Partial least squares for function-on-function regression via Krylov subspaces

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Abstract

People employ the function-on-function regression (FoFR) to model the relationship between two random curves. Fitting this model, widely used strategies include algorithms falling into the framework of functional partial least squares (FPLS, typically requiring iterative eigendecomposition). Here we introduce an FPLS route for FoFR based upon Krylov subspaces. It can be expressed in two forms equivalent to each other (in exact arithmetic): one of them is non-iterative with explicit forms of estimators and predictions, facilitating the theoretical derivation and potential extensions (to more complex modelling); the other one stabilizes numerical outputs. The consistence of estimators and predictions is established with the aid of regularity conditions. Numerical studies illustrate the competitiveness of our proposal in terms of both accuracy and running time.

Keywords: functional data analysis; functional linear model; functional partial least squares; functional principal component analysis.

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1 Introduction

Sometimes one would like to model the relationship between two stochastic curves. To exemplify this type of interest, two instances are listed as below.

**Diffusion tensor imaging (DTI) data** (dataset `DTI` in R package `classiFunc`, Maierhofer and Pfisterer, 2018). DTI is powerful for characterizing microstructural changes for neuropathology (Alexander et al., 2007). One of widely used DTI measures is the fractional anisotropy (FA). An FA tract profile consists of FA values (ranging between zero and one) along a tract of interest in the brain. Originally collected at the Johns Hopkins University and the Kennedy-Krieger Institute, FA tract profiles for the corpus callosum (CCA) and the right corticospinal tract (RCST) for 142 individuals are included in dataset `DTI` in R package `refund` (Goldsmith et al., 2019). Imputing missing values among them, Maierhofer and Pfisterer (2018) created `DTI in classiFunc`. There are investigations on associations between these CCA and RCST trajectories; see, e.g., Ivanescu et al. (2015).

**Boys’ gait (BG) data** (dataset `gait` in R package `fda`, Ramsay et al., 2020). This dataset records hip and knee angles in degrees for 39 walking boys. For each individual, through a 20-point movement cycle, these angles form two curves. Then BG may be partially reflected by the relationship between hip and knee curves.

As a fundamental model in the functional data analysis (FDA), the function-on-function regression (FoFR, first proposed by Ramsay and Dalzell, 1991) may be helpful to the these scientific explorations. Let $X = X(s)$ and $Y = Y(t)$ be two $L_2$-processes defined, respectively, on closed intervals $\mathbb{I}_X, \mathbb{I}_Y \subset \mathbb{R}$. FoFR is formulated as

$$Y(t) = \mu_Y(t) + \int_{\mathbb{I}_X} \{X(s) - \mu_X(s)\} \beta^*(s,t)ds + \varepsilon(t),$$

where $\beta^* \in L_2(\mathbb{I}_X \times \mathbb{I}_Y)$ is the target unknown parameter function and $\mu_X(s)$ (resp. $\mu_Y(t)$) denotes $E\{X(s)\}$ (resp. $E\{Y(t)\}$). Zero-mean Gaussian process $\varepsilon(t)$ has a covariance function $r_\varepsilon$ continuous on $\mathbb{I}_Y \times \mathbb{I}_Y$ and is uncorrelated with $X(s)$, i.e., $E\{X(s), \varepsilon(t)\} = 0$ for all $(s,t) \in \mathbb{I}_X \times \mathbb{I}_Y$. This model becomes

$$Y(t) = \mu_Y(t) + L_X(\beta^*)(t) + \varepsilon(t),$$

(1)
defining a random integral operator \( \mathcal{L}_X : L_2(\mathbb{I}_X \times \mathbb{I}_Y) \rightarrow L_2(\mathbb{I}_Y) \) such that, for each \( f \in L_2(\mathbb{I}_X \times \mathbb{I}_Y) \),

\[
\mathcal{L}_X(f)(\cdot) = \int_{\mathbb{I}_X} \{ X(s) - \mu_X(s) \} f(s, \cdot) ds.
\]

Write \( r_{XX} = r_{XX}(s, t) = \text{cov}\{ X(s), X(t) \} \), and \( r_{YY} = r_{YY}(s, t) = \text{cov}\{ Y(s), Y(t) \} \), continuous respectively on \( \mathbb{I}_X \times \mathbb{I}_X \) and \( \mathbb{I}_Y \times \mathbb{I}_Y \). Also, we have continuous \( r_{XY} = r_{XY}(s, t) = \text{cov}\{ X(s), Y(t) \} \), \( (s, t) \in \mathbb{I}_X \times \mathbb{I}_Y \). Correspondingly, a linear integral operator \( \mathcal{R}_{XX} : L_2(\mathbb{I}_X) \rightarrow L_2(\mathbb{I}_X) \) is given by, for each \( f \in L_2(\mathbb{I}_X) \),

\[
\mathcal{R}_{XX}(f)(\cdot) = \int_{\mathbb{I}_X} r_{XX}(\cdot, t) f(t) dt.
\]

One more operator \( \mathcal{R}_{YY} : L_2(\mathbb{I}_Y) \rightarrow L_2(\mathbb{I}_Y) \) is defined in complete analogy to \( \mathcal{R}_{XX} \). Let \((\lambda_{i,X}, \phi_{i,X})\) (resp. \((\lambda_{i,Y}, \phi_{i,Y})\)) be the \( i \)-th leading eigenvalue and eigenfunction of \( \mathcal{R}_{XX} \) (resp. \( \mathcal{R}_{YY} \)). It is standard in FDA to assume that \( \sum_{i=1}^{\infty} \lambda_{i,X} < \infty \) and \( \sum_{i=1}^{\infty} \lambda_{i,Y} < \infty \), with positive \( \lambda_{i,X} \) and \( \lambda_{i,Y} \). Further assuming (C1) in Appendix, He et al. (2010, Theorem 2.3) confirmed the uniqueness of \( \beta^* \) in the sense of least squares, viz.

\[
\beta^*(s, t) = \Gamma_{XX}^{-1}(r_{XY})(s, t) = \sum_{i,j=1}^{\infty} \int_{\mathbb{I}_Y} \int_{\mathbb{I}_X} \phi_{i,X}(s) \phi_{i,Y}(t) ds dt \phi_{i,X}(s) \phi_{i,Y}(t),
\]

where \( \| \cdot \|_2 \) denotes the \( L_2 \)-norm (abused for all the \( L_2 \) spaces involved), and \( \Gamma_{XX} : L_2(\mathbb{I}_X \times \mathbb{I}_Y) \rightarrow L_2(\mathbb{I}_X \times \mathbb{I}_Y) \) is a linear integral operator defined as, for each \( f \in L_2(\mathbb{I}_X \times \mathbb{I}_Y) \),

\[
\Gamma_{XX}(f)(s, t) = \int_{\mathbb{I}_X} r_{XX}(s, w) f(w, t) dw, \quad (s, t) \in \mathbb{I}_X \times \mathbb{I}_Y.
\]

Hereafter, we stick to (C1) and take (2) as the true parameter-to-estimate, especially in the theoretical discussion.

Excellent contributions have been made to the investigation of FoFR. In general, due to the intrinsically infinite dimension, people have to consider an approximation to \( \beta^* \) within certain subspaces of \( L_2(\mathbb{I}_X \times \mathbb{I}_Y) \). Traditionally, these subspaces are constructed from predetermined functions, e.g., splines and Fourier basis functions. But a more prevailing option may be data-driven: the functional principal component regression (FPCR) drops the tail of the series on the farthest right-hand side of (2) and approximates \( \beta^* \) by its orthogonal projection to span\{ \( f_{ij} \in L_2(\mathbb{I}_X \times \mathbb{I}_Y) \mid f_{ij}(s, t) = \phi_{i,X}(s) \phi_{j,Y}(t), 1 \leq i \leq p, 1 \leq j \leq q \} \}, with \( p \) and \( q \) chosen by cross-validation and span\{ \} denoting the linear space spanned by
elements inside the braces; specifically, FPCR approximates $\beta^*$ by

$$
\beta_{p,q,\text{FPCR}}(s,t) = \sum_{i=1}^{p} \sum_{j=1}^{q} \int_{I_X} \int_{I_X} \phi_{i,X}(v)r_{XY}(v,w)\phi_{j,Y}(w)dv dw / \lambda_{i,X} \phi_{i,X}(s)\phi_{j,Y}(t).
$$

(3)

Accompanied with a penalized estimation, Lian (2015) and Sun et al. (2018) limited their discussions on coefficient estimators to reproducing kernel Hilbert spaces. The Tikhonov (viz. ridge-type) regularization in Benatia et al. (2017) yields a remedy for ill-posed $\beta^*$ when not all $\lambda_{i,X}$ are non-zero. Distinct from these works, our consideration is based on a subspace of $L_2(\mathbb{I}_X \times \mathbb{I}_Y)$ named after (Alexei) Krylov, viz.

