Covariance operators and integral operators

Without loss of generality, we restrict our attention to functions defined on $I \equiv [0, 1]$. Let the
Hilbert space $L_2(I)$ be the space of functions defined on $I$ and equipped with inner product
given by

$$
\langle u, v \rangle_{L_2} = \int_0^1 u(t)v(t) \, dt, \quad u, v \in L_2(I).
$$

Let $\Gamma(s, t)$ be a continuous bivariate function on $I \times I$. Then $\Gamma(s, t)$ induces a linear integral
operator, still written as $\Gamma(s, t)$, where its operation on a function $u(\cdot) \in L_2(I)$ is defined as

$$
(\Gamma u)(s) = \int_0^1 \Gamma(s, t)u(t) \, dt = \langle \Gamma(s, \cdot), u(\cdot) \rangle_{L_2} \quad \text{for} \quad u \in L_2(I).
$$

When $\langle u, \Gamma v \rangle_{L_2} = \langle \Gamma u, v \rangle_{L_2}$ for all $u, v \in L_2(I)$, $\Gamma(s, t)$ is said to be a symmetric linear integral
operator. Note that

$$
\langle u, \Gamma v \rangle_{L_2} = \int_0^1 \int_0^1 u(s)\Gamma(s, t)v(t) \, dt \, ds,
$$

$$
\langle \Gamma u, v \rangle_{L_2} = \int_0^1 \int_0^1 u(s)\Gamma(t, s)v(t) \, dt \, ds.
$$

Hence, as long as $\Gamma(s, t)$ is symmetric as a function of $(s, t)$ defined on $I \times I$, its induced
operator $\Gamma(s, t)$ is also a symmetric operator. When $\langle u, \Gamma u \rangle_{L_2} \geq 0$ for all $u \in L_2(I)$, $\Gamma$ is said
to be positive semi-definite (or non-negative definite). When the equality holds if and only if
$u = 0$ a.s., $\Gamma$ is said to be positive definite (or strictly positive definite). A positive (semi-
definite linear integral operator is also known as a covariance operator. Let $B$ denote the unit
ball in $L_2(I)$, i.e., $B \equiv \{ f \in L_2(I) : \| f \|_{L_2} \leq 1 \}$. An operator $\Gamma$ defined on $L_2(I)$ that maps
to $L_2(I)$ is said to be compact if the image of the unit ball, $\Gamma(B)$, is a compact set in $L_2(I)$.

Let $X(t)$, $t \in I$, be a random process with finite second moments and $Y$ be a univariate
random variable. We now consider three specific bivariate functions and their induced
operators,

$$
\Gamma(s, t) \equiv \text{cov}\{X(s), X(t)\}, \quad \Gamma_w(s, t) \equiv E[\text{cov}\{X(s), X(t)\} | Y],
$$

and

$$
\Gamma_e(s, t) \equiv \text{cov}[E\{X(s) \mid Y\}, E\{X(t) \mid Y\}].
$$
It is easy to verify that $\Gamma(s,t)$, $\Gamma_w(s,t)$ and $\Gamma_e(s,t)$ are all symmetric bivariate functions and $\Gamma(s,t) = \Gamma_w(s,t) + \Gamma_e(s,t)$. We further assume $\Gamma(s,t)$, $\Gamma_w(s,t)$, $\Gamma_e(s,t)$ to be continuous. The continuity of functions $\Gamma(s,t)$, $\Gamma_w(s,t)$ and $\Gamma_e(s,t)$ on $I \times I$ implies they are square integrable, and hence the continuity guarantees that, $\Gamma(s,t)$, $\Gamma_w(s,t)$ and $\Gamma_e(s,t)$ are compact operators on $L_2(I)$ Lax (2002) (Chapter 22, Theorem 4). The definitions of $\Gamma(s,t)$, $\Gamma_w(s,t)$ and $\Gamma_e(s,t)$ also ensure that, they are positive semi-definite. Mercer’s Theorem Lax (2002) (Chapter 30, Theorem 11) then implies that they have discrete spectra. Taking $\Gamma(s,t)$ for instance, it can be expanded in a uniformly convergent series of eigenvalues and eigenfunctions

$$
\Gamma(s,t) = \sum_{i=1}^{q} \xi_i \phi_i(s)\phi_i(t), \quad q \leq \infty, \tag{2}
$$

which we sometimes write in short as

$$
\Gamma = \sum_{i=1}^{q} \xi_i \phi_i \otimes \phi_i^T.
$$

Here $\xi_1 \geq \xi_2 \geq \cdots \geq \xi_q > 0$ are decreasing positive values. If $\Gamma(s,t)$ is strictly positive definite, then $q = \infty$ and $\{\phi_i(\cdot)\}_{i=1}^{q}$ form a complete orthonormal basis for $L_2(I)$. The above result critically relies on the strictly positive definiteness of $\Gamma$. Without the assumption of $\Gamma$ being strictly positive definite, we can still decompose $\Gamma(s,t)$ as in (2), and the corresponding $\{\phi_i(\cdot)\}_{i=1}^{q}$, $q \leq \infty$, always form a complete orthonormal basis for $R(\Gamma)$, the range of $\Gamma$. However, $R(\Gamma) \subsetneq L_2(I)$, when $\Gamma$ is not strictly positive definite. We further outline the following results which are relevant to the functional inverse regression study.

**Proposition 1.** A continuous, symmetric, positive (semi-) definite integral operator $\Gamma(s,t) = \sum_{i=1}^{q} \xi_i \phi_i(s)\phi_i(t)$ is a trace-class operator, i.e.,

$$
\sum_{i=1}^{q} \xi_i < \infty.
$$

**Proof.** Because $\Gamma(s,t)$ is a continuous function on $I \times I$, for $s = t$, $f(t) \equiv \Gamma(t,t)$ is a continuous function of $t$ in $I$, thus is integrable. Hence, $\sum_{i=1}^{q} \xi_i = \int f(t)dt < \infty$. \hfill $\Box$

