## MIXTURE INNER PRODUCT SPACES AND THEIR APPLICATION TO FUNCTIONAL DATA ANALYSIS

BY ZHENHUA LIN\*, 1,2, HANS-GEORG MÜLLER<sup>†,3</sup> AND FANG YAO\*,<sup>‡,1</sup>
University of Toronto\*, University of California, Davis<sup>†</sup> and Peking University<sup>‡</sup>

We introduce the concept of mixture inner product spaces associated with a given separable Hilbert space, which feature an infinite-dimensional mixture of finite-dimensional vector spaces and are dense in the underlying Hilbert space. Any Hilbert valued random element can be arbitrarily closely approximated by mixture inner product space valued random elements. While this concept can be applied to data in any infinite-dimensional Hilbert space, the case of functional data that are random elements in the  $L^2$  space of square integrable functions is of special interest. For functional data, mixture inner product spaces provide a new perspective, where each realization of the underlying stochastic process falls into one of the component spaces and is represented by a finite number of basis functions, the number of which corresponds to the dimension of the component space. In the mixture representation of functional data, the number of included mixture components used to represent a given random element in  $L^2$  is specifically adapted to each random trajectory and may be arbitrarily large. Key benefits of this novel approach are, first, that it provides a new perspective on the construction of a probability density in function space under mild regularity conditions, and second, that individual trajectories possess a trajectory-specific dimension that corresponds to a latent random variable, making it possible to use a larger number of components for less smooth and a smaller number for smoother trajectories. This enables flexible and parsimonious modeling of heterogeneous trajectory shapes. We establish estimation consistency of the functional mixture density and introduce an algorithm for fitting the functional mixture model based on a modified expectation-maximization algorithm. Simulations confirm that in comparison to traditional functional principal component analysis the proposed method achieves similar or better data recovery while using fewer components on average. Its practical merits are also demonstrated in an analysis of egg-laying trajectories for medflies.

**1. Introduction.** Introducing the concept of mixture inner product spaces is motivated by one of the basic problems in functional data analysis, namely to ef-

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ficiently represent functional trajectories by dimension reduction. Functional data correspond to random samples  $\{\tilde{X}_1, \tilde{X}_2, \dots, \tilde{X}_n\}$  drawn from a square-integrable random process defined on a finite interval  $D, \ \tilde{X} \in L^2(D)$ . Random functions  $\tilde{X}_i$  are generally considered to be inherently infinite-dimensional and, therefore, finite-dimensional representations are essential. A commonly employed approach for dimension reduction is to expand the functional data in a suitable basis in function space and then to represent the random functions in terms of the sequence of expansion coefficients. This approach has been very successful and has been implemented with B-spline bases [Ramsay and Silverman (2005)] and eigenbases, which consist of the eigenfunctions of the covariance operator of the underlying stochastic process that generates the data. The estimated eigenbasis expansion then gives rise to functional principal component analysis, which was introduced in a rudimentary form in Rao (1958) for the analysis of growth curves. Earlier work on eigendecompositions of square integrable stochastic processes [Gikhman and Skorokhod (1969), Grenander (1950)] paved the way for statistical approaches.

There has been a substantial literature on functional principal component analysis, including basic developments [Besse and Ramsay (1986), Castro, Lawton and Sylvestre (1986)], advanced smoothing methods and modes of variation [Rice and Silverman (1991), Silverman (1996)], theoretical investigations [Boente and Fraiman (2000), Hall and Hosseini-Nasab (2006), Kneip and Utikal (2001)] and a unified framework that covers functional principal component analysis for functional data with both sparse and dense designs and, therefore, brings many longitudinal data under this umbrella [Li and Hsing (2010), Yao, Müller and Wang (2005), Zhang and Wang (2016)]. One of the attractions of functional principal component analysis is that for any number of included components the resulting finite-dimensional approximation to the infinite-dimensional process explains most of the variation. This has contributed to the enduring popularity of functional principal component analysis [Chen and Lei (2015), Li and Guan (2014)], which differs in essential ways from classical multivariate principal component analysis, due to the smoothness and infinite dimensionality of the functional objects.

Existing methods assume a common structural dimension for this approximation [Hall and Vial (2006), Li, Wang and Carroll (2013)], where for asymptotic consistency it is assumed that the number of included components, which is the same for all trajectories in the sample, increases with sample size to ensure asymptotic unbiasedness. To determine an adequate number of components based on observed functional data that is applied across the sample to approximate the underlying processes reasonably well is crucial for the application of functional principal component analysis. This is challenging for applications in which the trajectories recorded for different subjects exhibit different levels of complexity. We introduce here an alternative to the prevailing paradigm that the observed functional data are all infinite-dimensional objects, which are then approximated through a one-size-fits-all sequence of increasingly complex approximations. The proposed alternative model is to assume that each observed random trajectory is composed of only

finitely many components, where the number of components that constitutes an observed trajectory may be arbitrarily large without upper bound and varies across the observed trajectories. This means that while each trajectory can be fully represented without residual by its projections on a finite number of components, the overall process is still infinite-dimensional as no finite dimension suffices to represent it: For each fixed dimension d, there generally exist trajectories that require more than d components for adequate representation. A key feature of this new model is that the number of components used to represent a trajectory depends on the trajectory to be represented.

In this paper, we develop the details of this model and show in data analysis and simulations that its implementation leads to more parsimonious representations of heterogeneous functional data when compared with classical functional principal component analysis. Its relevance for functional data analysis motivates us to develop this model in the context of a general infinite-dimensional separable Hilbert space; we note that all Hilbert spaces considered in this paper are assumed to be separable. For any given infinite-dimensional Hilbert space and an orthonormal basis of this space, we construct an associated *mixture inner product space* (MIPS). The mixture inner product space consists of an infinite mixture of vector spaces with different dimensions d,  $d = 1, 2, 3, \ldots$ . We investigate properties of probability measures on these dimension mixture spaces and show that the mixture inner product space associated with a given Hilbert space is dense in the Hilbert space and is well suited to approximate individual Hilbert space elements as well as probability measures on the Hilbert space.

The mixture inner product space concept has direct applications in functional data analysis. It is intrinsically linked to a trajectory-adaptive choice of the number of included components, and moreover, can be harnessed to construct a density for functional data. The density problem when viewed in the Hilbert space  $L^2$ arises due to the well-known nonexistence of a probability density for functional data with respect to Lebesgue measure in  $L^2$ , which is a consequence of the low small ball probabilities [Dabo-Niang (2002), Li and Linde (1999)] in this space. The lack of a density is a drawback that negatively impacts various methods of functional data analysis. For example, it is difficult to rigorously define modes, likelihoods or other density-dependent methods, such as functional clustering or functional Bayes classifiers. It has therefore been proposed to approach this problem by defining a sequence of approximating densities, where one considers the joint density of the first K functional principal components, as K increases slowly with sample size. This leads to a sequence of finite-dimensional densities that can be thought of as a surrogate density [Bongiorno and Goia (2016), Delaigle and Hall (2010)]. This approach bypasses but does not resolve the key issue that a density in the functional space  $L^2$  does not exist.

In contrast, if the random functions lie in a mixture inner product space, which includes functions of arbitrarily large dimension, one can construct a well-defined

target density by introducing a suitable measure for mixture distributions. This density is a mixture of densities on vector spaces of various dimensions d and its existence follows from the fact that a density exists with respect to the usual Lebesgue measure for each component space, which is a finite-dimensional vector space. Therefore, the proposed mixture inner product space approach is of relevance for the foundations of the theory of functional data analysis.

The paper is organized as follows. We develop the concept of mixture inner product spaces and associated probability measures on such spaces in Section 2 and then apply it to functional data analysis in Section 3. This is followed by simulation studies in Section 4 and an application of the proposed method to a real data set in Section 5. Conclusions are in Section 6. All proofs and technical details are in the Appendix.

- 2. Random elements in mixture inner product spaces. In the theory of functional data analysis, functional data can be alternatively viewed as random elements in  $L^2$  or as realizations of stochastic processes. Under joint measurability assumptions, these perspectives coincide; see Chapter 7 of Hsing and Eubank (2015). We adopt the random element perspective in this paper, which is more convenient as we will develop the concept of a mixture inner product space (MIPS) first for general infinite-dimensional Hilbert spaces, and will then take up the special case of functional data and  $L^2$  in Section 3. In this section, we consider probability measures on Hilbert spaces and random elements that are Hilbert space valued random variables.
- 2.1. Mixture inner product spaces. Let H be an infinite-dimensional Hilbert space with inner product  $\langle \cdot, \cdot \rangle$  and induced norm  $\| \cdot \|$ . Let  $\Phi = (\phi_1, \phi_2, \ldots)$  be a complete orthonormal basis (CONS) of H. We also assume that the ordering of the sequence  $\phi_1, \phi_2, \ldots$  is given and fixed. Define  $H_k, k = 0, 1, \ldots$ , as the linear subspace spanned by  $\phi_1, \phi_2, \ldots, \phi_k$ , where  $H_0 = \emptyset$ , and set  $S_k = H_k \setminus H_{k-1}$  for  $k = 1, 2, \ldots$  and  $S = \bigcup_{k=1}^{\infty} S_k$ , where also  $S = \bigcup_{k=1}^{\infty} H_k$ . Then S is an infinite-dimensional linear subspace of H with inner product inherited from H. Since S has an inner product and is a union of the k-dimensional subsets  $S_k$ , we refer to S as mixture inner product space (MIPS). The definition of  $S_k$  depends on  $\Phi$ , and thus on the ordered sequence  $\phi_1, \phi_2, \ldots$ , while S depends on  $\Phi$  only in the sense that any permutation of  $\phi_1, \phi_2, \ldots$  yields the same space  $S = S(\Phi)$ . It is easy to see that two CONS  $\Phi = (\phi_1, \phi_2, \ldots)$  and  $\Psi = (\psi_1, \psi_2, \ldots)$  result in the same MIPS, that is,  $S(\Phi) = S(\Psi)$ , if and only if for each  $k = 1, 2, \ldots$ , there exists a positive integer  $n_k < \infty$ , positive integers  $k_1, k_2, \ldots, k_{n_k} < \infty$  and real numbers  $a_{k_1}, a_{k_2}, \ldots, a_{k_{n_k}}$ , such that  $\phi_k = \sum_{j=1}^{n_k} a_{k_j} \psi_{k_j}$ .