$$
\text{KS}_p(\Gamma_{XX}, \beta^*) = \text{span}\{\Gamma_{XX}^i(\beta^*) \mid 1 \leq i \leq p\},
$$

(4)

where $\Gamma_{XX}^0$ is indeed the identity operator $I$, while $\Gamma_{XX}^i : L_2(\mathbb{I}_X \times \mathbb{I}_Y) \rightarrow L_2(\mathbb{I}_X \times \mathbb{I}_Y)$, $i \geq 1$, is defined recursively as, for each $f \in L_2(\mathbb{I}_X \times \mathbb{I}_Y)$ and each $(s,t) \in \mathbb{I}_X \times \mathbb{I}_Y$,

$$
\Gamma_{XX}^i(f)(s,t) = (\Gamma_{XX} \circ \Gamma_{XX}^{i-1})(f)(s,t)
= \Gamma_{XX}\{\Gamma_{XX}^{i-1}(f)\}(s,t)
= \int_{I_X} r_{XX}(s,w)\{\Gamma_{XX}^{i-1}(f)(w,t)\}dw.
$$

Noting that $\Gamma_{XX}^i(\beta^*) = \Gamma_{XX}^{i-1}(r_{XY})$ for all $i \in \mathbb{Z}^+$, the ($p$-dimensional) Krylov subspace at (4) incorporates both $X$ and $Y$ and hence overcomes the unsupervision of truncated eigenspace used in FPCR.

(4) is a natural generalization of Delaigle and Hall (2012, (3.4)), expanding as well the Krylov subspace method for the (multivariate) partial least squares (PLS). In the multivariate context, PLS is a terminology shared by a series of algorithms yielding supervised (i.e., related-to-response) basis functions; Bissett (2015, Section 2.2) briefed several well-known examples of them, including the nonlinear iterative PLS (NIPALS, Wold, 1975) and the statistically inspired modification of PLS (SIMPLS, de Jong, 1993). For single-vector-response, these two lead to outputs identical to that from the Krylov subspace method; but they are known to yield different results when the response is of more than one vectors; see Cook and Forzani (2019, Section 7.2). Likewise, their respective functional counterparts are equivalent to each other for scalar-response but become diverse again for FoFR. We
refer readers to Beyaztas and Shang (2020) for a straightforward extension of NIPALS and SIMPLS for FoFR. Shooting at the same model, SigComp (Luo and Qi, 2017) embeds penalties into NIPALS. It is Proposition 1 that drives us to pick up the Krylov subspace method as our route.

**Proposition 1.** Under (C1), true parameter \( \beta^* \in \overline{\text{KS}}_\infty(\Gamma_{XX}, \beta^*) = \text{span}\{\Gamma_{XX}^i(\beta^*) | i \geq 1\} \), with the overline representing the closure.

**Remark 1.** It is worth noting that Proposition 1 is not a corollary of Delaigle and Hall (2012, Theorem 3.2); the latter one merely implies an identity weaker than Proposition 1: fixing arbitrary \( t_0 \in I_Y \), univariate function \( \beta^*(\cdot, t_0) \in \text{span}\{\Gamma_{XX}^i(\beta^*)(\cdot, t_0) | i \geq 1\} \).

As an extension of the alternative PLS (APLS, Delaigle and Hall, 2012, designed for the scalar-on-function regression), our proposal is abbreviated as fAPLS, with letter “f” emphasizing its application to FoFR. The remaining portion of this paper is organized as below. Section 2 details two equivalent expressions of fAPLS estimators, facilitating the empirical implementation and theoretical derivation, respectively. In Section 3 fAPLS is compared with competitors in applications to both simulated and authentic datasets. The framework of fAPLS is potential to be extended to more complex settings, e.g., correlated subjects and non-linear modelling; we include three promising directions in Section 4. More assumptions and proofs are relegated to Appendix for conciseness.

## 2 Method

We propose to project \( \beta^* \) to (4) and to utilize the least squares solution

\[
\beta_{p,fAPLS} = \arg \min_{\beta \in \text{KS}_p(\Gamma_{XX}, \beta^*)} \mathbb{E} \| Y - \mu_Y - \mathcal{L}_X(\beta) \|^2_2 = [\Gamma_{XX}(\beta^*), \ldots, \Gamma_{XX}^p(\beta^*)] H_p^{-1} \alpha_p.
\]

where \( H_p = [h_{ij}]_{1 \leq i, j \leq p} \) and \( \alpha_p = [\alpha_1, \ldots, \alpha_p]^\top \) denote \( p \times p \) and \( p \times 1 \) matrices, respectively, with

\[
h_{ij} = \int_{I_Y} \left\{ \int_{I_X} \int_{I_X} r_{XX}(s, w) \Gamma_{XX}^i(\beta^*)(s, t) \Gamma_{XX}^j(\beta^*)(w, t) ds dw \right\} dt
\]
\[
\int_{I_Y} \int_{I_X} \Gamma_{XX}^i(\beta^*)(s,t)\Gamma_{XX}^{i+1}(\beta^*)(s,t)dsdt,
\]

(6)

\[
\alpha_i = \int_{I_Y} \left\{ \int_{I_X} \int_{I_X} r_{XX}(s,w)\Gamma_{XX}^i(\beta^*)(s,t)\beta^*(w,t)dsdw \right\}dt
\]
\[
= \int_{I_Y} \int_{I_X} \Gamma_{XX}(\beta^*)(s,t)\Gamma_{XX}'(\beta^*)(s,t)dsdt.
\]

Proposition 1 justifies (5) by entailing that \(\lim_{p \to \infty} \|\beta_{p,\text{FAPLS}} - \beta^*\|_2 = 0\), which is crucial to the consistency of our estimators delivered later.

Suppose \(n\) two-tuples \((X_i, Y_i), 1 \leq i \leq n\), are all independent realizations of \((X, Y)\). Nobody is aware of the analytical expressions of these trajectories. So it is impossible to compute corresponding integrals exactly. Nevertheless, numerical tools like quadrature rules are available and satisfactory, as long as observed points at each curve are sufficiently dense. Errors are introduced in these approximations. Though they are bounded, it is inevitable to assume smoothness of original trajectories; see, e.g., Tasaki (2009) for the trapezoidal rule. To fulfill the requirement on smoothness, interpolations, e.g., various splines, are often involved; refer to, e.g., Xiao (2019) for theoretical results on certain penalized splines. For convenience, we assume curves to be observed densely enough and abuse integral signs for corresponding empirical approximations.

It is natural to estimate \(r_{XX}(s, t)\) and \(r_{XY}(s, t) (= \Gamma_{XX}(\beta^*)(s, t))\), respectively, by

\[
\hat{r}_{XX}(s, t) = \frac{1}{n} \sum_{i=1}^{n} X_i^\text{cent}(s)X_i^\text{cent}(t)
\]

(7)

\[
\hat{\Gamma}_{XX}(\beta^*) = \hat{r}_{XY}(s, t) = \frac{1}{n} \sum_{i=1}^{n} X_i^\text{cent}(s)Y_i^\text{cent}(t)
\]

(8)

in which \(X_i^\text{cent} = X_i - \bar{X}\) and \(Y_i^\text{cent} = Y_i - \bar{Y}\), with \(\bar{X} = n^{-1} \sum_{i=1}^{n} X_i\) and \(\bar{Y} = n^{-1} \sum_{i=1}^{n} Y_i\). Given \(\hat{\Gamma}_{XX}(\beta^*)\), one can estimate \(\Gamma_{XX}^{i+1}(\beta^*)(s, t)\) by

\[
\hat{\Gamma}_{XX}^{i+1}(\beta^*)(s, t) = \int_{I_X} \hat{r}_{XX}(s, w)\hat{\Gamma}_{XX}^i(\beta^*)(w, t)dw.
\]

(9)

Plugging (7), (8) and (9) all into (5), an estimator for both \(\beta_{p,\text{FAPLS}}\) and \(\beta^*\) comes:

\[
\hat{\beta}_{p,\text{FAPLS}} = [\hat{\Gamma}_{XX}(\beta^*), \ldots, \hat{\Gamma}_{XX}^p(\beta^*)]\hat{\mathbf{H}}^{-1}\hat{\alpha}_p,
\]

(10)

where \(\hat{\mathbf{H}} = [\hat{h}_{ij}]_{1 \leq i, j \leq p}\) and \(\hat{\alpha}_p = [\hat{\alpha}_1, \ldots, \hat{\alpha}_p]^{\top}\) are respectively consisting of

\[
\hat{h}_{ij} = \int_{I_Y} \int_{I_X} \hat{\Gamma}_{XX}^i(\beta^*)(s, t)\hat{\Gamma}_{XX}^{i+1}(\beta^*)(s, t)dsdt,
\]

(11)
\[
\hat{\alpha}_i = \int_{I_Y} \int_{I_X} \hat{\Gamma}_{XX}(\beta^*)(s,t)\hat{\Gamma}_{XX}(\beta^*)(s,t)dsdt.
\]