**Proposition 2.** For any positive (semi-) definite operator $\Gamma(s,t) = \sum_{i=1}^{q} \xi_i \phi_i(s)\phi_i(t)$, there exists a mean zero random process $X(s)$ satisfying $\int E\{X^2(s)\}ds < \infty$ such that $\Gamma(s,t) = \text{cov}\{X(s),X(t)\}$ and

$$
X(s) = \sum_{i=1}^{q} A_i \phi_i(s),
$$

where $A_i$’s are independent random variables with mean zero and variances $\xi_i$’s.
Proof. For $i = 1, 2, \ldots, q$, let $A_i = \xi_i^{1/2}Z_i$, where $Z_i$’s are independent standard normal random variables. Obviously the resulting $X(s)$ is a mean zero process that satisfies $\text{cov}\{X(s), X(t)\} = \Gamma(s, t)$. In addition, $\int E\{X^2(s)\}ds = \sum_{i=1}^{q} \xi_i < \infty$. $\square$

Note that, in our construction of the Gaussian process in the above proof, the sample path $X(\cdot|\omega)$ may not be in $L^2(I)$ for a given realization $\omega$. However, $\int E\{X^2(s)\}ds < \infty$ ensures that the probability of this kinds of $\omega$ is 0. That is, $X(\cdot|\omega) \in L^2(I)$ almost surely. In the following, we may simply use $X \in L^2(I)$ to denote that $X(\cdot|\omega) \in L^2(I)$ almost surely.

2.2 RKHS relevant for functional inverse regression

Let $H_\Gamma$ be the RKHS generated by $\Gamma(s, t)$. Specifically,

$$H_\Gamma \equiv \text{closure}\left\{ \sum_{i=1}^{q} \Gamma(s, t_i)\alpha_i : q \in \mathbb{N}, \alpha_i \in \mathbb{R}, t_i \in [0, 1] \right\},$$

where the closure is taken with respect to the norm induced by the following inner product

$$\langle \Gamma(s, \cdot), \Gamma(t, \cdot) \rangle_{H_\Gamma} = \Gamma(s, t).$$

Note that $H_\Gamma$ is a proper subset of $L^2(I)$. For $f \in H_\Gamma \subset L^2(I)$, $f$ has the expansion

$$f(t) = \sum_i f_i \phi_i(t), \text{ where } f_i = \langle f, \phi_i \rangle_{L^2}.$$

In addition to its $L^2$-norm defined as $\|f\|_{L^2} = \sum_i f_i^2$, the $H_\Gamma$-norm is given by

$$\|f\|^2_{H_\Gamma} = \sum_i \frac{f_i^2}{\xi_i}.$$

For $u, v \in H_\Gamma$, the $H_\Gamma$-inner product is given by

$$\langle u, v \rangle_{H_\Gamma} = \sum_i \frac{u_i v_i}{\xi_i}, \quad (3)$$

where $u(t) = \sum_i u_i \phi_i(t)$, $v(t) = \sum_i v_i \phi_i(t)$.

3 Motivating Examples

Throughout our development of a rigorous framework for functional inverse regression, we set up a space,

$$R(\Gamma^{-1/2}) \equiv \left\{ f : f = \sum_{i=1}^{\infty} f_i \phi_i, f_i \in \mathbb{R} \text{ such that } \sum_i \xi_i f_i^2 < \infty \right\} \supseteq L^2(I),$$
which is the range space of the operator $\Gamma^{-1/2}$ and is larger than $L_2(I)$. Below we give a few examples, wherein the dimension reduction functions fall out of $L_2(I)$ and reside in $R(\Gamma^{-1/2})$. These examples motivate us to consider an enlarged space for functional dimension reduction. Interestingly, this enlarged space $R(\Gamma^{-1/2})$ is the space considered by Grenander (1950) and Rao and Varadarajan (1963) in the study of linear discriminant analysis of Gaussian measures on a separable Hilbert space.

Example 1 (Binary response). Let $Y$ be a binary random variable having probabilities $P(Y = 1) = P(Y = -1) = \frac{1}{2}$, and let $\{\psi_i\}_{i=1}^\infty$ be a complete orthonormal basis for $L_2(I)$. Given $Y = y$, consider

$$X_y(t) = \alpha y \sum_{i=1}^\infty \frac{1}{\sqrt{2+\delta}} \psi_i(t) + \sum_{i=1}^\infty \frac{1}{\sqrt{2+\delta}} Z_i \psi_i(t), \quad t \in I,$$

where $0 < \delta \leq 1/2$ and $\alpha$ is some scalar that controls the separation of two groups. Here $Z_i$'s are independent standard normal random variables that are independent of $Y$. Let $\Gamma_e$ be the between-group covariance and $\Gamma_w$ be the within-group covariance. Then $\Gamma = \Gamma_e + \Gamma_w$. We can easily calculate the within-group covariance function as

$$\Gamma_w(s, t) \equiv E[\text{cov}\{X(s), X(t)|Y\}] = \sum_{i=1}^\infty \frac{1}{\sqrt{2+\delta}} \psi_i(s) \psi_i(t),$$

and the between-group covariance function as

$$\Gamma_e(s, t) = \text{cov}\{\alpha Y \sum_{i=1}^\infty \frac{1}{\sqrt{2+\delta}} \psi_i(s), \alpha Y \sum_{i=1}^\infty \frac{1}{\sqrt{2+\delta}} \psi_i(t)\}$$

$$= \alpha^2 \left[ \sum_{i=1}^\infty \frac{1}{\sqrt{2+\delta}} \psi_i(s) \right] \left[ \sum_{i=1}^\infty \frac{1}{\sqrt{2+\delta}} \psi_i(t) \right].$$

Proposition 3. The following two optimization problems

$$\arg\max_\beta \langle \Gamma_e \beta, \beta \rangle_{L_2} \equiv \arg\max_\beta \langle \Gamma_e \beta, \beta \rangle_{L_2}$$

have the same solution $\beta$ given by

$$\beta(t) = c \sum_{i=1}^\infty \frac{1}{\sqrt{\delta}} \psi_i(t), \quad (4)$$

for any constant $c$.