In the sequel, we assume a CONS  $\Phi$  is pre-determined, and  $S(\Phi)$  is simply denoted by S. Let  $\mathcal{B}(H)$  be the Borel  $\sigma$ -algebra of H and  $(\Omega, \mathcal{E}, P)$  a probability space. A H-valued random element  $X_H$  is a  $\mathcal{E}$ - $\mathcal{B}(H)$  measurable mapping from

 $\Omega$  to H. Recall that S is an inner product space, and hence it has its own Borel  $\sigma$ -algebra  $\mathcal{B}(S)$ . Therefore, S-valued random elements can be defined as  $\mathcal{E}$ - $\mathcal{B}(S)$  measurable maps from  $\Omega$  to S. The following proposition establishes some basic properties of MIPS, where it should be noted that S is a proper subspace of H; for example,  $h = \sum_{k=1}^{\infty} 2^{-k} \phi_k$  is in H but not S.

PROPOSITION 1. Let S be a MIPS of H. Then:

- 1. S is a dense subset of H.
- 2.  $S \in \mathcal{B}(H)$  and  $\mathcal{B}(S) \subset \mathcal{B}(H)$ .
- 3. Every S-valued random element  $X_S$  is also an H-valued random element.

An important consequence of the denseness of S is that any H-valued random element can be uniformly approximated by S-valued random elements to an arbitrary precision: Consider  $\xi_j = \langle X, \phi_j \rangle$  and  $X_k = \sum_{j=1}^k \xi_j \phi_j$ . For each  $j, k = 1, 2, \ldots$ , define  $\Omega_{j,k} = \{\omega \in \Omega : \|X - X_k\|_H < j^{-1}\} \setminus \Omega_{j,k-1}$ , with  $\Omega_{1,0} = \varnothing$ . Because  $\|X(\omega) - X_k(\omega)\|_H \to 0$  for each  $\omega \in \Omega$ ,  $\Omega_{j,1}, \Omega_{j,2}, \ldots$  form a measurable partition of  $\Omega$  for each j. Defining  $Y_j(\omega) = \sum_{k=1}^\infty X_k(\omega) 1_{\omega \in \Omega_{j,k}}$ , where  $1_{\omega \in \Omega_{j,k}}$  is the indicator function of  $\Omega_{j,k}$ , for each  $\omega$ , there is a k such that  $Y_j(\omega) = X_k(\omega) \in S$ . Moreover, if  $A \in \mathscr{B}(S)$ , then  $Y_j^{-1}(A) = \bigcup_{k=1}^\infty (X_k^{-1}(A) \cap \Omega_{j,k}) \in \mathscr{E}$ , as each  $X_k$  is measurable. Therefore, each  $Y_j$  is  $\mathscr{E}$ - $\mathscr{B}(S)$  measurable, and hence an S-valued random element. Finally, the construction of  $Y_j$  guarantees that  $\sup_{\omega \in \Omega} \|X(\omega) - Y_j(\omega)\|_H < j^{-1} \to 0$  as  $j \to \infty$ . This leads to the following uniform approximation result.

THEOREM 1. If X is a H-valued random element and S is a MIPS of H, there exists a sequence of S-valued random elements  $Y_1, Y_2, \ldots$ , such that  $\sup_{\omega \in \Omega} \|X(\omega) - Y_j(\omega)\|_H \to 0$  as  $j \to \infty$ .

From the above discussion, we see that in approximating X with precision  $j^{-1}$ , the number of components used for different  $\omega$  might be different. For example, if  $\omega \in \Omega_{j,k}$ , then k components are used. This adaptivity of S-valued random elements can lead to an overall more parsimonious approximation of X compared to approximations with fixed choice of k. We characterize this property in the following result. For each S-valued random element Y, the average number of components of Y is naturally given by  $\mathcal{K}(Y) = \sum_{k=1}^{\infty} k P(Y \in S_k)$ .

PROPOSITION 2. Suppose k > 1 and  $1 \le p < \infty$ . Let X be a H-valued random element,  $\xi_j = \langle X, \phi_j \rangle$  and  $X_k = \sum_{j=1}^k \xi_j \phi_j$ . If  $\{E(\|X - X_k\|_H^p)\}^{1/p} < \varepsilon$ , then there exists an S-valued random element Y such that  $\{E(\|X - Y\|_H^p)\}^{1/p} < \varepsilon$  and  $\mathcal{K}(Y) < \mathcal{K}(X_k)$ , provided that the probability density  $f_k$  of  $\xi_j$  is continuous at 0 and  $f_k(0) > 0$ .

We note that the above result can be extended to the case  $p = \infty$ , where  $\{E(\|Z\|_H^p)\}^{1/p}$  is replaced by  $\inf\{w \in \mathbb{R} : P(\omega \in \Omega : \|Z(\omega)\|_H \le w) = 1\}$ .

2.2. Probability densities on mixture inner product spaces. For S-valued random elements X, defining  $K = K(X) = \sum_{k=1}^{\infty} k 1_{X \in S_k}$  and  $X_k = \sum_{j=1}^{k} \langle X, \phi_j \rangle \phi_j$ , then  $X = \sum_{k=1}^{\infty} X_k 1_{K=k}$ , and  $X = X_k$  with probability  $\pi_k = P(K = k)$ . Since each  $X_k$  is of finite dimension, if the conditional density  $f(X_k \mid K = k)$  exists for each k, then it is possible to define a probability density for X with respect to a base measure whose restriction to each  $S_k$  coincides with the k-dimensional Lebesgue measure. In contrast, for general random processes, it is well known that the small ball probability density does not exist [Delaigle and Hall (2010), Li and Linde (1999)]. An intuitive explanation is that with the mixture representation the probability mass of X is essentially concentrated on the mixture components  $S_k$ , each of which has a finite dimension, with high concentration on the leading components. The decay of the mixture proportions  $\pi_k$  as k increases then prevents the overall probability mass from escaping to infinity. Below we provide the details of this concept of a mixture density associated with MIPS.

It is well known that each  $H_k$  is isomorphic to  $\mathbb{R}^k$ , with associated Lebesgue measure  $\tau_k$ . Defining a base measure  $\tau(A) = \sum_{k=1}^{\infty} \tau_k(A \cap S_k)$  for  $A \in \mathcal{B}(S)$ , where we note that  $\tau$  depends on the choice of the CONS, as change in the CONS leads to a different MIPS, the restriction of  $\tau$  to each  $S_k$  is  $\tau_k$ . Therefore, although  $\tau$  itself is not a Lebesgue measure, the restriction to each finite-dimensional subspace  $H_k$  is.

For the random variables  $\xi_j = \langle X, \phi_j \rangle$ ,  $j \ge 1$ , for a *S*-valued random element *X* assume that the conditional densities  $f_k(\xi_1, \xi_2, \dots, \xi_k) = f(\xi_1, \xi_2, \dots, \xi_k \mid K = k)$  exist. With  $\pi_k = P(X \in S_k) = P(K = k)$ , we then define the mixture density function

(1) 
$$f(x) = \sum_{k=1}^{\infty} \pi_k f_k(\langle x, \phi_1 \rangle, \langle x, \phi_2 \rangle, \dots, \langle x, \phi_k \rangle) 1_{x \in S_k} \quad \forall x \in S.$$

Note that even though there are infinitely many terms in (1), for any given realization  $x = X(\cdot, \omega)$ , only one of these terms is nonzero due to the presence of the indicator  $1_{x \in S_k}$  and the fact that  $X \in S$ . Therefore, f is well defined for all  $x \in S$  given  $\sum_k \pi_k = 1$ .

The presence of the indicator function  $1_{x \in S_k}$  implies that the mixture density in (1) is distinct from any classical finite mixture model, where each component might have the same full support, while here the support of the each mixture component is specific to the component. The key difference to usual mixture models is that our model entails a mixture of densities that are defined on disjoint subsets, rather than on a common support. The following result implies that the problem of nonexistence of a probability density in  $L^2$  can be addressed by viewing functional data as elements of a mixture inner product space.

THEOREM 2. The measure  $\tau$  is a  $\sigma$ -finite measure on S. In addition, if the conditional density  $f_k(\xi_1, \xi_2, \dots, \xi_k)$  exists for each k, then the probability distri-

bution  $P_X$  on S induced by X is absolutely continuous with respect to  $\tau$ . Moreover, the function f defined in (1) is a probability density of  $P_X$  with respect to  $\tau$ .

We note that the domain of f is S. Although S is dense in H, since f is not continuous, there is no natural extension of f to the whole space H. Nevertheless, we can extend both  $\tau$  and f to H in the following straightforward way. Define the extended measure  $\tau^*$  on H by  $\tau^*(A) = \tau(A \cap S)$  for all  $A \in \mathcal{B}(H)$ . To extend f, we simply define f(x) = 0 if  $x \in H \setminus S$ . One can easily verify that  $\tau^*$  is a measure on H extending  $\tau$ , and f is a density function of X with respect to  $\tau^*$ .