Finally, given trajectory \(X_0 \sim X\) and \(t \in I_Y\),

\[
g(X_0)(t) = \mathbb{E}\{Y(t) \mid X = X_0\} = \mu_Y(t) + \mathcal{L}_{X_0}(\beta^*)(t)
\]

is predicted by

\[
\hat{g}_{p,\text{APLS}}(X_0)(t) = \hat{\bar{Y}}(t) + \int_{I_X} X_0^{\text{cent}}(s)\hat{\beta}_{p,\text{APLS}}(s,t)ds.
\]

\(\hat{H}\) at (10) is always invertible if we were able to work in exact arithmetic. But it is not the case for finite precision arithmetic: as \(p\) increases, the linear system from \(\hat{\Gamma}_{XX}(\beta^*), \ldots, \hat{\Gamma}_{XX}^p(\beta^*)\) may be close to singular. To overcome this numerical difficulty, as suggested by Delaigle and Hall (2012, Section 4.2), we orthonormalize \(\hat{\Gamma}_{XX}(\beta^*), \ldots, \hat{\Gamma}_{XX}^p(\beta^*)\) (with respect to \(\hat{r}_{XX}\)) into \(\hat{\psi}_1, \ldots, \hat{\psi}_p\) (see Algorithm 1 or Lange 2010, pp. 102) and reformulate the optimization problem at (5) into the empirical version:

\[
\max_{[c_1, \ldots, c_p] \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^n \int_{I_Y} \left\{ Y_i(t) - \hat{\bar{Y}}(t) - \sum_{j=1}^p c_j \int_{I_X} X_i^{\text{cent}}(s)\hat{\psi}_j(s,t)ds \right\}^2 dt.
\]

We then reach a numerically stabilized estimator for \(\beta^*:\)

\[
\hat{\beta}_{p,\text{APLS}} = [\hat{\psi}_1, \ldots, \hat{\psi}_p][\hat{\gamma}_1, \ldots, \hat{\gamma}_p]^\top = \sum_{i=1}^p \hat{\gamma}_i \hat{\psi}_i,
\]

where \([\hat{\gamma}_1, \ldots, \hat{\gamma}_p]^\top\) is the maximizer of (14), with

\[
\hat{\gamma}_i = \int_{I_Y} \int_{I_X} \hat{r}_{XY}(s,t)\hat{\psi}_i(s,t)dsdt.
\]

A prediction for \(g(X_0)\) at (12), alternative to \(\hat{g}_{p,\text{APLS}}(X_0)\) at (13), is thus given by

\[
\hat{g}_{p,\text{APLS}}(X_0)(t) = \hat{\bar{Y}}(t) + \int_{I_X} X_0^{\text{cent}}(s)\hat{\beta}_{p,\text{APLS}}(s,t)ds.
\]

It is worth emphasizing that, in exact arithmetic, \(\hat{\beta}_{p,\text{APLS}}\) at (10) (resp. \(\hat{g}_{p,\text{APLS}}\) at (13)) is identical to \(\tilde{\beta}_{p,\text{APLS}}\) at (15) (resp. \(\tilde{g}_{p,\text{APLS}}\) at (16)), because \(\{\hat{\Gamma}_{XX}(\beta^*) \mid 1 \leq i \leq p\}\) and \(\{\hat{\psi}_i \mid 1 \leq i \leq p\}\) literally span the same space. Nevertheless, in practice \(\tilde{\beta}_{p,\text{APLS}}\) and \(\tilde{g}_{p,\text{APLS}}\) stand out due to their numerical stability for finite precision arithmetic, whereas the
Algorithm 1 Modified Gram-Schmidt orthonormalization with respect to $\hat{r}_{XX}$

\begin{algorithm}
\begin{algorithmic}
\For{$i$ in $1,\ldots,p$}
\State $\hat{\psi}_i^{[1]} \leftarrow \hat{\Gamma}_{XX}(\beta^*)$.
\If{$i \geq 2$}
\For{$j$ in $1,\ldots,i-1$}
\State $\hat{\psi}_i^{[j+1]} \leftarrow \hat{\psi}_i^{[j]} - \left\{ \int_{I_Y} \int_{I_X} \int_{I_X} \hat{r}_{XX}(s,w)\hat{\psi}_i^{[j]}(s,t)\hat{\psi}_j(w,t) \, ds \, dw \, dt \right\} \hat{\psi}_j$.
\EndFor
\EndIf
\State $\hat{\psi}_i \leftarrow \left\{ \int_{I_Y} \int_{I_X} \int_{I_X} \hat{r}_{XX}(s,w)\hat{\psi}_i^{[i]}(s,t)\hat{\psi}_i^{[i]}(w,t) \, ds \, dw \, dt \right\}^{-1/2} \hat{\psi}_i^{[i]}$.
\EndFor
\end{algorithmic}
\end{algorithm}

more explicit expressions of $\hat{\beta}_{p,fAPLS}$ and $\hat{g}_{p,fAPLS}$ make themselves preferred in theoretical derivations.

We have one hyper-parameter to tune. We use generalized cross validation (GCV, Craven and Wahba, 1979), i.e., $p$ is chosen as the minimizer of

$$\text{GCV}(p) = (n - p - 1)^{-2} \sum_{i=1}^{n} \int_{I_Y} \{ Y_i(t) - \tilde{g}_{p,fAPLS}(X_i)(t) \}^2 \, dt.$$ 

Define the fraction of variance explained (FVE) as $\text{FVE}(p) = \sum_{i=1}^{p} \lambda_{i,X} / \sum_{i=1}^{\infty} \lambda_{i,X}$; then the search for $p$ is limited within $[1, p_{\text{max}}]$, where $p_{\text{max}}$ is set to be the smallest integer such that $\text{FVE}(p_{\text{max}})$ exceeds a pre-determined close-to-one threshold, e.g., 99%. This FVE criterion is commonly used in truncating the Karhunen-Loève series, e.g., FPCR. Since FPLS algorithms are typically more parsimonious than FPCR in terms of number of basis functions, $p_{\text{max}}$ formed in this way tends to be reasonable.

2.1 Asymptotic properties

Under regularity conditions, Proposition 2 (resp. Proposition 3) verifies the consistency in $L_2$ and/or supremum metric (in probability) of $\hat{\beta}_{p,fAPLS}$ (resp. $\hat{g}_{p,fAPLS}(X_0)$). In these results, we allow $p$ to diverge as a function of $n$, but its rate is capped to be at most $O(\sqrt{n})$ if $\|r_{XX}\|_2 < 1$ and even slower otherwise. More discussion of the technical assumptions may be found at the beginning of Appendix.
Proposition 2. Holding (C1)–(C5), as \( n \) diverges, \( \|\hat{\beta}_{\text{p,APLS}} - \beta^*\|_2 = o_p(1) \). If upgrade (C5) to (C6), then the convergence becomes uniform, i.e., \( \|\hat{\beta}_{\text{p,APLS}} - \beta^*\|_\infty = o_p(1) \), with \( \cdot \|_\infty \) denoting the supremum metric.

Proposition 3. Given \( X_0 \sim X \), conditions (C1)–(C5) suffice for the zero-convergence (in probability) of \( \|\hat{g}_{\text{p,APLS}}(X_0) - g(X_0)\|_2 \) (i.e., \( \|\hat{g}_{\text{p,APLS}}(X_0) - g(X_0)\|_2 = o_p(1) \)), while the uniform version (viz. \( \|\hat{g}_{\text{p,APLS}}(X_0) - g(X_0)\|_\infty = o_p(1) \)) is entailed jointly by (C1)–(C4) and (C6)–(C7).

3 Numerical study

Our proposal fAPLS was compared with competitors in terms of the relative integrated squared estimation error (ReISEE) and/or relative integrated squared prediction error (ReISPE):

\[
\text{ReISEE} = \frac{\|\beta^* - \hat{\beta}\|_2^2}{\|\beta^*\|_2^2},
\]

\[
\text{ReISPE} = \frac{\sum_{i \in I_{\text{test}}} \|Y_i - \hat{Y}_i\|_2^2}{\sum_{i \in I_{\text{test}}} \|Y_i - \sum_{i \in I_{\text{train}}} Y_i/\#I_{\text{train}}\|_2^2},
\]

where \( \hat{\beta} \) estimates \( \beta \) and \( \hat{Y}_i \) predicts \( Y_i \), \( 1 \leq i \leq n \); where \( \# \) represents the cardinality, and \( I_{\text{train}} \) and \( I_{\text{test}} \) are respective index sets for training and testing. Subsequent comparisons involved other FPLS routes for FoFR, including SigComp (Luo and Qi, 2017) and (functional) NIPALS and SIMPLS (Beyaztas and Shang, 2020). We referred to their original source codes posted respectively at R package FRegSigCom (Luo and Qi, 2018) and GitHub (https://github.com/hanshang/FPLSR; accessible on May 12, 2020). Code trunks for our implementation are currently available at GitHub too (https://github.com/ZhiyangGeeZhou/fAPLS; accessible on May 12, 2020).