Proof. From $\Gamma = \Gamma_e + \Gamma_w$, we have

$$\frac{\langle \Gamma \beta, \beta \rangle_{L_2}}{\langle \Gamma_e \beta, \beta \rangle_{L_2}} = \frac{\langle \Gamma_e \beta, \beta \rangle_{L_2} + \langle \Gamma_w \beta, \beta \rangle_{L_2}}{\langle \Gamma_e \beta, \beta \rangle_{L_2}} = 1 + \frac{\langle \Gamma_w \beta, \beta \rangle_{L_2}}{\langle \Gamma_e \beta, \beta \rangle_{L_2}}.$$
Therefore, 
\[
\argmax_{\beta} \langle \Gamma e \beta, \beta \rangle_{L_2} \equiv \argmax_{\beta} \langle \Gamma w \beta, \beta \rangle_{L_2}.
\]

Let \( \beta = \sum_i b_i \psi_i \). Then
\[
\Gamma e \beta = \alpha^2 \left( \sum_{i=1}^{\infty} \frac{b_i}{i^{2+\delta}} \right) \left( \sum_{i=1}^{\infty} \frac{1}{i^{2+\delta}} \psi_i \right),
\]
\[
\langle \Gamma e \beta, \beta \rangle_{L_2} = \alpha^2 \left( \sum_{i=1}^{\infty} \frac{b_i}{i^{2+\delta}} \right)^2,
\]
\[
\Gamma w \beta = \sum_{i=1}^{\infty} \frac{b_i}{i^{2}} \psi_i,
\]
\[
\langle \Gamma w \beta, \beta \rangle_{L_2} = \sum_{i=1}^{\infty} \frac{b_i^2}{i^{2}}.
\]

Therefore, the optimization problem becomes to maximize
\[
\frac{\alpha^2 \left( \sum_{i=1}^{\infty} \frac{b_i}{i^{2+\delta}} \right)^2}{\sum_{i=1}^{\infty} \frac{b_i^2}{i^{2}}}.
\]

From Cauchy-Schwarz inequality,
\[
\left( \sum_{i=1}^{\infty} \frac{b_i}{i^{2+\delta}} \right)^2 \leq \left( \sum_{i=1}^{\infty} \frac{b_i^2}{i^{2}} \right) \left( \sum_{i=1}^{\infty} \frac{1}{i^{2+2\delta}} \right).
\]

The equality holds when \( b_i \propto 1/i^{\delta} \), which means
\[
\beta(t) \propto \sum_{i=1}^{\infty} \frac{1}{i^{\delta}} \psi_i(t)
\]
is the maximum eigenfunction. \(\square\)

The dimension reduction function \( \beta(t) \) is obtained from solving the eigenvalue problem \( \Gamma e \beta = \lambda \Gamma \beta \). The corresponding optimal linear classification rule is via
\[
\text{sign} \left( \langle \beta, X \rangle_{L_2} \right).
\]

This result can be linked to some prior study of linear discriminant analysis of two Gaussian measures on a separable Hilbert space by Grenander (1950) and Rao and Varadarajan (1963). Let
\[
m_y(t) = E \{ X(t) \mid Y = y \} = \alpha_y \sum_{i=1}^{\infty} \frac{1}{i^{2+\delta}} \psi_i(t) = \Gamma^{1/2}_w \left( \alpha_y \sum_{i=1}^{\infty} \frac{1}{i^{1+\delta}} \psi_i \right)(t) \in R(\Gamma^{1/2}_w).
\]
Note that $\beta$ given in (4) is not in $L^2(I)$, but in $R(\Gamma_{w}^{-1/2})$, since

\[
\|\Gamma_{w}^{1/2}\beta\|^2_{L^2} = \left\| \sum_{i} \frac{1}{i^{\delta+1}} \psi_i(t) \right\|^2_{L^2} = \sum_{i} \frac{1}{i^{2+2\delta}} < \infty.
\]

We also have $\|\Gamma_{w}^{-1/2}m_y\|^2_{L^2} = \alpha^2 \sum_{i=1}^{\infty} \frac{1}{i^{2+2\delta}} < \infty$, i.e., $m_y$ is in $R(\Gamma_{w}^{1/2})$. Furthermore, from Proposition 3 and its proof, we have $\Gamma_{w}\beta = c_1m_y$, where $c_1 = c\alpha y \sum_{i=1}^{\infty} 1/(i^{2+2\delta})$, $\Gamma_{w}\beta = c_2m_y$, where $c_2 = c(\alpha y)^{-1}$. Therefore

\[
\langle \Gamma_{w}^{1/2}\beta, \Gamma_{w}^{1/2}\beta \rangle_{L^2} = \langle \Gamma\beta, \beta \rangle_{L^2}
\]

\[
= \langle (\Gamma_{w} + \Gamma_{e})\beta, \beta \rangle_{L^2} = \langle \Gamma_{w}\beta, \beta \rangle_{L^2} + \langle \Gamma_{e}\beta, \beta \rangle_{L^2}
\]

\[
= \|\Gamma_{w}^{1/2}\beta\|^2_{L^2} + c_1c_2\langle m_y, \Gamma_{w}^{-1}m_y \rangle_{L^2}
\]

\[
= \|\Gamma_{w}^{1/2}\beta\|^2_{L^2} + c^2 \left( \sum_{i=1}^{\infty} \frac{1}{i^{2+2\delta}} \right) \|\Gamma_{w}^{-1/2}m_y\|^2_{L^2} < \infty.
\]

Hence, $\beta \in R(\Gamma_{w}^{-1/2})$.

This is an example that $X \in L^2(I)$, $\beta \in R(\Gamma_{w}^{-1/2})$, but $\beta \notin L^2(I)$, and the classification rule sign ($\langle \beta, X \rangle_{L^2}$) is well-defined. This indicates that, to solve for a linear discriminant analysis problem in $L^2(I)$, we cannot restrict $\beta$ to $L^2(I)$. We are obliged to enlarge the domain of $\beta$ to $R(\Gamma_{w}^{-1/2})$. On the other hand, requiring $\beta \in R(\Gamma_{w}^{-1/2})$ is indeed sufficient for the purpose of linear discriminant analysis given in (4) for classifying the observations into two groups.