2.3. Constructing mixture inner product space valued random elements. In this section, we focus on an important class of MIPS-valued random elements. Let  $\tilde{\xi}_1, \tilde{\xi}_2, \ldots$  be a sequence of uncorrelated centered random variables such that joint probability densities  $\tilde{f}_k$  of  $\tilde{\xi}_1, \tilde{\xi}_2, \ldots, \tilde{\xi}_k$  exist for all k. Suppose K is a positive random integer with distribution  $\pi = (\pi_1, \pi_2, \ldots)$  where K is independent of  $\tilde{\xi}_1, \tilde{\xi}_2, \ldots$ , and  $\pi_k = \Pr(K = k)$ . Then we construct a random element  $K = \mu + \sum_{k=1}^K \tilde{\xi}_k \phi_k$ , where  $\mu \in H$ . We refer to a MIPS with random elements constructed in this way as a generative MIPS. Note that the mean element  $\mu$  is allowed to be in the space K. Therefore, the centered process  $K - \mu$ , which is the primary object that the MIPS framework targets, takes value in a MIPS. This feature enhances the practical applicability of the MIPS framework. A generative MIPS has particularly useful properties that we discuss next.

In order to define mean and covariance of X, we also need that  $E(\|X\|_H^2) < \infty$ ; a simple condition that implies this assumption is  $\sum_{j=1}^{\infty} (\sum_{k=j}^{\infty} \pi_k) \operatorname{var}(\tilde{\xi}_j) < \infty$ . Indeed, with  $\pi_j^* = \sum_{k=j}^{\infty} \pi_k$ ,

$$\begin{split} E(\|X - \mu\|_H^2) &= E\left(\sum_{j=1}^K \tilde{\xi}_j^2\right) = EE\left(\sum_{j=1}^K \tilde{\xi}_j^2 \mid K\right) = \sum_{k=1}^\infty \pi_k E\left(\sum_{j=1}^k \tilde{\xi}_j^2\right) \\ &= \sum_{k=1}^\infty \pi_k \sum_{j=1}^k \operatorname{var}(\tilde{\xi}_j) = \sum_{j=1}^\infty \left(\sum_{k=j}^\infty \pi_k\right) \operatorname{var}(\tilde{\xi}_j) = \sum_{j=1}^\infty \pi_j^* \operatorname{var}(\tilde{\xi}_j) < \infty, \end{split}$$

 $E(\|X\|_H^2) \le E(\|X - \mu\|_H^2) + \|\mu\|_H^2 < \infty$ , and  $(X - \mu)$  is seen to be a *S*-valued random element. Under the condition  $E(\|X - \mu\|_H^2) < \infty$ ,  $E(X - \mu) = 0$ , and hence  $E(X) = \mu$ . Without loss of generality, we assume  $\mu = 0$  in the following.

To analyze the covariance structure of  $X = \sum_{k=1}^K \tilde{\xi}_k \phi_k$ , consider  $\xi_k = \langle X, \phi_k \rangle$ . Then  $\xi_k = \tilde{\xi}_k 1_{K \geq k}$ ,  $E(\xi_k) = 0$ ,  $\operatorname{var}(\xi_k) = \pi_k^* \operatorname{var}(\tilde{\xi}_k)$  and  $E(\xi_j \xi_k) = 0$ , and  $\xi_1, \xi_2, \ldots$  are seen to be uncorrelated centered random variables with variance  $\pi_k^* \operatorname{var}(\tilde{\xi}_k)$ . Furthermore, because K is independent of the  $\tilde{\xi}_k$ , the conditional density of  $\xi_1, \xi_2, \ldots, \xi_k$  given K = k is the joint density of  $\tilde{\xi}_1, \tilde{\xi}_2, \ldots, \tilde{\xi}_k$ . If  $E(\|X\|_H^2) < \infty$ , the covariance operator  $\Gamma$  for X exists [Hsing and Eubank

(2015)]. The  $\phi_k$  are eigenelements of  $\Gamma$ , as

$$\Gamma \phi_k = E(X\langle X, \phi_k \rangle) = E(X\xi_k) = E(X\tilde{\xi}_k 1_{K \ge k}) = EE(X\tilde{\xi}_k 1_{K \ge k} \mid K)$$

(2) 
$$= \sum_{j=1}^{\infty} \pi_j E(X\tilde{\xi}_k 1_{K \ge k} \mid K = j) = \sum_{j=k}^{\infty} \pi_j E\left(\tilde{\xi}_k \sum_{m=1}^j \tilde{\xi}_m \phi_m\right)$$
$$= \pi_k^* \operatorname{var}(\tilde{\xi}_k) \phi_k,$$

where the last equality is due to uncorrelatedness of  $\tilde{\xi}_1, \tilde{\xi}_2, \dots$ . From (2), the eigenvalue  $\lambda_k$  corresponding to the kth eigenelement  $\phi_k$  is

(3) 
$$\lambda_k = \pi_k^* \operatorname{var}(\tilde{\xi}_k).$$

Since  $\phi_1, \phi_2, \ldots$  is a CONS of H,  $\Gamma$  has no other eigenelement in H. Therefore,  $\Gamma$  admits the eigendecomposition  $\Gamma = \sum_{k=1}^{\infty} \lambda_k \phi_k \otimes \phi_k$ , where  $(x \otimes y)z = \langle x, z \rangle y$  for  $x, y, z \in H$ . For the special case where  $H = L^2$ , this feature establishes a connection to traditional functional principal component analysis and suggests implementation of MIPS in this special case by adopting well studied functional principal component analysis methods; see the next section for details.

An important consequence of these considerations is that for each random element  $\tilde{X} \in H$  with  $E(\|\tilde{X}\|_H^2) < \infty$  and for which the covariance operator  $\tilde{\Gamma}$  has an eigendecomposition  $\tilde{\Gamma} = \sum_{k=1}^{\infty} \tilde{\lambda}_k \tilde{\phi}_k \otimes \tilde{\phi}_k$  (assuming w.l.o.g. that  $\tilde{\phi}_1, \tilde{\phi}_2, \ldots$  form a CONS of H), there exists a MIPS  $\tilde{S}$  and a  $\tilde{S}$ -valued random element Z, such that the covariance operator  $\Gamma$  of Z has the same set of eigenelements. To see this, define  $\tilde{S}$  to be the MIPS generated by  $\tilde{\phi}_1, \tilde{\phi}_2, \ldots$  and note that  $\zeta_k = \langle \tilde{X}, \tilde{\phi}_k \rangle, k \geq 1$ , are uncorrelated random variables with variances  $\tilde{\lambda}_k$  [Hsing and Eubank (2015)]. Choose an independent random positive integer K with distribution  $\pi = (\pi_1, \pi_2, \ldots)$  and  $\pi_k > 0$  for all k, and set  $Z = \sum_{k=1}^K \zeta_k \tilde{\phi}_k$ . Since  $\sum_{j=1}^{\infty} \pi_j^* \operatorname{var}(\zeta_j) \leq \sum_{j=1}^{\infty} \operatorname{var}(\zeta_j) < \infty$ , we have  $E(\|Z\|_H^2) < \infty$ . Therefore, the derivation in (2) applies to Z and shows that the covariance operator of Z has exactly the eigenelements  $\tilde{\phi}_1, \tilde{\phi}_2, \ldots$ 

- **3. Application to functional data analysis.** In this section, we demonstrate how the MIPS concept can be applied to provide a new approach for the analysis of functional data and demonstrate how this can be utilized to define a density function for functional data via the density function (1), thus providing a new perspective on one of the foundational issues of functional data analysis. In the following sections, we show how to apply the theory of MIPS to analyze functional data.
- 3.1.  $L^p$ -denseness of mixture inner product space valued random processes. Theorem 1 implies that any given H-valued random element can be uniformly approximated by MIPS-valued random elements. An important consequence is

that the set of MIPS-valued random elements is dense in an  $L^p$  sense, as follows. For  $1 \le p < \infty$ , let  $L^p(\Omega, \mathscr{E}, P; H)$  be the space of H-valued random elements X such that  $E(\|X\|_H^p) < \infty$ . It is well known [Vakhania, Tarieladze and Chobanyan (1987)] that  $L^p(\Omega, \mathscr{E}, P; H)$  (with elements defined as equivalence classes) is a Banach space with norm  $\|X\|_{L^p} = \{E(\|X\|_H^p)\}^{1/p}$  for every  $X \in L^p(\Omega, \mathscr{E}, P; H)$ , where for  $p = \infty$ ,  $L^\infty(\Omega, \mathscr{E}, P; H)$  denotes the Banach space with the essential supremum norm. Since each S-valued random element is also an H-valued random element according to Proposition 1, the space  $L^p(\Omega, \mathscr{E}, P; S)$  is a subspace of  $L^p(\Omega, \mathscr{E}, P; H)$ . The following corollary states that  $L^p(\Omega, \mathscr{E}, P; S)$  is dense in  $L^p(\Omega, \mathscr{E}, P; H)$ , which is an immediate consequence of Theorem 1.

COROLLARY 1. If X is a H-valued random element and S is a MIPS of H, there exists a sequence of S-valued random elements  $Y_1, Y_2, \ldots$ , such that  $\|X - Y_j\|_{L^p} \to 0$  as  $j \to \infty$  for  $1 \le p \le \infty$ , that is,  $L^p(\Omega, \mathcal{E}, P; S)$  is a dense subset of  $L^p(\Omega, \mathcal{E}, P; H)$ .