3.1 Simulation

Each of the 200 toy samples consisted of \( n \) (\( = 300 \)) independent and identically distributed (iid) pairs of trajectories (with 80\% used for training). For simplicity, assume \( \mu_X = \mu_Y = 0 \).
(a) $\beta^* = (17)$, SNR = 1 & $\rho = 0.1$. 
(b) $\beta^* = (17)$, SNR = 1 & $\rho = 0.9$.

(c) $\beta^* = (17)$, SNR = 5 & $\rho = 0.1$. 
(d) $\beta^* = (17)$, SNR = 5 & $\rho = 0.9$.

Figure 1: Boxplots of ReISEE values for simulation with $\beta^*$ at (17). The four boxes in each subfigure, from left to right, correspond to fAPLS, SigComp, NIPALS and SIMPLS, respectively. All the plots come with the identical scale.

We took 100, 10 and 1 as the top three eigenvalues of $\Gamma_{XX}$, whereas $\lambda_{i,X} = 0$ for all $i \geq 4$. Correspondingly, the first three eigenfunctions of $\Gamma_{XX}$ were respectively set to be (normalized) shifted Legendre polynomials of order 2 to 4 (say $P_2$, $P_3$ and $P_4$; see Hochstrasser, 1972, pp. 773–774), viz.

$$\phi_{1,X}(t) = P_2(t) = \sqrt{5}(6t^2 - 6t + 1),$$
Figure 2: Boxplots of ReISPE values for simulation with $\beta^* = (17)$. The four boxes in each subfigure, from left to right, correspond to fAPLS, SigComp, NIPALS and SIMPLS, respectively. All the plots come with the identical scale.

$$\phi_{2,X}(t) = P_3(t) = \sqrt{7}(20t^3 - 30t^2 + 12t - 1),$$

$$\phi_{3,X}(t) = P_4(t) = 3(70t^4 - 140t^3 + 90t^2 - 20t + 1).$$
Figure 3: Boxplots of ReISEE values for simulation with $\beta^*$ at (18). The four boxes in each subfigure, from left to right, correspond to fAPLS, SigComp, NIPALS and SIMPLS, respectively. All the plots come with the identical scale.

As is known, they are of unit norm and mutually orthogonal on $[0, 1]$ (employed as both $I_X$ and $I_Y$ in simulation). Two sorts of slope functions were respectively given by

$$\beta^*(s, t) = P_2(s)P_2(t),$$  \hspace{1cm} (17)

$$\beta^*(s, t) = P_4(s)P_4(t).$$  \hspace{1cm} (18)
Figure 4: Boxplots of ReISPE values for simulation with $\beta^* = (18)$. The four boxes in each subfigure, from left to right, correspond to fAPLS, SigComp, NIPALS and SIMPLS, respectively. All the plots come with the identical scale.

For zero-mean Gaussian process $\varepsilon$, the covariance function $r_\varepsilon = r_\varepsilon(s, t) = \sigma^2 \rho^{|s-t|}$, with $\rho$ controlling the autocorrelation of $\varepsilon$ and $\sigma$ determined by the value of signal-noise-ratio (SNR = $\sigma^{-1} \sqrt{\text{var}(\|Y\|_2^2)}$). Different values of $\rho$ (resp. SNR) were involved: 0.1 and 0.9 (resp. 1 and 5). In total there were eight combinations on $(\beta^*, \text{SNR}, \rho)$.

A common point shared by Figures 1–4 was that the two plots of the same line differ
little. That is, $\rho$, the degree of autocorrelation of error process, impacted little on the estimation or prediction. This phenomenon was consistent to the one in the multivariate context. Fixing levels of $\beta^*$ and $\rho$, as SNR became larger, each approach led to relatively higher accuracy (or equivalently, lower values of ReISEE and ReISPE). Profiting from the smoothness penalty, SigComp was the most accurate strategy under almost all the settings; in general the prediction and estimation accuracy of fAPLS was comparable to that of NIPALS and SIMPLS. In particular, when the signal was absolutely strong (viz. $\beta^*$ at (17)), fAPLS output satisfactory estimators (see Figure 1) and was fully competitive in terms of prediction (see Figure 2). Encountering the weakest (both absolutely and relatively) signal (viz. $\beta^*$ at (18) and SNR = 1), fAPLS performed the worst: its estimation error was the most fluctuating (see Figures 3a and 3b), though in this case fAPLS prediction errors were still comparable with those given by NIPALS and SIMPLS (see Figures 4a and 4b).

The biggest advantage of fAPLS was on the running time: under all the eight simulation settings, it ran much faster than the other three (see Table 1). This phenomenon was not surprising, because, compared with the other three competing routes, fAPLS involves no eigendecomposition nor tuning parameter for penalty.

### 3.2 Application

Revisit the two datasets described in Section 1. For DTI (resp. BG) data, we took CCA FA tract profiles (resp. hip angle curves) as predictors and RCST FA tract profiles (resp. knee angle curves) as responses. For each dataset, repeat the random split for 200 times: take roughly 20% of all the data points for testing and the remaining for training. After analyzing these training subsets, corresponding to each approach, we generated 200 ReISPE values.

Outputs for DTI data from the four approaches were fairly close to each other in terms of ReISPE (see Figure 5a), while BG data seemed in favor of SIMPLS (see Figure 5b). We guess the relatively small sample size (= 39) of BG data was a cause deteriorating fAPLS predictions.

There was a lack of dominant eigenvalues of $R_{XX}$ for DTI data. As a consequence,
Figure 5: Boxplots of ReISPE values for the two applications. Both plots come with the identical scale.

Table 1: Time consumed (in seconds) by 200 repeats in numerical studies (running on a laptop with Intel® Core™ i5-5200U CPU @2×2.20 GHz and 8 GB RAM)

|       | SNR = 1  | SNR = 5  |               | DTI    | BG    |
|-------|----------|----------|---------------|--------|-------|
|       | ρ = 0.1  | ρ = 0.9  | ρ = 0.1       | ρ = 0.9|       |
| fAPLS | 6.0      | 6.1      | 6.1           | 6.2    | 6.4   |
|       | 363.4    | 372.7    | 365.2         | 377.5  | 376.5 |
|       | 197.6    | 199.1    | 195.0         | 205.0  | 206.1 |
|       | 183.2    | 187.9    | 181.2         | 188.0  | 191.3 |

$p_{\text{max}}$ became as high as 23, slowing down the implementation of fAPLS. That is, as is seen in Table 1 that, compared with other cases, DTI dataset consumed much more time in running fAPLS.

4 Conclusion & discussion

Fitting FoFR, we suggest fAPLS, a route of FPLS via Krylov subspaces. The fAPLS estimator owns a concise and explicit expression. Meanwhile, we introduce an alternative and equivalent form of it, stabilizing numerical outputs. fAPLS is competitive to existing
FPLS routes in terms of estimation and prediction errors and is also less computationally involved. This approach is potential to be further extended, as illustrated in the following paragraphs.

For now we avoid involving applications to geodata. The spatial correlation (i.e., \( X_i \) and \( X_j, i \neq j \), no longer mutually independent) can lead to inconsistency of PLS estimators; see Singer et al. (2016, Theorem 1) for the multivariate context with single-vector-response. A naive correction, transplanted from Singer et al. (2016, Section 4.1), is to instead implement the regression on transformed observations \((X_i^*, Y_i^*), i = 1, \ldots, n\), such that, for all \((s, t) \in \mathbb{I}_X \times \mathbb{I}_Y\), \([X_i^*(s), \ldots, X_n^*(s)]^\top = V_{XX}^{-1/2}(s)[X_1(s), \ldots, X_n(s)]^\top\) and \([Y_1^*(t), \ldots, Y_n^*(t)]^\top = V_{YY}^{-1/2}(t)[Y_1(t), \ldots, Y_n(t)]^\top\), with \( n \times n \) matrices \( V_{XX}(s) = [\text{cov}\{X_i(s), X_j(s)\}] \) and \( V_{YY}(t) = [\text{cov}\{Y_i(t), Y_j(t)\}]\). But it is even challenging to recover \( V_{XX} \) and \( V_{YY} \) sufficiently accurately without specifying the dependence structure, since there is only one observation for each \( i \). Alternatively and more practically, one can target at correcting naive \( \hat{\Gamma}_{XX} \) and \( \hat{r}_{XY} \) for dependent subjects; Paul and Peng (2011) offered a solution to it.