**Example 2** (Categorical response). The feature revealed in Example 1 is not unique for binary response variable $Y$. When the response variable $Y$ is categorical, similar phenomenon can be observed. For example, consider the case, where the response variable $Y$ is categorical with possible values $y_1, \ldots, y_k$. We normalize the $y$ values so that $Y$ has mean zero and variance 1. Let

\[
X_y(t) = \alpha y \sum_{i=1}^{\infty} \frac{1}{i^{2+2\delta}} \psi_i(t) + \sum_{i=1}^{\infty} \frac{1}{i} Z_i \psi_i(t), \quad t \in I.
\]

We can easily verify that the within-group covariance function is

\[
\Gamma_{w}(s, t) \equiv E \left[ \text{cov} \{ X(s), X(t) \mid Y \} \right] = \sum_{i=1}^{\infty} \frac{1}{i^{2}} \psi_i(s) \psi_i(t),
\]

and the between-group covariance function is

\[
\Gamma_{e}(s, t) = \text{cov} \left\{ \alpha Y \sum_{i=1}^{\infty} \frac{1}{i^{2+2\delta}} \psi_i(s), \alpha Y \sum_{i=1}^{\infty} \frac{1}{i^{2+2\delta}} \psi_i(t) \right\}
\]

\[
= \alpha^2 \left\{ \sum_{i=1}^{\infty} \frac{1}{i^{2+2\delta}} \psi_i(s) \right\} \left\{ \sum_{i=1}^{\infty} \frac{1}{i^{2+2\delta}} \psi_i(t) \right\}.
\]
Let $\Gamma = \Gamma_w + \Gamma_e$. Note that the forms of $\Gamma_w(s,t)$ and $\Gamma_e(s,t)$ here are exactly the same as those in Example 1. Thus, when we perform the functional sliced inverse regression by solving for the first eigenfunction,

$$\beta_1 = \arg \max_v \frac{\langle \Gamma_e \beta, \beta \rangle_{L^2}}{\langle \Gamma_w \beta, \beta \rangle_{L^2}},$$

we have exactly the same analysis as that in Example 1. It then leads to the same conclusion. That is, we are obliged to enlarge the domain of $\beta$ to $R(\Gamma^{-1/2})$. On the other hand, requiring $\beta \in R(\Gamma^{-1/2})$ is also sufficient for our purpose of classifying the observations into $k$ groups.

**Example 3 (Continuous response).** Finally we provide an example with continuous response variable $Y$. Let $Y$ have mean zero and variance 1, and let

$$X_y(t) = \alpha y \sum_{i=1}^{\infty} \frac{1}{i^{2+\delta}} \psi_i(t) + \sum_{i=1}^{\infty} \frac{1}{i} Z_i \psi_i(t), \quad t \in I. \quad (7)$$

We can easily verify that the within-group covariance function is

$$\Gamma_w(s,t) \equiv E \text{cov}\{X(s), X(t)|Y\} = \sum_{i=1}^{\infty} \frac{1}{i^2} \psi_i(s) \psi_i(t).$$

The between-group covariance function is

$$\Gamma_e(s,t) = \text{cov}\left\{ \alpha Y \sum_{i=1}^{\infty} \frac{1}{i^{2+\delta}} \psi_i(s), \alpha Y \sum_{i=1}^{\infty} \frac{1}{i^{2+\delta}} \psi_i(t) \right\} = \alpha^2 \left\{ \sum_{i=1}^{\infty} \frac{1}{i^{2+\delta}} \psi_i(s) \right\} \left\{ \sum_{i=1}^{\infty} \frac{1}{i^{2+\delta}} \psi_i(t) \right\}. $$

Let $\Gamma = \Gamma_w + \Gamma_e$. Now the same analysis as that in Examples 1 and 2 leads to the conclusion that, regardless of how many slices one decides to use, $\beta$ is in $R(\Gamma^{-1/2})$.

4 Enlarged dimension reduction space and main results

In this section, we present our main results. First, we establish in Theorem 1 an interesting link between covariance operators on $L^2(I)$ and on $H_\Gamma$. Next, we extend the functional dimension reduction to a relaxed model with enlarged space given in (10). The reproducing kernel Hilbert space $H_\Gamma$, induced from the covariance operator $\Gamma$, defines a proper range space for the sliced mean (see Proposition 6 and Theorem 2(a) below). It also plays the parallel role as the span of $X$ in finite dimension (see Proposition 6). Note that, $H_\Gamma$ is equipped with an inner product $\langle \cdot, \cdot \rangle_{H_\Gamma}$. Interestingly, this inner product refers to the standardization (see equation (3) above and equation (11) below) similar to the Mahalanobis distance and the standardization by the covariance matrix in finite vector case. We also study the linear design condition under the relaxed model in Proposition 7.
4.1 Bounded operators on $L_2(I)$ and on $\mathcal{H}_\Gamma$

**Theorem 1.** Assume $\Gamma$ and $\Gamma_e$ are continuous, and respectively strict positive definite and positive semi-definite. Then, $\Gamma^{-1/2}\Gamma_e^{-1/2}$ is a well-defined bounded linear operator on $L_2(I)$ if and only if $\Gamma_e$ is a well-defined bounded linear operator on $\mathcal{H}_\Gamma$.

**Proof.** Let $h = \sum_i c_i \phi_i$. Then,

$$\|\Gamma^{-1/2}h\|_{L_2}^2 = \|\Gamma^{-1/2} \sum_i c_i \phi_i(\cdot)\|_{L_2}^2 = \sum_i c_i^2 / \xi_i = \|h\|_{\mathcal{H}_\Gamma}^2. \quad (8)$$

That is,

$$\Gamma^{-1/2}h \in L_2(I) \Leftrightarrow h \in \mathcal{H}_\Gamma. \quad (9)$$

For any $g \in L_2(I)$, there exists $h = \Gamma^{1/2}g \in \mathcal{H}_\Gamma$. Then

$$\|\Gamma^{-1/2}\Gamma_e^{-1/2}g\|_{L_2} = \|\Gamma^{-1/2}\Gamma_e h\|_{L_2} = \|\Gamma_e h\|_{\mathcal{H}_\Gamma}.$$ 

Together with (8), we have

$$\frac{\|\Gamma^{-1/2}\Gamma_e^{-1/2}g\|_{L_2}}{\|g\|_{L_2}^2} = \frac{\|\Gamma_e h\|_{\mathcal{H}_\Gamma}}{\|h\|_{\mathcal{H}_\Gamma}^2},$$

which yields the statement of the theorem. \qed

**Remark 1.** From (8), $\Gamma^{-1/2}$ is bounded when it is defined as a linear operator from $\mathcal{H}_\Gamma$ to $L_2(I)$. Here boundedness is referred to its induced operator norm, $\sup_{f \in \mathcal{H}_\Gamma} \|\Gamma^{-1/2}f\|_{L_2}^2 / \|f\|_{\mathcal{H}_\Gamma}^2 < \infty$. However, when it operates on $f \in L_2(I)$, $\Gamma^{-1/2}f$ may not belong to $L_2(I)$. For example, $\Gamma^{-1/2} \phi_i(t) = \xi_i^{-1/2} \phi_i(t)$, hence $\|\Gamma^{-1/2} \phi_i\|_{L_2}^2 / \|\phi_i\|_{L_2}^2 = \xi_i^{-1} \to \infty$, as $i \to \infty$. When combined with the additional covariance operator $\Gamma_e$, **Theorem 1** ensures the resulting operator $\Gamma^{-1/2}\Gamma_e^{-1/2}$ is a bounded linear operator on $L_2(I)$, i.e., $\Gamma^{-1/2}\Gamma_e^{-1/2} : L_2(I) \to L_2(I)$ is a well-defined bounded operator. Note that $L_2(I)$ is a much larger space than $\mathcal{H}_\Gamma$. Thus, the new operator composed of the three operators can be well-defined in a larger domain than the original operator $\Gamma^{-1/2}$ can.