Applying this result to the Hilbert space  $H = L^2(D)$ , which is the set of real functions  $f: D \to \mathbb{R}$  such that  $\int_D |f(t)|^2 dt < \infty$ , where D is a compact subset of  $\mathbb{R}$ , for example, D = [0, 1], we conclude that the set of MIPS-valued random processes is dense in the space of all  $L^2(D)$  random processes. This denseness implies that when modeling functional data with MIPS-valued random processes, the results are arbitrarily close to those one would have obtained with the traditional  $L^2$  based functional data analysis approaches in the  $L^2$  sense. A major difference between the two approaches is that each functional element is always finite-dimensional in the MIPS framework, as it belongs to one of the subspaces  $S_k$ , where the MIPS is  $S = \bigcup_{k=1}^{\infty} S_k$ , as defined above, while in the classical  $L^2$  framework each element is infinite-dimensional. The denseness of MIPS in  $L^2$  provides additional justification for the adoption of this new approach.

As we will demonstrate below, modeling functional data in the MIPS framework enjoys extra flexibility and parsimony in representing observed functional data. And, as mentioned before, it provides a way to define probability densities for functional data within the full MIPS space, avoiding ad hoc truncation approaches to which one must resort when tackling the density problem directly in the traditional functional data space  $L^2$ .

3.2. Model and estimation. In the following, we develop a MIPS based functional mixture model from a practical modeling perspective. A practical motivation to adopt a mixture model is that it enables adaptive choice of the number of components that are included to represent a given functional trajectory. This adaption is with respect to the complexity of the trajectory that is to be represented. The basic idea is that trajectories that have more features and shape variation relatively to other trajectories require a larger number of components to achieve a good representation, while those that are flat and have little shape variation will require

fewer components. This contrasts with the "one size fits all" approach of functional principal component analysis or other expansions in basis functions, where the expansion series always includes infinitely many terms.

To implement MIPS based shape-adaptive modeling, we require that the process X underlying the observed data is a generative MIPS random process, as defined in the beginning of Section 2.3. This requirement is formalized in the following assumption:

(A0) The observed functional data  $X_1, X_2, \ldots, X_n$  are i.i.d. realizations of a generative MIPS random process X, that is,  $X = \sum_{k=1}^K \tilde{\xi}_k \phi_k$  for a sequence of uncorrelated centered random variables  $\tilde{\xi}_k$  and a CONS  $\Phi = \{\phi_1, \phi_2, \ldots\}$  of the space  $L^2$ . Here, K is an integer valued random variable that is independent of the  $\tilde{\xi}_k$  and has the distribution  $P(K = k) = \pi_k > 0$  for a sequence  $\pi_k, k \ge 1$ , such that  $0 \le \pi_k \le 1$  and  $\sum_k \pi_k = 1$ . The sequence  $\lambda_k = \text{var}(\tilde{\xi}_k)$  is strictly decreasing with increasing k, that is,  $\lambda_1 > \lambda_2 > \cdots$ .

Under this assumption, the CONS  $\Phi = \{\phi_1, \phi_2, ...\}$  is exactly the one featured in the Karhunen–Loève decomposition, according to the discussion in Section 2.3.

We demonstrate that the probability density for functional mixtures as defined in the previous section can be consistently estimated under suitable regularity conditions. For convenience, the functions  $X_1, \ldots, X_n$  are considered fully observed; densely sampled functional data can be individually pre-smoothed to produce asymptotically equivalent estimates [Hall, Müller and Wang (2006)]. The eigenfunctions  $\phi_1, \phi_2, \ldots$  and associated eigenvalues are unknown and need to be estimated from the data.

We consider the case where the component densities  $f_k$ ,  $k \ge 1$ , are parametrizable by set of parameters  $\theta_k = (\theta_{k,1}, \theta_{k,2}, \dots, \theta_{k,d_k})^T \in \mathbb{R}^{d_k}$  for some sequence of integers  $d_k$ , and the distribution of the mixture proportions  $\pi$  is governed by a sequence of parameters  $\theta_{\pi} \in \mathbb{R}^{d_{\pi}}$ . Although we develop here a parametric approach to model each component density  $f_k$ , it is worth noting that a nonparametric approach might be taken in a similar spirit as the nonparametric estimation of finite mixtures, developed by Benaglia, Chauveau and Hunter (2009) and Levine, Hunter and Chauveau (2011), where substantial additional technicalities are involved. We leave this topic for future research.

For notational convenience, let  $\theta_{[k]}$  be the sequence of parameter sets, containing distinct parameters  $\theta_1, \theta_2, \ldots, \theta_k$ , as well as the parameters in  $\theta_{\pi}$  that determine  $\pi_1, \ldots, \pi_{k-1}$ , with the dimension denoted by  $d_{[k]}$ , where  $\theta_{[\infty]}$  stands for the sequence of all distinct parameters, such that

(4) 
$$\theta_{[k]} = (\theta_{[\infty],1}, \theta_{[\infty],2}, \dots, \theta_{[\infty],d_{[k]}}),$$

where  $\theta_{[\infty],j}$  is the jth coordinate of  $\theta_{[\infty]}$ . Let  $I_{[\infty],j}$  denote the domain of  $\theta_{[\infty],j}$ , and define  $\Theta = \prod_{j=1}^{\infty} I_{[\infty],j}$ . We write  $f_k(\cdot)$  as  $f_k(\cdot \mid \theta_k)$  to emphasize the dependence on  $\theta_k$ . Similarly,  $f(\cdot)$  is written as  $f(\cdot \mid \theta_{[\infty]})$  to indicate that f is

parametrized by  $\theta_{[\infty]}$ , that is,

(5) 
$$f(X(\omega) \mid \theta_{[\infty]}) = \sum_{k=1}^{\infty} \pi_k f_k(\xi_1(\omega), \xi_2(\omega), \dots, \xi_k(\omega) \mid \theta_k) 1_{X(\omega) \in S_k}.$$

For a generic parameter  $\theta$ , we use  $\theta_0$  to denote its true value, and  $\hat{\theta}$  to denote corresponding maximum likelihood estimators, for example,  $\theta_{\infty,0}$  denotes the true parameters of  $\theta_{[\infty]}$ .

To illustrate the key idea, we make the simplifying assumption of compactness of the parameter space, which may be relaxed by introducing more technicalities. The condition below characterizes the compactness of the parameter space  $\Theta =$  $\prod_{i=1}^{\infty} I_{[\infty], i}$  as a product of compact spaces, using Tychonoff's theorem.

(A1) For each  $j = 1, 2, ..., I_{[\infty], j}$  is a nonempty compact subset of  $\mathbb{R}$ , and thus  $\Theta = \prod_{i=1}^{\infty} I_{[\infty],j}$  is compact (by Tychonoff's theorem).

With eigenfunctions  $\phi_1, \phi_2, \dots$  estimated by decomposing the sample covariance operator, the principal component scores  $\xi_{ik}$  are estimated by  $\hat{\xi}_{ik} = \langle X_i, \hat{\phi}_k \rangle$ for each i = 1, 2, ..., n and k = 1, 2, ..., where  $\hat{\phi}_k$  are the standard estimates of  $\phi_k$ . To quantify the estimation quality, we postulate a standard regularity condition for X [Hall and Hosseini-Nasab (2006)] and a polynomial decay assumption for the eigenvalues  $\lambda_1 > \lambda_2 > \cdots > 0$  [Hall and Horowitz (2007)].

- (A2) For all C > c' and some  $\varepsilon' > 0$ , where c' > 0 is a constant,  $\sup_{t \in D} E\{|X(t)|^C\} < \infty \text{ and } \sup_{s,t \in D} E[\{|s-t|^{-\varepsilon'}|X(s)-X(t)|\}^C] < \infty.$ (A3) For all  $k \ge 1$ ,  $\lambda_k - \lambda_{k+1} \ge C_0 k^{-b-1}$  for constants  $C_0 > 0$  and b > 1, and
- also  $\pi_k = O(k^{-\beta})$  for a constant  $\beta > 1$ .

Note that  $\sum_k \lambda_k < \infty$  and  $\sum \pi_k = 1$  imply b > 1 and  $\beta > 1$  and one also has  $\pi_k^* = \sum_{j=k}^\infty \pi_k = O(k^{-\beta+1})$ . Condition (A3) also implies that  $\lambda_k \ge C' k^{-b}$  for a constant C' > 0 for all k. Therefore, if  $\rho_k = \text{var}(\tilde{\xi}_k)$ , the relation  $\lambda_k = \pi_k^* \text{var}(\tilde{\xi}_k)$ that was derived in (3) implies  $\rho_k = \lambda_k/\pi_k^* \ge C_\rho k^{-b+\beta-1}$  for a constant  $C_\rho > 0$ and for all k. Note that the case  $-b + \beta - 1 > 0$ , for which the variances of the  $\tilde{\xi}_k$ diverge, is not excluded.

Our next assumption concerns the regularity of mixture components  $f_k(\tilde{\xi}_1, \tilde{\xi}_2,$  $\ldots, \tilde{\xi}_k$ ) and  $g_k(\tilde{\xi}_1, \tilde{\xi}_2, \ldots, \tilde{\xi}_k) = \log f_k(\tilde{\xi}_1, \tilde{\xi}_2, \ldots, \tilde{\xi}_k)$ , where the dependence on  $\theta_k$  is suppressed when no confusion arises.