fAPLS has got a heuristic extension to multiple functional covariates, i.e., associated with each realization \( Y_i \sim Y \), there are \( m > 1 \) functional covariates, say \( X_{ij} \sim X_j, 1 \leq j \leq m \), and correspondingly \( m \) coefficient functions \( \beta^{*}(j), 1 \leq j \leq m \). In particular,

\[
Y_i(t) = \mu_Y(t) + \sum_{i=1}^{m} \mathcal{L}_{X_{ij}}(\beta^{*}(j)) + \varepsilon_i(t),
\]

where \( Y_i \) and \( X_{ij} \) are assumed to be independent across all \( i \). Following the idea of (5), an ad hoc estimator for true \((\beta^{*(1)}, \ldots, \beta^{*(m)})\) is thus

\[
(\hat{\beta}^{(1)}_{\text{APLS}}, \ldots, \hat{\beta}^{(m)}_{\text{APLS}}) = \arg\min_{(\beta^{(j)}) \in \mathcal{KS}_{\mu}(\hat{\Gamma}_{X_{j}X_{j}}, \beta^{*(j)}), 1 \leq j \leq m} \frac{1}{m} \sum_{i=1}^{m} \int_{I_Y} \left\{ Y_i(t) - \bar{Y}_i(t) \right. \\
- \sum_{j=1}^{m} \int_{I_{X_{j}}} (X_{ij} - \bar{X}_j)(s)\beta^{(j)}(s,t)ds \left. \right\}^2 dt,
\]

with \( \bar{X}_j = m^{-1} \sum_{j=1}^{m} X_{ij} \) and domains \( I_{X_{j}} \) varying with \( j \). Of course, it becomes necessary to introduce penalties once the above minimizer is not uniquely defined.

Although fAPLS appears to only work for linear models, it is possible to be utilized in fitting the (functional) generalized linear models and proportional hazard (PH) models.
The basic idea, inherited from Marx (1996), is to embed fAPLS into steps of the iteratively reweighted LS (IRLS, Green, 1984) in maximizing likelihood. In a recent work, Wang et al. (2020) jointly modeled the trajectory of the Alzheimer’s Disease Assessment Scale-Cognitive (ADAS-Cog) score and the time of conversion from the mild cognition impairment to Alzheimer’s disease; incorporating APLS with IRLS, their joint model consisted of a functional linear mixed-effects model and a PH model. Maybe it is more natural to consider fAPLS (with an adaption to sparse observations in analogy to Zhou and Lockhart, 2020), because, after all, the two responses (i.e., the ADAS-Cog score and the hazard) both vary with time.

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Appendix

In detail our assumptions are summarized as below.

(C1) \( \sum_{i,j=1}^{\infty} \lambda_{i,X}^{-2} \left\{ \int_{I_Y} \int_{I_X} \phi_{i,X}(s) r_{XY}(s,t) \phi_{j,Y}(t) ds dt \right\}^2 < \infty \). \( \beta^* \) belongs to the range of \( \Gamma_{XX} \), say range(\( \Gamma_{XX} \)).

(C2) \( \mathbb{E}(\|X\|_2^4) < \infty \) for all \( t \in I_Y \).

(C3) Let \( I_X = [0,1] \). Both \( \|\xi_{XX}\|_{\infty,2} \) and \( \|\eta_{XX}\|_{\infty,2} \) are of order \( O_p(1) \) as \( n \to \infty \), with \( \xi_{XX} \) and \( \eta_{XX} \) defined in the statement of Lemma 1 and \( \|\cdot\|_{\infty,2} \) defined such that \( \|f\|_{\infty,2} = \sup_{s \in I_X} \left\{ \int_{I_X} f^2(s,t) dt \right\}^{1/2} \) for \( f \in L_2(I_X \times I_X) \).

(C4) As \( n \to \infty \), \( p = p(n) = O(n^{1/2}) \). Meanwhile, \( \|\widehat{H}_p - H_p\|_2^2 / \tau_p \leq \rho \) for certain \( \rho \in (0,1) \) when \( n \) is sufficiently large. (Here \( \|\cdot\|_2 \) is abused for the matrix norm induced by the Euclidean norm, i.e., for arbitrary \( A \in \mathbb{R}^{p \times q} \) and \( b \in \mathbb{R}^{q \times 1} \) \( \|A\|_2 = \sup_{b,\|b\|_2 = 1} \|Ab\|_2 \) is actually the largest eigenvalue of \( A \). It reduces to the Euclidean norm for vectors.)
(C5) Additional requirements on \( p \) vary with the magnitude of \( \|r_{XX}\|_2 \); they also depend on \( \tau_p \), the smallest eigenvalue of \( H_p \).

- If \( \|r_{XX}\|_2 \geq 1 \), then, as \( n \to \infty \),
  \[
  n^{-1} \tau_p^{-2} p^4 \max(1, \tau_p^{-2} p^2 \|r_{XX}\|_2^4) \quad \text{and} \quad n^{-1} \tau_p^{-3} p^5 \|r_{XX}\|_2^6
  \]
  are both of order \( o(1) \);
- if \( \|r_{XX}\|_2 < 1 \), then \( (n \tau_p^4)^{-1} = o(1) \) as \( n \) diverges.

(C6) Keep everything in (C5) but substitute \( \|r_{XX}\|_\infty \) for \( \|r_{XX}\|_2 \). Meanwhile, require that
  \[ \|\beta_{p,\text{APLS}} - \beta^*\|_\infty = o(1) \]
  as \( p \) diverges, viz. an enhanced version of Proposition 1.

(C7) Stochastic process \( Y \) is “eventually totally bounded in mean” (as defined by Hoffmann-Jørgensen, 1985, (5)–(7)); i.e., in our context,

- \( \mathbb{E}(\|Y\|_\infty) < \infty \);
- for each \( \epsilon > 0 \), there is a finite cover of \( \mathbb{T} \), say \( \text{Co}(\mathbb{T}) \), for each set \( A \in \text{Co}(\mathbb{T}) \), such that
  \[
  \inf_{n \in \mathbb{Z}^+} n^{-1} \mathbb{E}\{\sup_{s,t \in A} |Y(s) - Y(t)|\} < \epsilon.
  \]

Introduced by He et al. (2010), (C1) is set up to guarantee the uniqueness and identifiability of \( \beta^* \) in FoFR (1). It is also adopted by Yao et al. (2005). Assumptions (C2)–(C4) are prerequisites for \( L_2 \)-convergence results in Delaigle and Hall (2012). One may feel unclear about the technical conditions stated in (C5) for the scenario of \( \|r_{XX}\|_2 \geq 1 \): virtually a special case for is that \( n^{-1} \max(\tau_p^{-4}, \tau_p^{-6}, \tau_p^{-8}) = o(1) \) and \( p = O(\ln \ln n) \). Apparently, \( p \) is more restricted when \( \|r_{XX}\|_2 \geq 1 \) than in the case of \( \|r_{XX}\|_2 < 1 \) (for the latter case \( p \) is allowed to diverge at the rate of \( O(n^{1/2}) \)); that is why Delaigle and Hall (2012) suggested changing the scale on which \( X \) is measured. (C6) is an upgrade of (C5), handling the uniform convergence (in probability). At last, we add (C7) as a prerequisite of the uniform law of large numbers for \( \{Y_i \mid i \geq 1 \} \).

**Lemma 1.** For each \((s, w, t) \in \mathbb{I}_X \times \mathbb{I}_X \times \mathbb{I}_Y\),

\[
\hat{r}_{XX}(s, w) = r_{XX}(s, w) + n^{-1/2} \xi_{XX}(s, w) + n^{-1} \eta_{XX}(s, w),
\]

\[
\hat{r}_{XY}(s, t) = r_{XY}(s, t) + n^{-1/2} \xi_{XY}(s, t) + n^{-1} \eta_{XY}(s, t)
\]

(19)

where, with identity operator \( I : \mathbb{R} \to \mathbb{R} \),

\[
\xi_{XX}(s, w) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (I - \mathbb{E})[\{X_i(s) - \mu_X(s)\}\{X_i(w) - \mu_X(w)\}],
\]
\[
\eta_{XX}(s, w) = -n\{-X(s) - \mu_X(s)\}\{X(w) - \mu_X(w)\},
\]
\[
\xi_{XY}(s, t) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} (I - E)\{X_i(s) - \mu_X(s)\}\{Y_i(t) - \mu_Y(t)\},
\]
\[
\eta_{XY}(s, t) = -n\{-X(s) - \mu_X(s)\}\{Y(t) - \mu_Y(t)\},
\]
and \(\|\xi_{XX}\|_2, \|\eta_{XX}\|_2, \|\xi_{XY}\|_2\) and \(\|\eta_{XY}\|_2\) all equal \(O_p(1)\) as \(n\) diverges.