4.2 Relaxed model and extended estimation

We are now in a position to revisit the functional dimension reduction problem studied in [Jiang et al. (2014)], describe the problem more rigorously and extend it. Let $X(t), t \in I$, be a stochastic process satisfying $E \int X^2(t)dt < \infty$. Denote its covariance function and spectrum by

$$\Gamma(s, t) = \text{cov}\{X(s), X(t)\} = \sum_{i=1}^{\infty} \xi_i \phi_i(s) \phi_i(t).$$
Then, $X$ can be expressed by an expansion as

$$X(s) = \sum_{i=1}^{\infty} A_i \phi_i(s),$$

where $A_i$’s are independent random variables with mean zero and variances $\xi_i$’s. Below we give a Proposition, which ensures that we can exchange the order of double integrals.

**Proposition 4.**

$$E \langle X, \phi_i \rangle_{L^2} = \langle E(X), \phi_i \rangle_{L^2}.$$

**Proof.** From Cauchy-Schwarz inequality, we have

$$E \int |X(s)\phi_i(s)|ds \leq E \left[ \left( \int X^2(s)ds \right)^{1/2} \left( \int \phi_i^2(s)ds \right)^{1/2} \right] = E \left( \int X^2(s)ds \right)^{1/2}.$$

From Jensen’s inequality,

$$E \left( \int X^2(s)ds \right)^{1/2} \leq \left( E \int X^2(s)ds \right)^{1/2} < \infty.$$

Thus, with $E \int |X(s)\phi_i(s)|ds < \infty$, we can apply Fubini’s Theorem and get

$$E \int X(s)\phi_i(s)ds = \int E[X(s)]\phi_i(s)ds.$$

Our proposed model is

$$Y = f \left( \langle \beta_1, X \rangle_{L^2}, \ldots, \langle \beta_d, X \rangle_{L^2}, \epsilon \right), \text{ where } \beta(\cdot) \in R(\Gamma^{-1/2}). \quad (10)$$

Note that a critical difference of our formulation here from that in Jiang et al. (2014) is that, we only require $\beta$ to be in $R(\Gamma^{-1/2})$, which is larger than $L^2(I)$. This extension allows more flexibility in the dimension reduction functions.

**Proposition 5.** For $\beta \in R(\Gamma^{-1/2})$, $\langle \beta, X \rangle_{L^2}$ is well-defined almost surely.

**Proof.** Let $\delta \equiv \Gamma^{1/2} \beta \in L^2(I)$ and $\delta_i = \langle \delta, \phi_i \rangle_{L^2}$. We have

$$E \langle \beta, X \rangle_{L^2}^2 = E \left( \sum_i \langle \Gamma^{-1/2} \delta, \phi_i \rangle_{L^2} \cdot \langle X, \phi_i \rangle_{L^2} \right)^2$$

$$= \sum_i \langle \xi_i^{-1/2} \delta_i \rangle^2 E A_i^2$$

$$= \sum_i \xi_i^{-1} \delta_i^2 \xi_i = \sum_i \delta_i^2 = \|\delta\|_{L^2}^2 < \infty,$$

which implies that $|\langle \beta, X \rangle_{L^2}| < \infty$ a.s. \qed
Remark 2. Proposition 5 reveals an interesting result regarding the space where \( X \) belongs to. The finite second moment condition is commonly used in statistical analysis. In the finite dimensional case, a random vector with finite second moment can have arbitrary variation for each component of the random vector, hence the random vector can take values in the entire space. However, this is not the case in the infinite dimensional functional space. To ensure finite integrated variance, a random function cannot have arbitrary variation along each dimension. In fact, the variations along all dimensions, except a finite set of dimensions, have to degenerate sufficiently fast to guarantee finite total variant. In fact, the set of dimensions in which almost all variation accumulate is fixed for a single random function. As a consequence, the random function cannot take values everywhere in \( L_2(I) \). This is why the resulting space of the random function \( X \) is in fact a much smaller subspace of \( L_2(I) \). A feature of this subspace is that it ensures finite inner-product with elements in \( R(\Gamma^{-1/2}) \), where \( \Gamma \) is the covariance function of \( X \). We define this space as

\[
R(\Gamma^{1/2})^+ \equiv \{ f : \langle f, \beta \rangle_{L_2} < \infty, \text{a.s.} \ \forall \beta \in R(\Gamma^{-1/2}) \}.
\]

Obviously \( R(\Gamma^{1/2}) \subset R(\Gamma^{1/2})^+ \subset L_2(I) \). We will encounter this space again when we present an equivalent linearity condition later in Section 4.3. Note that although a single random function \( X \) belongs to a much smaller space \( R(\Gamma^{1/2})^+ \), the (uncountable) union of all such spaces of all random functions is the entire \( L_2(I) \).

Remark 3. For any \( f \in R(\Gamma^{1/2}) \), Proposition 5 ensures that the quantity \( \langle \Gamma^{-1/2} f, X \rangle_{L_2} \) is well-defined a.s. It is easy to verify the identity

\[
\langle \Gamma^{-1/2} f, \Gamma^{-1/2} X \rangle_{L_2} = \langle \Gamma^{-1} f, X \rangle_{L_2} = \langle f, X \rangle_{H_\Gamma}.
\]

In the classical SIR, the main problem can be viewed as solving the eigenvalue problem of \( \Gamma_e \) in the space scaled by \( \Gamma^{-1/2} \). Now in Functional Sliced Inverse Regression (FSIR), (11) indicates that \( \Gamma^{-1/2} \) can be again viewed as the scaled operator from \( L_2(I) \) to \( H_\Gamma \).