(A4) For  $k = 1, 2, ..., f_k(\cdot \mid \theta_k)$  is continuous at all arguments  $\theta_k$ . There exist constants  $C_1, C_2, C_3 \ge 0, -\infty < \alpha_1, \alpha_2 < \infty, 0 < \nu_1 \le 1, 0 < \nu_2 \le 2$ and functions  $H_k(\cdot)$  such that, for all  $k = 1, 2, ..., g_k$  satisfies  $|g_k(u)|$  $|g_k(v)| \le C_1 H_k(v) \|u - v\|^{\nu_1} + C_2 k^{\alpha_2} \|u - v\|^{\nu_2}$  for all  $u, v \in \mathbb{R}^k$ , and  $E\{H_k(\xi_1,\xi_2,\ldots,\xi_k)\}^2 < C_3 k^{2\alpha_1}.$ 

In the following, we use  $\alpha = \max\{\alpha_1, \alpha_2\}$  and  $\nu = \min(2\nu_1, \nu_2)$ . Note that Hölder continuity is a special case for  $C_1 = 0$ . Given (A3), one can verify that (A4) is satisfied for the case of Gaussian component densities with  $C_1$ ,  $C_2$ ,  $C_3 > 0$ ,  $v_1 = 1$ ,  $v_2 = 2$ ,  $\alpha_1 > 2^{-1} \max(1 - b, 2b - 3\beta + 4)$  and  $\alpha_2 = \max(0, b - \beta + 1)$ . The condition on  $|g_k(u) - g_k(v)|$  in (A4) implicitly assumes a certain growth rate of  $d_{[k]}$  as k goes to infinity. For instance,  $E\{H_k(\xi_1, \xi_2, \ldots, \xi_k)\}^2$  is a function of the parameter set  $\theta_{[k]}$ . By the compactness assumption on  $\theta_{[\infty]}$ , the parameters have a common upper bound. With this upper bound,  $E\{H_k(\xi_1, \xi_2, \ldots, \xi_k)\}^2$  can be bounded by some function R of  $d_{[k]}$ . By postulating  $E\{H_k(\xi_1, \xi_2, \ldots, \xi_k)\}^2 \leq C_3 k^{2\alpha_1}$  in (A4), we implicitly assert that the function  $R(d_{[k]})$  can be bounded by a polynomial of k, with the exponent  $2\alpha_1$ . We would need a larger value for  $\alpha_1$  when  $d_{[k]}$  grows faster with k. A similar argument applies to  $\alpha_2$ .

To state the needed regularity conditions for the likelihood function, we need some notation. Let  $Q_r = \min(K, r)$ , and define  $Z_i = \sum_{j=1}^{Q_r} \langle X_i, \phi_j \rangle \phi_j$ , so that  $Z_i \in S_q$ ,  $q \le r$ . The log-likelihood of a single observation Z is

(6) 
$$L_{r,1}(Z \mid \theta_{[r]}) = \log \left\{ \left( 1 - \sum_{k=1}^{r-1} \pi_k \right) f_r(Z \mid \theta_{[r]}) 1_{Z \in S_r} + \sum_{k=1}^{r-1} \pi_k f_k(Z \mid \theta_{[k]}) 1_{Z \in S_k} \right\}.$$

The log-likelihood function of  $\theta_{[r]}$  for a sample  $Z_1, \ldots, Z_n$  accordingly is

(7) 
$$L_{r,n}(\theta_{[r]}) = n^{-1} \sum_{i=1}^{n} L_{r,1}(Z_i \mid \theta_{[r]}),$$

with maximizer  $\hat{\theta}_{[r]}$ . We impose the following regularity condition on  $L_r(\theta_{[r]}) = E\{L_{r,1}(Z \mid \theta_{[r]})\}$ .

(A5) There exist constants  $h_1, h_2, h_3, a_1, a_2, a_3 > 0$  such that for all  $r \ge 1$ ,  $U_r = \{\theta_{[r]}: L_r(\theta_{[r],0}) - L_r(\theta_{[r]}) < h_1 r^{-a_1}\}$  is contained in a neighborhood  $\mathcal{B}_r = \{\theta_{[r]}: \|\theta_{[r],0} - \theta_{[r]}\| < h_2 r^{-a_2}\}$  of  $\theta_{[r],0}$ , where  $\theta_{[r],0}$  denotes the true parameters of  $\theta_{[r]}$ . Moreover,  $L_r(\theta_{[r],0}) - L_r(\theta_{[r]}) \ge h_3 r^{-a_3} \|\theta_{[r],0} - \theta_{[r]}\|^2$  for all  $\theta_{[r]} \in U_r$ .

Writing  $a = \max\{a_1, a_3\}$ , we observe that (A5) is satisfied when each component  $f_k$  is Gaussian for any a > 1, and (A1) and (A3) hold. (A5) essentially states that the global maximizer of  $L_r$  is unique and uniformly isolated from other local maximizers with an order  $r^{-a}$ . Such a condition on separability is necessary when there are infinitely many mixture components in a model. We note that (A5) also ensures identifiability of the global maximizer.

The next assumption is used to regulate the relationship between the mixture proportions  $\pi_k$  and the magnitude of  $g_k(\tilde{\xi}_1, \tilde{\xi}_2, \dots, \tilde{\xi}_k)$ , by imposing a bound on  $g_k$  for increasing k.

(A6) For a constant  $c < \beta - 1$ ,  $E[g_k(\tilde{\xi}_1, \tilde{\xi}_2, \dots, \tilde{\xi}_k)] = O(k^{c-a})$ , where a is defined in (A5) and  $\beta$  in (A3) and  $g_k(\tilde{\xi}_1, \tilde{\xi}_2, \dots, \tilde{\xi}_k) = \log f_k(\tilde{\xi}_1, \tilde{\xi}_2, \dots, \tilde{\xi}_k)$ .

The constraint  $\beta > c+1$  in (A6) guarantees that in light of  $\pi_k = O(k^{-\beta})$ , as per (A3), the mixture proportions  $\pi_k$  decay fast enough relative to average magnitude of  $g_k(\tilde{\xi}_1, \tilde{\xi}_2, \ldots, \tilde{\xi}_k)$  to avoid a singularity that might arise in the summing operation to construct the density f in (1) when the magnitude of  $g_k(\tilde{\xi}_1, \tilde{\xi}_2, \ldots, \tilde{\xi}_k)$  grows too fast. This bound will prevent that too much mass is allocated to the components with higher dimensions in the composite mixture density f. Such a scenario would preclude the existence of a density and is avoided by tying the growth of  $g_k$  to the decline rate of the  $\pi_k$ , as per (A6).

From a practical perspective, faster decay of the  $\pi_k$  that places more probability mass on the lower-order mixture components will help stabilize the estimation procedure, as it is difficult to estimate the high-order eigenfunctions that are needed for the higher order components. For the case of Gaussian component densities, a simple calculation gives  $E|g_k(\tilde{\xi}_1,\tilde{\xi}_2,\ldots,\tilde{\xi}_k)|=O(k\log k)$ , thus (A6) is fulfilled for any c>a+1. This will also imply that  $\beta>a+2$ . An extreme situation arises when  $\pi_k=0$  for  $k\geq k_0$  for some  $k_0>0$ , that is, the dimension of the functional space is finite and the functional model essentially becomes parametric. In this case, the construction of the mixture density in functional space is particularly straightforward.

The following theorem establishes estimation consistency for a growing sequence of parameters  $\theta_{[r_n]}$  as the sample size n increases, and consequently the consistency of the estimated probability density at any functional observation  $x \in S$  as argument. Define constants  $\gamma_1 = (2b + 3)\nu/2 + \alpha - 2\beta$ ,  $\gamma_2 = a + (\gamma_1 + 2)1_{\{\gamma_1 > -2\}}$ , and  $\gamma = \min\{\nu/(2\gamma_2), 1/(2b + 2)\}$ .

THEOREM 3. If assumptions (A0)–(A6) hold and  $r_n = O(n^{\gamma - \varepsilon})$  for any  $0 < \varepsilon \le \gamma$ , then the global maximizer  $\hat{\theta}_{[r_n]}$  of  $\hat{L}_{r,n}(\theta_{[r_n]})$  satisfies

$$\|\hat{\theta}_{[r_n]} - \theta_{[r_n],0}\| \xrightarrow{p} 0,$$

where  $\theta_{[r_n]}$  is defined in (4), and  $\hat{L}_{r,n}(\theta_{[k]})$  is the likelihood function obtained by plugging the estimated quantities  $\hat{\phi}_k$  and  $\hat{\xi}_{ik}$  into  $L_{r,n}(\theta_{[r_n]})$  defined in (7). Consequently, for any  $x \in S = \bigcup_{k=1}^{\infty} S_k$ , one has

$$|f(x \mid \hat{\theta}_{[r_n]}) - f(x \mid \theta_{[\infty],0})| \xrightarrow{p} 0,$$

where f is the mixture probability density defined in (5).

We see from Theorem 3 that the number of consistently estimable mixture components,  $r_n$ , grows with a polynomial rate in terms of the sample size n. From (A4), the proximity to a singularity of the component density  $f_k$  is seen to increase as  $\alpha$  increases, indicating more difficulty in estimating  $f_k$ , and thus restricting the

rate of increase in  $r_n$ . Faster decay rates of the eigenvalues  $\lambda_k$ , relative to the decline rates in the mixture proportions  $\pi_k$  and quantified by b and  $(b-\beta+1)$ , respectively, lead to limitations in the number of eigenfunctions that can be reliably estimated and this is reflected in a corresponding slowing of the rise of the number of mixture components  $r_n$  that can be included. The rate at which  $r_n$  can increase also depends on the decay of the  $\pi_k$  as quantified by  $\beta$ .