**Proof of Lemma 1.** It is an immediate implication of Delaigle and Hall (2012, (5.1)). □

**Lemma 2.** Assume (C1) and (C2) and that there is \(C > 0\) such that, for all \(n\), we have \(p \leq Cn^{-1/2}\). Then, for each \(\epsilon > 0\), there are positive \(C_1, C_2\) and \(n_0\) such that, for each \(n > n_0\),

\[
\Pr\left[\bigcap_{i=1}^{p} \{\|\hat{\Gamma}^i_{XX}(\beta^*) - \Gamma^i_{XX}(\beta^*)\|_2 \leq n^{-1/2}\|r_{XX}\|_2^{-1}\{C_1 + C_2(i - 1)\}\} \right] \geq 1 - \epsilon.
\]

Assuming one more condition (C3),

\[
\Pr\left[\bigcap_{i=1}^{p} \{\|\hat{\Gamma}^i_{XX}(\beta^*) - \Gamma^i_{XX}(\beta^*)\|_\infty \leq n^{-1/2}\|r_{XX}\|_\infty^{-1}\{C_1 + C_2(i - 1)\}\} \right] \geq 1 - \epsilon.
\]

**Proof of Lemma 2.** Since \(\Gamma_{XX}(\beta^*) = r_{XY}\) and \(\hat{\Gamma}_{XX}(\beta^*) = \hat{r}_{XY}\), Lemma 2 is simply implied by Lemma 1 when \(p = 1\). For integer \(i \geq 2\) and each \((s, t) \in \bar{I}_X \times \bar{I}_Y\),

\[
|\hat{\Gamma}^i_{XX}(\beta^*)(s, t) - \Gamma^i_{XX}(\beta^*)(s, t)|
\]
\[
= |\hat{\Gamma}^i_{XX}\{\hat{\Gamma}^{i-1}_{XX}(\beta^*) - \Gamma^{i-1}_{XX}(\beta^*)\}(s, t) + (\hat{\Gamma}^i_{XX} - \Gamma^i_{XX})\{\Gamma^{i-1}_{XX}(\beta^*)\}(s, t)|
\]
\[
\leq \left(\int_{\bar{I}_X} \hat{r}^2_{XX}(s, w)dw\right)^{1/2} \left(\int_{\bar{I}_X} \{\hat{\Gamma}^{i-1}_{XX}(\beta^*) - \Gamma^{i-1}_{XX}(\beta^*)\}(w, t)dw\right)^{1/2}
\]
\[
+ \left(\int_{\bar{I}_X} \{\hat{r}_{XX}(s, w) - r_{XX}(s, w)\}^2dw\right)^{1/2} \left(\int_{\bar{I}_X} \Gamma^{i-1}_{XX}(\beta^*)(w, t)dw\right)^{1/2}.
\]

It implies that, by the triangle inequality,

\[
\|\hat{\Gamma}^i_{XX}(\beta^*) - \Gamma^i_{XX}(\beta^*)\|_2 \leq \|\hat{r}_{XX}\|_2\|\hat{\Gamma}^{i-1}_{XX}(\beta^*) - \Gamma^{i-1}_{XX}(\beta^*)\|_2 + \|\hat{r}_{XX} - r_{XX}\|_2\|\Gamma^{i-1}_{XX}(\beta^*)\|_2.
\]

On iteration it gives that

\[
\|\hat{\Gamma}^i_{XX}(\beta^*) - \Gamma^i_{XX}(\beta^*)\|_2 \leq \|\hat{r}_{XX}\|_2^{-1}\|\hat{\Gamma}_{XX}(\beta^*) - \Gamma_{XX}(\beta^*)\|_2.
\]

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For each $\epsilon > 0$, there is $n_0 > 0$ such that, for all $n > n_0$, we have

\[
1 - \epsilon/2 \leq \Pr(\|\hat{r}_{XX} - r_{XX}\|_2 \leq C_0 n^{-1/2}) \leq \Pr(\|\hat{r}_{XX}\|_2 + C_0 n^{-1/2}),
\]

\[
1 - \epsilon/2 \leq \Pr(\|\hat{r}_{XY} - r_{XY}\|_2 \leq C_0 n^{-1/2}),
\]

with constant $C_0 > 0$, by Lemma 1. It follows (20) that

\[
1 - \epsilon \leq \Pr \left[ \bigcap_{i=1}^{p} \left\{ \|\hat{\Gamma}^{i}_{XX} - \Gamma^{i}_{XX}(\beta^{*})\|_2 \leq C_0 n^{-1/2} \left\{ (\|r_{XX}\|_2 + C_0 n^{-1/2})^{i-1}ight.ight. \\
+ \left. \left. \sum_{j=1}^{i-1} \|r_{XX}\|_2^{j} \|\beta^{*}\|_2 \|r_{XX}\|_2 + C_0 n^{-1/2})^{i-j-1} \right\} \right\} \right]
\]

\[
\leq \Pr \left[ \bigcap_{i=1}^{p} \left\{ \|\hat{\Gamma}^{i}_{XX}(\beta^{*}) - \Gamma^{i}_{XX}(\beta^{*})\|_2 \leq C_0 n^{-1/2} \|r_{XX}\|_2^{i-1} \left\{ 1 + C_0 n^{-1/2}/\|r_{XX}\|_2 \right\}^{i-1}ight.ight. \\
+ \left. \left. \|\beta^{*}\|_2 \sum_{j=1}^{i-1} \left( 1 + C_0 n^{-1/2}/\|r_{XX}\|_2 \right)^{i-j-1} \right\} \right\} \right]
\]

\[
\leq \Pr \left[ \bigcap_{i=1}^{p} \left\{ \|\hat{\Gamma}^{i}_{XX}(\beta^{*}) - \Gamma^{i}_{XX}(\beta^{*})\|_2 \leq \|r_{XX}\|_2^{i-1} \left\{ C_1 + C_2(i-1) \right\} \right\} \right], \quad \text{(since } p \leq C n^{1/2})
\]

where $C_1 = C_0 \exp(CC_0/\|r_{XX}\|_2)$ and $C_2 = \|\beta^{*}\|_2 C_1$.

Suppose (C3) holds. Similar to (20),

\[
\|\hat{\Gamma}^{i}_{XX}(\beta^{*}) - \Gamma^{i}_{XX}(\beta^{*})\|_{\infty} \leq \|\hat{r}_{XX}\|_{\infty}^{i-1} \|\hat{\Gamma}^{i}_{XX}(\beta^{*}) - \Gamma^{i}_{XX}(\beta^{*})\|_{\infty}
\]

\[
+ \|\hat{r}_{XX} - r_{XX}\|_{\infty} \sum_{j=1}^{i-1} \|\hat{r}_{XX}\|_{\infty}^{i-j-1} \|\Gamma^{j}_{XX}(\beta^{*})\|_{\infty}
\]

\[
\leq \|\hat{r}_{XX}\|_{\infty}^{i-1} \|\hat{\Gamma}^{i}_{XX}(\beta^{*}) - \Gamma^{i}_{XX}(\beta^{*})\|_{\infty}
\]

\[
+ \|\hat{r}_{XX} - r_{XX}\|_{\infty} \sum_{j=1}^{i-1} \|\hat{r}_{XX}\|_{\infty}^{i-j-1} \|r_{XX}\|_{\infty}^{2} \|\beta^{*}\|_{\infty}.
\]

Mimicking the argument above for the $L_2$ sense, one obtains that

\[
\Pr \left[ \bigcap_{i=1}^{p} \left\{ \|\hat{\Gamma}^{i}_{XX}(\beta^{*}) - \Gamma^{i}_{XX}(\beta^{*})\|_{\infty} \leq n^{-1/2}\|r_{XX}\|_{\infty}^{i-1} \left\{ C_1 + C_2(i-1) \right\} \right\} \right] \geq 1 - \epsilon,
\]
with, at this time, $C_1 = C_0 \exp(CC_0/\|r_{XX}\|_{\infty})$ and $C_2 = \|\beta^*\|_{\infty}C_1$. The finiteness of $\|\beta^*\|_{\infty}$ originates from the continuity of eigenfunctions $\phi_{i,X}$’s and $\phi_{i,Y}$’s (refer to the Mercer’s theorem).