In fact, the relaxed model leads to more flexible requirements on subsequent operators needed in the estimation procedure, which in turn leads to less stringent conditions on quantities such as mean covariates conditional on the response, etc. For example, in the FSIR approach, we would search for \( \beta \) from the functional eigenvalue problem

\[
\Gamma_e \beta = \lambda \Gamma \beta,
\]

where \( \Gamma(s,t) \equiv \text{cov}\{X(s), X(t)\} \) as before, \( m_Y(s) \equiv E\{X(s) \mid Y\} \) and

\[
\Gamma_e(s,t) \equiv \text{cov}[E\{X(s) \mid Y\}, E\{X(t) \mid Y\}] = \text{cov}\{m_Y(s), m_Y(t)\}.
\]

Letting \( \eta = \Gamma^{1/2} \beta \in L_2(I) \), rewriting (12) as

\[
\Gamma^{-1/2} \Gamma_e \Gamma^{-1/2} \eta = \Gamma^{-1/2} \Gamma_e \Gamma^{-1/2} (\Gamma^{1/2} \beta) = \lambda (\Gamma^{1/2} \beta) = \lambda \eta,
\]
we would naturally require $\Gamma^{-1/2} \Gamma_e \Gamma^{-1/2}$ to be a well-defined operator from $L_2(I)$ to $L_2(I)$. However, $\Gamma^{-1/2} \Gamma_e \Gamma^{-1/2}$ is restricted to operate on $R(\Gamma_e)$ in Jiang et al. (2014). This restriction, comes naturally from their condition that $\beta \in L_2(I)$, leads to a conclusion that the slice mean can only be in a restricted space $R(\Gamma)$ (Theorem 2(b) below) instead of in the space $R(\Gamma^{-1/2})$. In Theorem 2(a), we show that our relaxation on the domain of $\Gamma^{-1/2} \Gamma_e \Gamma^{-1/2}$ leads to a more flexible condition on the conditional mean functions $m_Y(s)$.

Here, we first state a useful result in Proposition 6

**Proposition 6.** $R(\Gamma^{1/2}) \equiv \mathcal{H}_\Gamma$.

**Proof.** A function $g \in R(\Gamma^{1/2})$ is equivalent to $g = \Gamma^{1/2}h$ and $h \in L_2(I)$. Now

$$
\|g\|_{\mathcal{H}_\Gamma}^2 = \|\Gamma^{1/2}h\|_{\mathcal{H}_\Gamma}^2 = \|\sum_i \xi_i^{1/2}\phi_i(s)\langle \phi_i(t), h(t)\rangle\|_{\mathcal{H}_\Gamma}^2 = \|\sum_i \{\xi_i^{1/2}\langle \phi_i(t), h(t)\rangle\}^2 / \xi_i\|_{\mathcal{H}_\Gamma} = \|h\|_{L_2}^2.
$$

Thus $\|g\|_{\mathcal{H}_\Gamma}^2 < \infty$ is equivalent to $\|h\|_{L_2}^2 < \infty$, hence $g \in R(\Gamma^{1/2})$ is equivalent to $g \in \mathcal{H}_\Gamma$. \qed

**Remark 4.** Proposition 6 implies that, if $m_y \in \mathcal{H}_\Gamma$, then $m_y \in R(\Gamma^{1/2})$, and thus $\Gamma^{-1}m_y$ is in $R(\Gamma^{-1/2})$. In those examples in Section 3, we have shown that the relaxation from $\beta \in L_2(I)$ to $\beta \in R(\Gamma^{-1/2})$ is crucial and that the condition $\beta \in R(\Gamma^{-1/2})$ is sufficient for $\langle \beta, X \rangle_{L_2}$ being well-defined a.s. Furthermore, from the proof of Proposition 6 we have

$$
|\langle \beta, m_y \rangle_{L_2}| = |\langle \beta, E(X|Y = y) \rangle_{L_2}| = |E(\langle \beta, X \rangle_{L_2}|Y = y)| \leq \left[ E(\langle \beta, X \rangle_{L_2}^2|Y = y) \right]^{1/2} < \infty,
$$

which means that $m_y \in R(\Gamma^{1/2})$. Therefore, our relaxed condition on $\beta$ is sufficient to include all possible $m_y$. In fact, it is also necessary since for any proper subset $\Omega \subsetneq R(\Gamma^{-1/2})$, there always exists some $m_y$ so that the optimal $\beta = \Gamma^{-1}m_y \notin \Omega$.

**Theorem 2.** Let $Y$ take values in a discrete finite set, say $\{1, \ldots, k\}$, with equal probability.

(a) If $\Gamma^{-1/2} \Gamma_e \Gamma^{-1/2}$ is a bounded operator from $L_2(I)$ to $L_2(I)$, then $m_y \in R(\Gamma^{1/2})$.

(b) Alternatively, if $\Gamma^{-1/2} \Gamma_e \Gamma^{-1/2}$ is a bounded operator from $R(\Gamma^{1/2})$ to $R(\Gamma^{1/2})$, then $m_y \in R(\Gamma)$.

**Proof.** (a) From Theorem 1 if $\Gamma^{-1/2} \Gamma_e \Gamma^{-1/2}$ is a bounded operator on $L_2(I)$, then $\Gamma_e$ is a bounded operator on $\mathcal{H}_\Gamma$, which means $h \equiv \Gamma_e g \in \mathcal{H}_\Gamma$ for any $g \in \mathcal{H}_\Gamma$. Thus,

$$
h = \Gamma_e g = \frac{1}{k} \sum_{y=1}^k m_y \otimes m_y^\top g = \frac{1}{k} \sum_{y=1}^k \langle m_y, g \rangle_{L_2} m_y.
$$
In order for the above function to be in \( \mathcal{H}_\Gamma \) for arbitrary \( g \in \mathcal{H}_\Gamma, m_y \)'s have to be in \( \mathcal{H}_\Gamma \).

(b) For an arbitrary \( g \in R(\Gamma^{1/2}), g_1 \equiv \Gamma^{-1/2}g \) is in \( L_2(I) \). Since \( h \equiv \Gamma^{-1/2}\Gamma e \Gamma^{-1/2}g \) is in \( R(\Gamma^{1/2}) \), we have \( \Gamma^{1/2}h \) is in \( R(\Gamma) \). Furthermore, \( \Gamma^{1/2}h \) can be expressed as

\[
\Gamma^{1/2}h = \Gamma e \Gamma^{-1/2}g = \frac{1}{k} \sum_{y=1}^{k} m_y \otimes m_y^T g_1 = \frac{1}{k} \sum_{y=1}^{k} \langle m_y, g_1 \rangle_{L_2} m_y.
\]

In order for the above function to be in \( R(\Gamma) \) for arbitrary function \( g_1 \in L_2(I) \), \( m_y \)'s have to be in \( R(\Gamma) \).