3.3. Fitting algorithm. We present an estimation method based on the expectation-maximization algorithm to determine the mixture probabilities  $\pi_k$  for  $k=1,2\ldots$ , and the number  $K_i$  of components that are associated with each individual trajectory  $X_i$ . For simplicity, we assume that the mixture proportions  $\pi_k$  are derived from a known family of discrete distributions that can be parametrized with one or few unknown parameters, denoted here by  $\vartheta$ , simplifying the notation introduced in Section 3.2. A likelihood for fitting individual trajectories with K components can then be constructed. The following algorithm is based on fully observed  $X_i$ . Modifications for the case of discretely observed data are discussed at the end of the section.

To be specific, we outline the algorithm for the mixture density of Gaussian processes, and use  $\pi \sim \text{Poisson}(\vartheta)$ , that is,  $P(K = k \mid \vartheta) = \vartheta^k e^{-\vartheta}/k!$ . Versions for other distributions can be developed analogously. Assume that  $X_1, \ldots, X_n$  are centered without loss of generality. Projecting  $X_i$  onto each eigenfunction  $\phi_j$ , we obtain the functional principal component scores  $\xi_{i1}, \xi_{i2}, \ldots$  of  $X_i$ . Given  $K_i = k$ ,  $(\xi_{i1}, \xi_{i2}, \ldots, \xi_{ik}) = (\tilde{\xi}_{i1}, \ldots, \tilde{\xi}_{ik})$  and

(8) 
$$(\tilde{\xi}_{i1}, \dots, \tilde{\xi}_{ik})^T \sim N(0, \Sigma_{\rho}^{(k)}),$$

where  $\Sigma_{\rho}^{(k)}$  is the  $k \times k$  diagonal matrix with diagonal elements  $\rho_j = \text{var}(\tilde{\xi}_j)$ , j = 1, 2, ..., k. The likelihood  $f(X_i \mid K_i = k)$  of  $X_i$  conditional on  $K_i = k$  is then given by

(9) 
$$f(X_i \mid K_i = k) = \frac{1}{\sqrt{(2\pi)^k |\Sigma_{\rho}^{(k)}|}} \times \exp\left[-\frac{1}{2}(\xi_{i1}, \dots, \xi_{ik}) (\Sigma_{\rho}^{(k)})^{-1} (\xi_{i1}, \dots, \xi_{ik})^T\right].$$

Note that one needs the eigenvalues  $\rho_k$  to characterize the distribution of the observations  $X_i$  given  $K_i$ . Based on equation (3), one can adopt standard functional principal component analysis for the entire sample that contains realizations of X, that is, extract the eigenvalues  $\lambda_k$  of G first and then utilize  $\rho_k = \lambda_k/\pi_k^*$ . This however requires to infer the unknown mixture proportions  $\pi_k$ . To address this conundrum, we treat  $K_i$  as a latent variable or missing value and adopt the expectation-maximization paradigm, as follows:

- 1. Obtain consistent estimates  $\hat{\phi}_k(\cdot)$  of  $\phi_k(\cdot)$  and  $\hat{\lambda}_k$  of  $\lambda_k$ ,  $k=1,2,\ldots$ , from functional principal component analysis by pooling the data from all individuals, following some well-known procedures [Dauxois, Pousse and Romain (1982), Hall and Hosseini-Nasab (2006)], followed by projecting each observation  $X_i$  onto each  $\hat{\phi}_k$  to obtain estimated functional principal component scores  $\hat{\xi}_{ik}$ . As starting value for the Poisson parameter  $\vartheta$ , we set  $\vartheta=k$ , where k is the smallest integer such that the fraction of variation explained by the first k principal components exceeds 95%.
- 2. Plug in the estimate  $\hat{\lambda}_k$  for  $\lambda_k$  and calculate  $\hat{\rho}_k = \hat{\lambda}_k / \pi_k^*$ , with  $\pi_k = p(k \mid \vartheta)$  based on the current estimate of  $\vartheta$ , which we denote by  $\vartheta^{(t)}$ . Obtain the conditional expectation of  $K_i$  given  $X_i$ ,

(10) 
$$E(K_i \mid X_i) = \frac{\sum_{k=1}^{\infty} k f(X_i \mid K_i = k) P(K_i = k \mid \vartheta^{(t)})}{\sum_{k=1}^{\infty} f(X_i \mid K_i = k) P(K_i = k \mid \vartheta^{(t)})},$$

where  $f(X_i \mid K_i = k)$  is given by (9). It is natural to use the nearest integer, denoted by  $E_i(K_i \mid X_i)$ . The updated estimate of  $\vartheta$  is given by  $\vartheta^{(t+1)} = n^{-1} \sum_{i=1}^n E_i(K_i \mid X_i)$ . Repeat this step until  $\vartheta^{(t)}$  converges. By the ascent property of the EM algorithm,  $\vartheta^{(t)}$  converges to a local maximizer. In practice, this step is repeated until a specified convergence threshold is reached that may be defined in terms of the relative change of  $\vartheta$ , that is,  $|\vartheta^{(t+1)} - \vartheta^{(t)}|/\vartheta^{(t)}$ .

3. Each  $X_i$  is represented by  $X_i = \sum_{j=1}^{K_i} \hat{\xi}_{ij} \hat{\phi}_j$ , where  $K_i$  is obtained as in (10).

In the numerical implementation, it is advantageous to only keep the positive eigenvalue estimates  $\hat{\rho}_k^+$ , and to introduce a truncated Poisson distribution that is bounded by  $K_n^+ = \max\{k : \hat{\rho}_k^+ > 0\}$ ,

(11) 
$$p^{+}(k \mid \vartheta, K_{n}^{+}) = \frac{\vartheta^{k}}{k!(\sum_{\ell=0}^{K_{n}^{+}} \vartheta^{\ell}/\ell!)} \equiv \pi_{k}^{+}, \qquad k = 0, 1, \dots, K_{n}^{+}.$$

Since the maximum likelihood estimate of  $\vartheta$  in (11) based on the truncated Poisson distribution is complicated and does not have an analytical form, it is expedient to numerically maximize the conditional expectation of the log-likelihood with respect to  $\vartheta$  given the observed data  $X_i$ , i = 1, ..., n, and the current estimate  $\vartheta^{(t)}$ .

(12) 
$$\sum_{i=1}^{n} E\{\log p^{+}(K_{i} \mid \vartheta, K_{n}^{+}) \mid X_{i}, \vartheta^{(t)}\}$$

$$= \sum_{i=1}^{n} \frac{\sum_{k=1}^{K_{n}^{+}} \log p^{+}(k \mid \vartheta, K_{n}^{+}) f(X_{i} \mid K_{i} = k) p^{+}(k \mid \vartheta^{(t)}, K_{n}^{+})}{\sum_{k=1}^{K_{n}^{+}} f(X_{i} \mid K_{i} = k) p^{+}(k \mid \vartheta^{(t)}, K_{n}^{+})},$$

and to consider the modified eigenvalues  $\rho_k^+ = \lambda_k^+ / (\sum_{j=k}^{K_n^+} \pi_j^+)$ .

In many practical situations, the trajectories  $X_i$  are measured at a set of discrete points  $t_{i1}, \ldots, t_{im_i}$ , rather than fully observed. This situation requires some modifications of the estimation procedures. For step 1, the eigenfunctions  $\phi_k$ ,  $k=1,2,\ldots$ , can be consistently estimated via a suitable implementation of functional principal component analysis, where for this estimation step unified frameworks have been developed for densely or sparsely observed functional data [Li and Hsing (2010), Zhang and Wang (2016)]. If the design points are sufficiently dense, alternatively, individual smoothing as a preprocessing step may be applied and one may then treat the pre-smoothed functions  $\hat{X}_1, \ldots, \hat{X}_n$  as if they were fully observed.

In situations where the measurements are noisy, a possible approach is to compute the likelihoods conditional on the available observations  $U_i = (U_{i1}, \ldots, U_{im_i})$ , where  $U_{ij} = X_i(t_{ij}) + \varepsilon_{ij}$  with measurement errors  $\varepsilon_{ij}$  that are independently and identically distributed according  $N(0, \sigma^2)$  and independent of  $X_i$ . Under joint Gaussian assumptions on  $X_i^{(k)}$  and the measurement errors, the  $m_i \times m_i$  covariance matrix of  $U_i$  is

(13) 
$$\operatorname{cov}(U_i \mid k) = \left\{ \sum_{r=1}^k \rho_r \phi_r(t_{ij}) \phi_r(t_{i\ell}) \right\}_{1 \le j, \ell \le m_i} + \sigma^2 I_{m_i} \equiv \Sigma_{U_i}^{(k)},$$

where  $I_{m_i}$  denotes the  $m_i \times m_i$  identity matrix. The likelihood  $f(U_i \mid K)$  is then derived from  $N(\mu_i, \Sigma_{U_i}^{(k)})$  with  $\mu_i = \{\mu(t_{i1}), \dots, \mu(t_{im_i})\}^{\top}$  and the estimation procedure is modified by replacing  $f(X_i \mid K_i = k)$  with  $f(U_i \mid K_i = k)$  in equation (10). The following modifications are applied at steps 1 and 3: in step 1, the projections of the  $X_i$  onto the  $\phi_k$  are skipped; in step 3, the functional principal component scores  $\xi_{ik}, k = 1, \dots, K_i$ , are obtained in a final step by numerical integration for the case of densely sampled data,  $\xi_{ik} = \int X_i(t)\phi_k(t) dt$ , plugging in eigenfunction estimates  $\hat{\phi}_k$ , or by PACE estimates for the case of sparse data [Yao, Müller and Wang (2005)].