**Proof of Proposition 1.** Recall $\beta_{p,q,FPCR}$ at (3) and introduce $\beta_{p,\infty,FPCR} \in L_2(\mathbb{I}_X \times \mathbb{I}_Y)$ such that

$$\beta_{p,\infty,FPCR}(s,t) = \lim_{q \to \infty} \beta_{p,q,FPCR}(s,t) = \sum_{i=1}^{p} \frac{\phi_{i,X}(s)}{\lambda_{i,X}} \int_{\mathbb{I}_X} \phi_{i,X}(w)r_{XY}(w,t)dw.$$ 

It follows that

$$\Gamma_{XX}(\beta_{p,\infty,FPCR})(s,t) = \sum_{i=1}^{p} \phi_{i,X}(s) \int_{\mathbb{I}_X} \phi_{i,X}(w)r_{XY}(w,t)dw.$$ 

Now

$$[(\lambda_{1,X}I - \Gamma_{XX}) \circ \cdots \circ (\lambda_{p,X}I - \Gamma_{XX})](\beta_{p,\infty,FPCR}) = 0$$

in which the left-hand side equals $\sum_{i=1}^{p} a_i \Gamma_{XX}^{i}(\beta_{p,\infty,FPCR})$ with $a_0 = \prod_{i=1}^{p} \lambda_{i,X} > 0$. Therefore,

$$\beta_{p,\infty,FPCR} = -\sum_{i=1}^{p} \frac{a_i}{a_0} \Gamma_{XX}^{i}(\beta_{p,\infty,FPCR}).$$

Denote by $P_p : \text{range}(\Gamma_{XX}) \to \text{range}(\Gamma_{XX})$ the operator that projects elements in $\text{range}(\Gamma_{XX})$ to $\text{span}\{f_{ij} \in L_2(\mathbb{I}_X \times \mathbb{I}_Y) | f_{ij}(s,t) = \phi_{i,X}(s)\phi_{j,Y}(t), 1 \leq i \leq p, j \geq 1\}$. Thus $\beta_{p,\infty,FPCR} = P_p(\beta^*)$. Since $\Gamma_{XX}^{i}(\beta_{p,\infty,FPCR}) = P_p[\Gamma_{XX}^{i}(\beta^*)]$, one has

$$P_p \left[ \beta^* + \sum_{i=1}^{p} \frac{a_i}{a_0} \Gamma_{XX}^{i}(\beta^*) \right] = 0,$$

implying that, for all $p$,

$$P_p(\beta^*) \in \{P_p(f) | f \in \text{KS}_{\infty}(\Gamma_{XX},\beta^*)\}.$$ 

Taking limits as $p \to \infty$ on both sides of the above formula, we obtain $\beta^* \in \text{KS}_{\infty}(\Gamma_{XX},\beta^*)$ and accomplish the proof.

**Proof of Proposition 2.** Recall $\beta_{p,IAPLS}$ (5) and $\hat{\beta}_{p,IAPLS}$ (10) and notations in defining them. The Cauchy-Schwarz inequality implies that

$$|\hat{h}_{ij} - h_{ij}|$$
By Lemmas 1 and 2, for each \( \epsilon > 0 \) and \( p \leq Cn^{1/2} \), there are positive \( n_0, C_3 \) and \( C_4 \) such that, for all \( n > n_0 \),

\[
1 - \epsilon \leq \Pr \left[ \bigcap_{i,j=1}^p \left\{ |\hat{h}_{ij} - h_{ij}| \leq \|\hat{\Gamma}_{XX}(\beta^*) - \Gamma_{XX}(\beta^*)\|_2 (r_{XX}\|_2 + C_0 n^{-1/2})^{j+1} \|\beta^*\|_2 \right\} \right]
\]

Thus

\[
\|\hat{H}_p - H_p\|_2^2 \leq \sum_{j,k=1}^p |\hat{h}_{ij} - h_{ij}|^2 = O_p \left( n^{-1} \sum_{i,j=1}^p \|r_{XX}\|_2^{2i+2j} \right) + O_p \left\{ n^{-1} \sum_{i,j=1}^p \max(i^2, j^2) \|r_{XX}\|_2^{2i+2j} \right\}
\]

\[
= \begin{cases} O_p(n^{-1}p^2\|r_{XX}\|_2^{4p}) + O_p(n^{-1}p^4\|r_{XX}\|_2^{4p}) & \text{if } \|r_{XX}\|_2 \geq 1 \\ O_p(n^{-1}) & \text{if } \|r_{XX}\|_2 < 1 \end{cases}
\]

\[
= \begin{cases} O_p(n^{-1}p^4\|r_{XX}\|_2^{4p}) & \text{if } \|r_{XX}\|_2 \geq 1 \\ O_p(n^{-1}) & \text{if } \|r_{XX}\|_2 < 1 \end{cases}
\]

(21)

It is analogous to (21) to deduce that

\[
\|\hat{\alpha}_p - \alpha_p\|_2^2 = \sum_{j=1}^p |\hat{\alpha}_j - \alpha_j|^2 = \begin{cases} O_p(n^{-1}p^3\|r_{XX}\|_2^{2p}) & \text{if } \|r_{XX}\|_2 \geq 1 \\ O_p(n^{-1}) & \text{if } \|r_{XX}\|_2 < 1 \end{cases}
\]

(22)

Denote by \( \tau_p \) the smallest eigenvalue of \( H_p \). Noting that \( \|H_p^{-1}\|_2 = \tau_p^{-1} \), for \( p \leq Cn^{1/2} \),

\[
\| (\hat{H}_p - H_p) H_p^{-1} \|_2 \leq \tau_p^{-1} \|\hat{H}_p - H_p\|_2 = \begin{cases} O_p(n^{-1/2}\tau_p^{-1}p^2\|r_{XX}\|_2^{2p}) & \text{if } \|r_{XX}\|_2 \geq 1 \\ O_p(n^{-1/2}\tau_p^{-1}) & \text{if } \|r_{XX}\|_2 < 1 \end{cases}
\]

22
Introduce random matrix $M_p \in \mathbb{R}^{p \times p}$ such that $I - H_p^{-1}(\hat{H}_p - H_p) + M_p = \{I + H_p^{-1}(\hat{H}_p - H_p)\}^{-1}$, i.e., $M_p = \{I + H_p^{-1}(\hat{H}_p - H_p)\}^{-1}H_p^{-1}(\hat{H}_p - H_p)H_p^{-1}(\hat{H}_p - H_p)$. Therefore, 
\[
\|M_p\|_2 \leq \|I + H_p^{-1}(\hat{H}_p - H_p)\|_2^{-1}\|H^{-1}(\hat{H}_p - H_p)\|_2^{2} \leq (1 - \rho)^{-1}\|\hat{H}_p - H_p\|_2^2,
\]
provided that $\tau_p^{-1}\|\hat{H}_p - H_p\|_2 \leq \rho < 1$ (refer to (C4)). Revealed by the identity that $\hat{H}_p^{-1} = \{I + H_p^{-1}(\hat{H}_p - H_p)\}^{-1}H_p^{-1}$,
\[
\|\hat{H}_p^{-1} - H_p^{-1}\|_2 \leq \{\|H_p^{-1}(\hat{H}_p - H_p)\|_2 + \|M_p\|_2\}\|H_p^{-1}\|_2
\]
\[
= \begin{cases}
O_{p}(n^{-1/2}\tau_p^{-2}p^2\|r_{XX}\|_2^{2p}) + O_{p}(n^{-1}\tau_p^{-3}p^4\|r_{XX}\|_2^{4p}) & \text{if } \|r_{XX}\|_2 \geq 1 \\
O_{p}(n^{-1/2}\tau_p^{-2}) + O_{p}(n^{-1}\tau_p^{-3}) & \text{if } \|r_{XX}\|_2 < 1.
\end{cases}
\]
(23) Combining (22), (23) and the identity that
\[
\|\alpha_p\|_2 = \left[\sum_{i=1}^{p} \left\{ \int_{s} \int_{t} r_{XY}(s, t)\Gamma_{XX}(\beta^*)(s, t)dsdt \right\}^2 \right]^{1/2}
\]
\[
\leq \left[\sum_{i=1}^{p} \|r_{XY}\|_2\|\Gamma_{XX}(\beta^*)\|_2^2 \right]^{1/2}
\]
\[
= \begin{cases}
O_{p}(p^{1/2}\|r_{XX}\|_2^{p}) & \text{if } \|r_{XX}\|_2 \geq 1 \\
O(1) & \text{if } \|r_{XX}\|_2 < 1,
\end{cases}
\]
(24) we reach that
\[
\|\hat{H}_p^{-1}\alpha_p - H_p^{-1}\alpha_p\|_2
\]
\[
\leq \|\hat{H}_p^{-1}\|_2\|\alpha_p - \alpha_p\|_2 + \|\hat{H}_p^{-1} - H_p^{-1}\|_2\|\alpha_p\|_2
\]
\[
= \begin{cases}
O_{p}(n^{-1/2}\tau_p^{-1}p^{3/2}\|r_{XX}\|_2^{p}) + O_{p}(n^{-1}\tau_p^{-3}p^4\|r_{XX}\|_2^{4p}) & \text{if } \|r_{XX}\|_2 \geq 1 \\
O_{p}(n^{-1/2}\tau_p^{-1}) + O_{p}(n^{-1/2}\tau_p^{-2}) + O_{p}(n^{-1}\tau_p^{-3}) & \text{if } \|r_{XX}\|_2 < 1
\end{cases}
\]
\[
= \begin{cases}
O_{p}(n^{-1/2}\tau_p^{-1}p^{3/2}\|r_{XX}\|_2^{p}) + O_{p}(n^{-1}\tau_p^{-3}p^4\|r_{XX}\|_2^{4p}) & \text{if } \|r_{XX}\|_2 \geq 1 \\
O_{p}(n^{-1/2}\tau_p^{-2}) + O_{p}(n^{-1}\tau_p^{-3}) & \text{since } \tau_p \leq h_{ii} = O(1) \text{ if } \|r_{XX}\|_2 < 1.
\end{cases}
\]
(25)
For each \((s, t) \in \mathbb{I}_X \times \mathbb{I}_Y\),