We now examine how the formulation will affect the estimation procedure. Assume a discrete \( Y \) for simplicity. The \( j \)th slice mean function is given by

\[
m_j(t) = E\{X(t)|Y = j\} = \sum_i E(A_i|Y = j)\phi_i(t).
\]

Following Theorem 2 and Proposition 6, \( m_j \) is in RKHS \( \mathcal{H}_\Gamma \). Assume in the \( j \)th slice, we have observations \( D_j \equiv \{X_i(t), Y_i\}_{i=1}^{n_j} \), where \( Y_i = j \) and we consider two types of \( \mathcal{T} \). One is \( \mathcal{T} = I \), i.e., we observe the whole sample paths, and the other is \( \mathcal{T} = \{t_k\}_{k=1}^{q}, q < \infty \), i.e., we observe \( X_i(t) \) at some common discrete time points.

**Theorem 3** (Representer Theorem). Given the \( j \)th slice training sample \( D_j \) with \( \mathcal{T} = \{t_k\}_{k=1}^{q} \), an arbitrary empirical risk function \( \mathcal{Q} : \mathbb{R}^2 \mapsto \mathbb{R} \) and a scalar \( C > 0 \), consider the following minimization problem

\[
\operatorname*{argmin}_{m \in \mathcal{H}_\Gamma} \sum_{i=1}^{n_j} \sum_{t \in \mathcal{T}} \mathcal{Q}\{X_i(t), m(t)\} + C\|m\|^2_{\mathcal{H}_\Gamma}.
\]

(13)

Then the solution of the minimization problem exists and has the representation form

\[
\hat{m}_j(s) = \sum_{k=1}^{q} \Gamma(s, t_k)\alpha_{jk}, \quad t_k \in \mathcal{T}, \ \alpha_{jk} \in \mathbb{R}.
\]

(14)

**Proof.** For any function \( m(s) \in \mathcal{H}_\Gamma \), it can be expressed as

\[
m(s) = \sum_{k=1}^{q} \Gamma(s, t_k)\alpha_k + \nu(s),
\]

where \( \nu(s) \) is in \( \mathcal{H}_\Gamma \) and orthogonal to every \( \Gamma(s, t_k), j = 1, \ldots, k \). By the reproducing property of \( \mathcal{H}_\Gamma \),

\[
m(t_\ell) = \left< \Gamma(s, t_\ell), \sum_{k=1}^{q} \Gamma(s, t_k)\alpha_k + \nu(s) \right>_{\mathcal{H}_\Gamma} = \sum_{k=1}^{q} \Gamma(t_\ell, t_k)\alpha_k, \quad \ell = 1, \ldots, q,
\]
which does not involve $\nu(s)$. This implies that the empirical risk function $\mathbb{Q}$ in (13) also does not involve $\nu(s)$. Since

$$
\left\| \sum_{k=1}^{q} \Gamma(s,t_k)\alpha_k + \nu(s) \right\|_{\mathcal{H}_\Gamma}^2 = \left\| \sum_{k=1}^{q} \Gamma(s,t_k)\alpha_k \right\|_{\mathcal{H}_\Gamma}^2 + \left\| \nu \right\|_{\mathcal{H}_\Gamma}^2 \geq \left\| \sum_{k=1}^{q} \Gamma(s,t_k)\alpha_k \right\|_{\mathcal{H}_\Gamma}^2,
$$

the regularization term in (13) is minimized by $\nu(s) = 0$. Therefore, the minimizer takes the form $\hat{m}_j(s) = \sum_{k=1}^{q} \Gamma(s,t_k)\alpha_k$.

Remark 5. If we modify the minimization problem (13) by restricting the residing space of the slice mean to a smaller subspace $R(\Gamma)$,

$$
\arg\min_{m \in R(\Gamma)} \sum_{i=1}^{n_j} \sum_{t \in \mathcal{T}} \mathbb{Q}\{X_i(t), m(t)\} + C\|m\|_{\mathcal{H}_\Gamma}^2.
$$

(15)

then the representation form (14) might not be valid anymore.

Remark 6. When the observations are the entire paths, i.e., $\mathcal{T} = I$, we can choose $C = 0$ and modify the minimization (13) to

$$
\arg\min_{m \in \mathcal{H}_\Gamma} \sum_{i=1}^{n_j} \mathbb{Q}(X_i, m),
$$

(16)

where now $\mathbb{Q}$ is a bivariate risk functional. A typical bivariate risk functional is the quadratic one, i.e., $\mathbb{Q}(f,g) = \langle \Lambda(f-g), f-g \rangle_{L_2}$, where $\Lambda$ is a symmetric strictly positive definite linear integral operator with $\zeta_\ell$ and $\psi_\ell$ ($\ell = 1, \ldots, \infty$) as its eigenvalues and eigenfunctions. In this case, $\mathbb{Q}(f,g) = \sum_{\ell=1}^{\infty} \zeta_\ell (f_\ell - g_\ell)^2$ for $f = \sum_{\ell=1}^{\infty} f_\ell \psi_\ell$ and $g = \sum_{\ell=1}^{\infty} g_\ell \psi_\ell$. Write $X_i$ as $X_i = \sum_{\ell=1}^{\infty} x_{i\ell} \psi_\ell$ and $m = \sum_{\ell=1}^{\infty} m_\ell \psi_\ell$. Then

$$
\sum_{i=1}^{n_j} \mathbb{Q}(X_i, m) = \sum_{i=1}^{n_j} \sum_{\ell=1}^{\infty} \zeta_\ell (x_{i\ell} - m_\ell)^2 = \sum_{\ell=1}^{\infty} \zeta_\ell \sum_{i=1}^{n_j} (x_{i\ell} - m_\ell)^2.
$$

The above term is minimized when $m_\ell = \sum_{i=1}^{n_j} x_{i\ell}/n_j$ for all $\ell$. That is, the mean path is the minimizer of (16).
Remark 7. With a given covariance estimator, the slice means can be expressed as a linear combination of covariance functions at training data points, as presented in (14). When the covariance estimator is given, the estimation of slice means becomes less challenging. The most difficult part of estimation in FSIR is the estimation of covariance operator. High-dimensional covariance estimation is a difficult problem, and the functional case is even more challenging. Our aim here is to set up a right framework for the functional inverse regression in an enlarged space. Therefore, we do not further discuss the estimation of the covariance operator.