**4. Simulation study.** To demonstrate the performance of the proposed mixture approach, we conducted simulations for four different settings. For all settings, the simulations are based on n=200 trajectories from an underlying process X with mean function  $\mu(t)=t+\sin(t)$  and covariance function derived from the Fourier basis  $\phi_{2\ell-1}=\cos\{(2\ell-1)\pi t/10\}/\sqrt{5}$  and  $\phi_{2\ell}=\sin\{(2\ell-1)\pi t/10\}/\sqrt{5}$ ,  $\ell=1,2,\ldots,t\in T=[0,10]$ . For  $i=1,\ldots,n$ , the ith trajectory was generated as  $X_i(t)=\mu(x)+\sum_{k=1}^{K_i}\xi_{ik}\phi_k(t)$ . Two different cases for  $\xi_{ik}$  were considered. One is Gaussian, where  $\xi_{ik}\sim N(0,\rho_k)$  with  $\rho_k=16k^{-1.8}$ . The other is non-Gaussian, where  $\xi_{ik}$  follows a Laplace distribution with mean zero and variance  $16k^{-1.8}$ , which is included to illustrate the effect of mild deviations from the Gaussian case. Each trajectory was sampled at m=200 equally spaced time points  $t_{ij} \in T$ , and measurements were contaminated with independent measure-

ment errors  $\varepsilon_{ik} \sim N(0, \sigma^2)$ , that is, the actual observations are  $U_{ij} = X_i(t_{ij}) + \varepsilon_{ij}$ , j = 1, ..., m. Two different levels were considered for  $\sigma^2$ , namely, 0.1 and 0.25.

The four settings differ in the choice of the latent trajectory dimensions  $K_i$ . In the *multinomial* setting,  $K_i$  is independently sampled from a common distribution  $(\pi_1, \ldots, \pi_{15})$ , where the event probabilities  $\pi_1, \ldots, \pi_{15}$  are randomly generated according to a Dirichlet distribution. In the *Poisson* setting, each  $K_i$  is independently sampled from a Poisson distribution with mean  $\vartheta = 6$ . In the *finite* setting, each  $K_i$  is set to a common constant equal to 12, and in the *infinite* setting, each  $K_i$  is set to a large common constant equal to 25, which mimics the infinite nature of the process X. In the multinomial and Poisson settings the  $K_i$  vary from subject to subject, while in the finite and infinite settings, they are the same across all subjects. In the multinomial and finite settings, the  $K_1, \ldots, K_n$  are capped by a finite number that does not depend on n, whereas in the Poisson and infinite settings the  $K_i$  are in principle unbounded and can be arbitrarily large. In our implementation, we used the Gaussian–Poisson fitting algorithm described in Section 3.3 to obtain fits for the generated data in all four settings.

For evaluation purposes, we generated a test sample of size 20,000 for each setting. The population model components, such as the mean, covariance, eigenvalues and eigenfunctions and also the rate parameter  $\vartheta$  were estimated from the training sample, while the subject-level estimates,  $K_i$  and the estimates of the functional principal component were obtained from the generated data  $\{U_{ij}^*, j=1,\ldots,m\}$ that are observed for the ith subject in the test set  $X_i^*$ . Of primary interest is to achieve good trajectory recovery with the most parsimonious functional data representation possible, using as few components as possible to represent each trajectory. The performance of the trajectory recovery is measured in terms of the average integrated squared error obtained for the trajectories in the test set, AISE =  $n^{-1}\sum_{i=1}^n \int_T \{X_i^*(t) - \widehat{X}_i^*(t)\}^2 dt$ . The parsimoniousness of the representations is quantified by the average number of principal components  $K_{\text{avg}} = n^{-1} \sum_{i=1}^{n} K_i$ that are chosen for the subjects. For the traditional functional principal component analysis, this is always a common choice of  $K_i = K$  for all subjects. The results are presented in Table 1. For comparison, the minimized average integrated squared error for functional principal component analysis with its common choice K for the number of components across all trajectories is also included in the last column.

The results clearly show that in both Poisson and multinomial settings the proposed mixture method achieves often substantially smaller average integrated squared errors while utilizing fewer components on average than the traditional functional principal component analysis. In contrast, in the fixed and infinite settings, the proposed mixture method recovers trajectories with an error that is comparable to that of traditional functional principal component analysis, using roughly the same number of principal components. We conclude that the proposed mixture model is substantially better in some situations where trajectories are not homogeneous in terms of their structure, while the price to be paid for situations

## TABLE 1

Average integrated squared error (AISE) and average number  $K_{\rm avg}$  of principal components across all subjects. The first column denotes the type of data generation, either according to the mixture setting where the number of components varies from individual to individual, or according to the common setting, where the number of components is common for all subjects. The second column denotes the distribution of the number of principal components in the mixture setting and the number of common components in the common setting. The third column indicates the variance of the measurement error. The fifth and seventh columns show the AISE and the average number  $K_{\rm avg}$  of chosen components for the proposed mixture model (MIPS) for the Gaussian process and non-Gaussian process, respectively, while these values are displayed in the sixth and eighth columns for functional principal component analysis (FPCA), along with the common choice K for the number of components. The Monte Carlo standard error based on 100 simulation runs is given in parentheses, multiplied by 100

|                           |                     |                   |                       | Gaussian   |  | Non-Gaussian                                     |  |
|---------------------------|---------------------|-------------------|-----------------------|--|--|--|--|
| <b>Simulation setting</b> |                     |                   |                       | MIPS   | FPCA   | MIPS   | FPCA   |
| Mixture                   | Multinomial         | $\sigma^2 = 0.1$  | AISE<br>Kavg          | 7.01 <sub>(0.40)</sub><br>9.23 <sub>(1.21)</sub> | 7.67 <sub>(0.28)</sub><br>16.7 <sub>(1.76)</sub> | 6.98 <sub>(0.46)</sub><br>8.97 <sub>(1.12)</sub> | 7.70 <sub>(0.44)</sub><br>16.5 <sub>(1.93)</sub> |
|                           |                     | $\sigma^2 = 0.25$ | AISE $K_{\text{avg}}$ | 15.2 <sub>(1.02)</sub><br>8.66 <sub>(1.32)</sub> | 17.5 <sub>(0.81)</sub><br>16.7 <sub>(1.07)</sub> | 15.6 <sub>(1.04)</sub><br>8.58 <sub>(1.08)</sub> | 17.9 <sub>(1.19)</sub><br>16.8 <sub>(1.05)</sub> |
|                           | Poisson             | $\sigma^2 = 0.1$  | AISE $K_{\text{avg}}$ | 5.63 <sub>(0.21)</sub><br>6.78 <sub>(0.14)</sub> | 6.32 <sub>(0.23)</sub><br>13.7 <sub>(1.13)</sub> | 5.82 <sub>(0.65)</sub><br>6.68 <sub>(0.27)</sub> | 6.61 <sub>(0.89)</sub><br>13.4 <sub>(1.43)</sub> |
|                           |                     | $\sigma^2 = 0.25$ | AISE $K_{\text{avg}}$ | 12.1 <sub>(0.37)</sub><br>6.63 <sub>(0.16)</sub> | 13.9 <sub>(0.32)</sub><br>14.5 <sub>(1.17)</sub> | 12.2 <sub>(0.66)</sub><br>6.28 <sub>(0.23)</sub> | 14.0 <sub>(1.05)</sub><br>13.4 <sub>(1.94)</sub> |
| Common                    | Finite ( $K = 12$ ) | $\sigma^2 = 0.1$  | AISE Kavg             | 6.55 <sub>(0.07)</sub><br>13.6 <sub>(0.43)</sub> | 6.46 <sub>(0.07)</sub><br>12.1 <sub>(0.47)</sub> | 6.56 <sub>(0.07)</sub><br>13.5 <sub>(0.50)</sub> | 6.46 <sub>(0.07)</sub><br>12.2 <sub>(0.56)</sub> |
|                           |                     | $\sigma^2 = 0.25$ | AISE $K_{\text{avg}}$ | 15.7 <sub>(0.19)</sub><br>12.9 <sub>(1.00)</sub> | 15.5 <sub>(0.15)</sub><br>12.6 <sub>(1.03)</sub> | 15.8 <sub>(0.23)</sub><br>12.7 <sub>(0.81)</sub> | 15.5 <sub>(0.21)</sub><br>12.6 <sub>(0.99)</sub> |
|                           | Infinite $(K = 25)$ | $\sigma^2 = 0.1$  | AISE $K_{\text{avg}}$ | 13.2 <sub>(0.01)</sub><br>24.3 <sub>(0.05)</sub> | 12.9 <sub>(0.01)</sub><br>25.0 <sub>(0.00)</sub> | 13.3 <sub>(0.12)</sub><br>24.1 <sub>(0.09)</sub> | 12.9 <sub>(0.14)</sub><br>25.0 <sub>(0.00)</sub> |
|                           |                     | $\sigma^2 = 0.25$ | AISE $K_{\text{avg}}$ | 32.0 <sub>(0.53)</sub><br>23.8 <sub>(0.19)</sub> | 31.4 <sub>(0.51)</sub><br>25.0 <sub>(0.00)</sub> | 31.9 <sub>(0.38)</sub><br>23.6 <sub>(0.17)</sub> | 31.5 <sub>(0.70)</sub><br>25.0 <sub>(0.00)</sub> |

where the standard functional principal component analysis is the preferred approach is relatively small. We also note that a mild deviation from the Gaussian assumption does not have much impact on the performance. We also ran additional simulations for the *Poisson* settings with  $\sigma^2 = 0.1$  and different sample sizes. In comparison to the true value  $\vartheta = 6$  and the estimate  $\hat{\vartheta} = 6.78$  (0.14) for n = 200, the estimates 6.39 (0.13), 6.21 (0.10), 6.12 (0.06), 6.06 (0.04) for n = 500, 1000, 2000, 5000, respectively, provide empirical support for estimation consistency, where the standard errors in parentheses are based on 100 Monte Carlo runs.