\[
|\hat{\beta}_{p, \text{APLS}}(s, t) - \beta_{p, \text{APLS}}(s, t)|^2
= \left| \hat{\Gamma}_{XX}(\beta^*)(s, t) \right|^2 + \left| \hat{\Gamma}_{XX}(\beta^*)(s, t) \hat{H}_p^{-1} \hat{\alpha}_p \right|^2 - \left| [\sigma_{XX}(\beta^*)]^{(s, t)} \right| H_p^{-1} \alpha_p \right|^2
\leq \left| \|\hat{H}_p^{-1} \hat{\alpha}_p - H_p^{-1} \alpha_p\|_2 \left[ \sum_{i=1}^p \{\hat{\Gamma}_{XX}(\beta^*)(s, t)\} \right] \right|^{1/2}
+ \left| \|H_p^{-1} \alpha_p\|_2 \left[ \sum_{i=1}^p \{\hat{\Gamma}_{XX}(\beta^*)(s, t)\} \right] \right|^{1/2}
\leq 2\|\hat{H}_p^{-1} \hat{\alpha}_p - H_p^{-1} \alpha_p\|_2 \left[ \sum_{i=1}^p \{\hat{\Gamma}_{XX}(\beta^*)(s, t)\} \right]^{1/2}
+ 2\|H_p^{-1} \alpha_p\|_2 \left[ \sum_{i=1}^p \{\hat{\Gamma}_{XX}(\beta^*)(s, t)\} \right]^{1/2}.
\]

Thus \(\|\hat{\beta}_{p, \text{APLS}} - \beta_{p, \text{APLS}}\|_2^2\) is bounded as below:

\[
\|\hat{\beta}_{p, \text{APLS}} - \beta_{p, \text{APLS}}\|_2^2
\leq 2\|\hat{H}_p^{-1} \hat{\alpha}_p - H_p^{-1} \alpha_p\|_2 \sum_{i=1}^p \|\hat{\Gamma}_{XX}(\beta^*)\|^2_2 + 2\|H_p^{-1} \alpha_p\|_2 \sum_{i=1}^p \|\hat{\Gamma}_{XX}(\beta^*) - \hat{\Gamma}_{XX}(\beta^*)\|^2_2
\leq 2\|\hat{H}_p^{-1} \hat{\alpha}_p - H_p^{-1} \alpha_p\|_2 \sum_{i=1}^p \|\hat{\Gamma}_{XX}(\beta^*)\|^2_2
+ 2\tau^{-2}_p \|\alpha_p\|^2_2 \sum_{i=1}^p \|\hat{\Gamma}_{XX}(\beta^*) - \hat{\Gamma}_{XX}(\beta^*)\|^2_2,
\]

where, owing to (25),

\[
(26) = \begin{cases} 
O_p(n^{-1} \tau_p^{-2} p^4 \|r_{XX}\|_2^{4p}) \\
+ O_p(n^{-1} \tau_p^{-4} p^6 \|r_{XX}\|_2^{8p}) + O_p(n^{-2} \tau_p^{-6} p^{10} \|r_{XX}\|_2^{12p}) & \text{if } \|r_{XX}\|_2 \geq 1 \\
O_p(n^{-1} \tau_p^{-4}) + O_p(n^{-2} \tau_p^{-6}) & \text{if } \|r_{XX}\|_2 < 1;
\end{cases}
\]

the order of (27) is jointly given by (24) and Lemma 2, i.e.,

\[
(27) = \begin{cases} 
O(n^{-1} \tau_p^{-2} p^4 \|r_{XX}\|_2^{4p}) & \text{if } \|r_{XX}\|_2 \geq 1 \\
O_p(n^{-1} \tau_p^{-2}) & \text{if } \|r_{XX}\|_2 < 1.
\end{cases}
\]
In this way we deduce

\[ \| \hat{\beta}_{p,\text{APLS}} - \beta_{p,\text{APLS}} \|_2^2 = \begin{cases} 
O_p(n^{-1} \tau_p^{-2} p^4 \| r_{XX} \|_2^{4p}) & \text{if } \| r_{XX} \|_2 \geq 1 \\
O_p(n^{-1} \tau_p^{-4} p^6 \| r_{XX} \|_2^{8p}) + O_p(n^{-2} \tau_p^{-6} p^{10} \| r_{XX} \|_2^{12p}) & \text{if } \| r_{XX} \|_2 < 1.
\end{cases} \]

(28)

A set of necessary conditions for the zero-convergence (in probability) of (28) is contained in (C5). Once they are fulfilled, we conclude the \( L_2 \) convergence (in probability) of \( \hat{\beta}_{p,\text{APLS}} \) to \( \hat{\beta}^* \) following Proposition 1.

We complete the proof by bounding the estimating error in the supremum metric:

\[ \| \hat{\beta}_{p,\text{APLS}} - \beta_{p,\text{APLS}} \|_\infty = \left\| \hat{\Gamma}_{XX}(\beta^*), \ldots, \hat{\Gamma}_p(\beta^*) \right\|_\infty H_p^{-1} \hat{\alpha}_p - \left[ \Gamma_{XX}(\beta^*), \ldots, \Gamma_p(\beta^*) \right] H_p^{-1} \alpha_p \right\|_\infty^2 \]

\[ \leq 2 \| H_p^{-1} \hat{\alpha}_p - H_p^{-1} \alpha_p \|_2^2 \sum_{i=1}^p \| \Gamma_i(\beta^*) \|_\infty^2 + 2 \| H_p^{-1} \alpha_p \|_2^2 \sum_{i=1}^p \| \Gamma_i(\beta^*) - \hat{\Gamma}_i(\beta^*) \|_\infty^2 \]

\[ \leq 2 \| H_p^{-1} \hat{\alpha}_p - H_p^{-1} \alpha_p \|_2^2 \sum_{i=1}^p \| \Gamma_i(\beta^*) \|_\infty^2 \text{ (compare (26))} \]

\[ + 2 \tau_p^{-2} \| \alpha_p \|_2^2 \sum_{i=1}^p \| \hat{\Gamma}_i(\beta^*) - \Gamma_i(\beta^*) \|_\infty^2 \text{ (compare (27))} \]

\[ = \begin{cases} 
O_p(n^{-1} \tau_p^{-2} p^4 \| r_{XX} \|_\infty^{4p}) & \text{if } \| r_{XX} \|_\infty \geq 1 \\
O_p(n^{-1} \tau_p^{-4} p^6 \| r_{XX} \|_\infty^{8p}) + O_p(n^{-2} \tau_p^{-6} p^{10} \| r_{XX} \|_\infty^{12p}) & \text{if } \| r_{XX} \|_\infty < 1.
\end{cases} \]

converging to zero (in probability) with the satisfaction of (C6). The zero-convergence (in probability) of \( \| \hat{\beta}_{p,\text{APLS}} - \beta^* \|_\infty \) follows if we assume that \( \| \beta_{p,\text{APLS}} - \beta^* \|_\infty \to 0 \) as \( p \) diverges. \( \square \)

Proof of Proposition 3. Notice that

\[ \| g_{p,\text{APLS}}(X_0) - g(X_0) \|_2 \leq \| \bar{Y} - \mu_Y \|_2 + \| \bar{X} - \mu_X \|_2 \| \beta^* \|_2 + \| X_0 - \bar{X} \|_2 \| \hat{\beta}_{p,\text{APLS}} - \beta^* \|_2, \]

25
\[ \| \hat{g}_{p,tAPLS}(X_0) - g(X_0)\|_\infty \leq \| \bar{Y} - \mu_Y \|_\infty + \| \bar{X} - \mu_X \|_2 \| \beta^* \|_\infty + \| X_0 - \bar{X} \|_2 \| \hat{\beta}_{p,tAPLS} - \beta^* \|_\infty. \]

The finite trace of \( R_{XX} \) (resp. \( R_{YY} \)), viz. \( \sum_{i=1}^\infty \lambda_{i,X} = E(\| X - \mu_X \|_2^2) < \infty \) (resp. \( \sum_{i=1}^\infty \lambda_{i,Y} = E(\| Y - \mu_Y \|_2^2) < \infty \)), entails that \( \| \bar{X} - \mu_X \|_2 = o_{a.s.}(1) \) (resp. \( \| \bar{Y} - \mu_Y \|_2 = o_{a.s.}(1) \)); see Hoffmann-Jørgensen and Pisier (1976, (2.1.3)). The proof is complete once we verify the zero-convergence (in probability and under (C7)) of \( \| \bar{Y} - \mu_Y \|_\infty \) following Hoffmann-Jørgensen (1985, Theorem 2).

\[ \square \]

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