4.3 Linearity condition re-expressed

Recall that SIR requires a linearity condition, which, in the functional dimension reduction framework, is written as the following: For any \( b \in R(\Gamma^{-1/2}) \) there exist \( a_0, a_1, \ldots, a_k \in \mathbb{R} \) such that

\[
E (\langle b, X \rangle_{L_2} | \langle \beta_1, X \rangle_{L_2}, \ldots, \langle \beta_k, X \rangle_{L_2}) = a_0 + \sum_{j=1}^{k} a_j \langle \beta_j, X \rangle_{L_2},
\]

where \( \beta_1, \ldots, \beta_k \in R(\Gamma^{-1/2}) \). Below we give a more direct linearity condition statement, which is equivalent to the one given by (17).

\[
E (X(s) | \langle \beta_1, X \rangle_{L_2}, \ldots, \langle \beta_k, X \rangle_{L_2}) \text{ is linear in } \langle \beta_1, X \rangle_{L_2}, \ldots, \langle \beta_k, X \rangle_{L_2}, \quad \forall s \in I,
\]

where \( \beta_1, \ldots, \beta_k \in R(\Gamma^{-1/2}) \). That is, there exist \( a_j(s) \in R(\Gamma^{1/2})^+ \) such that

\[
E (X(s) | \langle \beta_1, X \rangle_{L_2}, \ldots, \langle \beta_k, X \rangle_{L_2}) = a_0(s) + \sum_{j=1}^{k} a_j(s) \langle \beta_j, X \rangle_{L_2}, \quad \forall s \in I.
\]

Remark 8. It is easy to check that \( R(\Gamma^{1/2})^+ \subset L_2(I) \). Since the functions \( a_j \)'s in (18) should belong to the same space where \( X \) resides, they belong to \( R(\Gamma^{1/2})^+ \) based on Proposition 4, which is smaller than \( L_2(I) \). This fact about \( a_j \)'s is masked when (17) is used to describe the linearity condition. However, we can see that this condition on \( a_j \)'s is indeed necessary and sufficient from the following proof of Proposition 7.

Proposition 7. The two versions of functional linearity condition given in (17) and (18) are equivalent.

Proof. Assume (17) holds. Consider the evaluation functional \( F_s(X) = X(s) \). Let \( b_s(\cdot) \equiv \sum_i \phi_i(s)\phi_i(\cdot) \). Since \( \|\Gamma^{1/2} b_s(\cdot)\|_{L_2}^2 = \sum_i \xi_i \phi_i^2(s) = \Gamma(s, s) < \infty \) for any \( s \), we have \( b_s(\cdot) \in R(\Gamma^{-1/2}) \) for any \( s \). Obviously

\[
\langle b_s, X \rangle_{L_2} = F_s(X) = X(s).
\]

(19)
Thus,
\[
E \{X(s)|\langle \beta_1, X \rangle_{L^2}, \ldots, \langle \beta_k, X \rangle_{L^2} \} = E (\langle b_s, X \rangle_{L^2}|\langle \beta_1, X \rangle_{L^2}, \ldots, \langle \beta_k, X \rangle_{L^2}) = a_0(s) + \sum_{j=1}^{k} a_j(s)\langle \beta_j, X \rangle_{L^2}.
\] (20)

By Proposition 5 we have \(X \in R(\Gamma^{1/2})^+\). It is then easy to see from the identities (20) that \(a_j\)'s are in \(R(\Gamma^{1/2})^+\). Hence (18) holds.

On the other hand, assume (18) holds, \(E (\langle b, X \rangle_{L^2}|\langle \beta_1, X \rangle_{L^2}, \ldots, \langle \beta_k, X \rangle_{L^2}) = a_0(s) + \sum_{j=1}^{k} a_j(s)\langle \beta_j, X \rangle_{L^2} \) holds.

Now for any \(b(s) \in R(\Gamma^{-1/2})\), take inner product with the above two sides, we obtain
\[
E (\langle b, X \rangle_{L^2}|\langle \beta_1, X \rangle_{L^2}, \ldots, \langle \beta_k, X \rangle_{L^2}) = \langle b, a_0 \rangle_{L^2} + \sum_{j=1}^{k} \langle b, a_j \rangle_{L^2}\langle \beta_j, X \rangle_{L^2}.
\]
Since \(b \in R(\Gamma^{-1/2})\) and \(a_j \in R(\Gamma^{1/2})^+\), \(\langle b, a_j \rangle_{L^2} < \infty\). Therefore, (17) holds.

**Remark 9.** We provide a neat expression (18) for the linearity condition. In the classical SIR, the corresponding condition of (17) is: For any \(b \in \mathbb{R}^p\), there exist \(a_0, a_1, \ldots, a_k \in \mathbb{R}\) such that
\[
E (b^T X|\beta_1^T X, \ldots, \beta_k^T X) = a_0 + \sum_{j=1}^{k} a_j \beta_j^T X.
\]
The corresponding condition of (18) is: There exist \(a_j\)'s in \(\mathbb{R}^p\) such that
\[
E (X|\beta_1^T X, \ldots, \beta_k^T X) = a_0 + \sum_{j=1}^{k} a_j \beta_j^T X.
\]
They are equivalent by similar arguments above. Interestingly, such equivalence description of the functional linearity condition seems only possible when we allow \(\beta \in R(\Gamma^{-1/2})\). In the original framework of Jiang et al. (2014), where \(\beta\) is required to be in \(L_2(I)\), we are unable to obtain such equivalence description, as the representation function \(b_s(\cdot)\) in (19) for the evaluation functional \(F_s\) is in \(R(\Gamma^{-1/2})\) but not in \(L_2(I)\).

5 Conclusion

We have described an extension of the dimension reduction models to the functional data framework. Our extension is based on careful and rigorous considerations in operator theory
and functional analysis. We mainly focused on generalizing concepts in the classical dimension reduction problems into the new framework and on enlarging the functional space of the reduction function \( \beta \). We found some interesting examples where such increased flexibility is indeed needed, and we discovered an equivalent expression of the popular linearity condition. While our analysis is based on FSIR, we believe similar analysis can be applied to other functional inverse regression based methods. It will be interesting to study how other methods in the classical dimension reduction models can be properly extended to the functional data framework.

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