**5. Application.** Longitudinal data on daily egg-laying for female medflies, Ceratitis Capitata, were obtained in a fertility study as described in Carey et al. (1998). The data set is available at http://anson.ucdavis.edu/~mueller/data/medfly1000.html. Selecting flies that survived for at least 25 days to ensure that there is no drop-out bias yielded a subsample of n = 750 medflies. For each of the flies, one has then trajectories corresponding to the number of daily eggs laid from birth to age 25 days. Shown in the top-left panel of Figure 1 are the daily egg-laying counts of 50 randomly selected flies. We apply a square-root transformation to the egg counts to symmetrize the errors as a pre-processing step. Applying standard functional principal component analysis yields estimates of the mean, covariance and eigenfunctions, as shown in the right and bottom panels of Figure 1.

Visual inspection indicates that the egg-laying trajectories possess highly variable shapes with different varying numbers of local modes. This motivates us to apply the proposed functional mixture model. The goal is to parsimoniously recover the complex structure of the observed trajectories. For evaluation, we conduct 100 runs of 10-fold cross-validation, where in each run, we shuffle the data independently, and use 10% of the flies as validation set for obtaining the subject-level estimates, which include the latent dimensions  $K_i$  and the functional principal component scores, and use the remaining 90% of the flies as training set. The

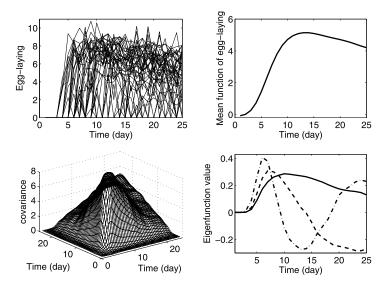


FIG. 1. Top-left: Daily egg-laying counts, after square-root transformation, for 50 randomly selected flies for the first 25 days of their lifespan. Top-right: Smooth estimate of the mean function. Bottom-left: Smooth nonnegative definite estimate of the covariance surface. Bottom-right: Smooth estimates of the first (solid), second (dashed) and third (dash-dotted) eigenfunctions, explaining 95% of the total variation.

TABLE 2

Egg-laying data: 10-fold cross-validated relative squared errors (CVRSE), as obtained for the proposed functional mixture model (MIPS) and for traditional functional principal component analysis (FPCA), where the latter uses a common number K of components across all subjects, for  $K=0,2,\ldots,18$  and  $K_{\rm avg}$  is the mean of the number of principal components used by the proposed method. The results are based on 100 random partitions with standard error in parentheses

FPCA 
$$K$$
 0 2 4 6 8  
CVRSE  $3.3914_{(0.0070)}$   $0.2038_{(0.0003)}$   $0.1549_{(0.0002)}$   $0.1388_{(0.0002)}$   $0.1347_{(0.0001)}$   
 $K$  10 12 14 16 18  
CVRSE  $0.1340_{(0.0001)}$   $0.1337_{(0.0001)}$   $0.1336_{(0.0001)}$   $0.1335_{(0.0001)}$   $0.1334_{(0.0001)}$   
MIPS  $CVRSE = 0.1319_{(0.0002)}$   $K_{avg} = 8.2684_{(0.0192)}$ 

resulting cross-validated relative squared errors are

$$CVRSE = n^{-1} \sum_{l=1}^{10} \sum_{i \in D_l} \left( \left[ \sum_{i=1}^m \{ U_{ij} - \widehat{X}_i^{-D_l}(t_{ij}) \}^2 \right] / \sum_{i=1}^m U_{ij}^2 \right),$$

where  $D_l$  is the *l*th validation set containing 10% of subjects.

The results are reported in Table 2 for the proposed functional mixture model and functional principal component analysis for different fixed values for the number of included components K. We find that the proposed method utilizes about 8 principal components on average ( $K_{\rm avg} = 8.27$ ) and with this number achieves better recovery, compared to the results obtained by the traditional functional principal component analysis using more components. Therefore, in this application, the proposed mixture model provides both better and more parsimonious fits.

Figure 2 displays egg-laying counts for 6 randomly selected flies, overlaid with smooth estimates obtained by the proposed mixture method and by traditional functional principal component analysis using 8 components (similar to  $K_{\rm avg}$ ) and also K=3, a choice that explains 95% of the variation of the data and, therefore, would be adopted by the popular fraction of variance explained selection criterion. This figure indicates that the functional mixture method appears to adapt better to the varying shapes of the trajectories. The estimated probability densities of the first three mixture components and their mixture proportions are depicted in Figure 3.

**6. Discussion and concluding remarks.** Density functions are important for many statistical applications that require the construction of a likelihood, for example, one could use maximum likelihood to find the best fit for a parametrized class of densities. Similarly, Bayes classifiers for functional data can be based on a density ratio. Densities can also be used for the estimation of modes and level contours and also to estimate the shape and location of ridges in functional data

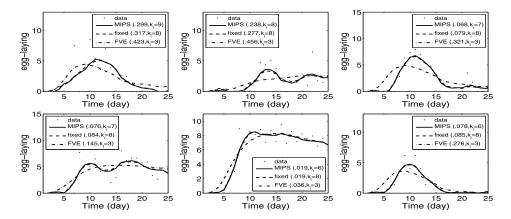


FIG. 2. Daily egg-laying counts for six randomly selected flies for the first 25 days of their lifespan, overlaid with the smooth estimates obtained from the proposed functional mixture model (MIPS), solid line, from functional principal component analysis with a fixed number of 8 components, dashed line, and for a fixed number of three components which explain 95% of the total variation, dash-dotted line. Shown in parentheses are the individual relative squared errors and the included number of components for that individual.

sets, extending the analogous problem for multivariate data. Specifically, the importance of constructing modes for functional data distributions has been recognized before [Gasser, Hall and Presnell (1998)]. One can consider related mode finding algorithms that can be used for clustering functional data [Liu and Müller

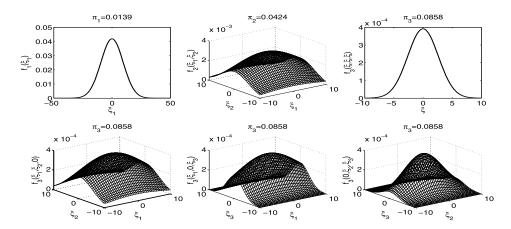


FIG. 3. Estimated probability density function for the first three mixture components and their corresponding mixture proportions  $\pi_k$ . Top: left, the probability density function of the first component; middle, the probability density function of the second component; right, the diagonal of the probability density function of the third component. Bottom: 2-dimension slices of the probability densities of the third component at  $\xi_1 = 0$ ,  $\xi_2 = 0$  and  $\xi_3 = 0$ , respectively, in the left, middle and right panels.

(2003)]. As clustering of functional data is attracting increasing attention [Chiou and Li (2007), Jacques and Preda (2014), Slaets, Claeskens and Hubert (2012)], density-based clustering for functional data likely will be of increasing interest for data analysis.

In addition to this relevance of densities in function space for functional data applications, the foundational issue of the existence and construction of densities in function space naturally puts the problem of obtaining a density for functional data into focus. The fact that such a density does not exist in the often considered function space  $L^2$  demonstrates the scope of the problem. This has led to the construction of a surrogate density, which can be based on a truncated expansion of the functional data into functional principal components [Bongiorno and Goia (2016), Delaigle and Hall (2010)]. This construction is a workaround that provides a practical solution but leaves open the problem of finding a theoretical solution, for which one has to move away from the whole space  $L^2$ .

Motivated by practical consideration from applications of functional data analysis, we propose here a construction that provides a theoretical solution to the density problem by essentially considering random functions in  $L^2$  whose distribution belongs to an infinite mixture of distributions on k-dimensional subspaces. Each of the component distributions has a finite dimension  $k < \infty$  and corresponds to functions that can be fully described by an expansion into k components only. The space is still infinite-dimensional overall, as the dimensions k are unlimited. This mixture distribution approach has the advantage that an overall density can be well defined theoretically under regularity assumptions. Moreover, the components of the expansion can be estimated by applying a usual eigen-expansion that gives the correct eigenfunctions even if the mixture structure is ignored. To obtain the correct eigenvalues, the mixture probabilities play a role, and they can be consistently estimated under additional assumptions. We develop the construction of mixture inner product spaces for which appropriate mixture densities can be found under certain conditions in a framework of general infinite dimensional Hilbert spaces that transcends functional data analysis and, therefore, may be of more general interest. In data applications, the proposed mixture model tends to use fewer components than standard functional principal component analysis, while achieving the same or sometimes better approximations to the observed trajectories, which demonstrates that mixture inner product spaces are also of practical interest.

## APPENDIX: TECHNICAL PROOFS

PROOF OF PROPOSITION 1. Let x be an arbitrary element of H and  $a_k = \langle x, \phi_k \rangle$ . Since  $\phi_1, \phi_2, \ldots$  form a complete orthonormal basis of H, we have  $\|x\|^2 = \sum_{k=1}^{\infty} a_k^2 < \infty$ . Now define  $x_k = \sum_{j=1}^k a_j \phi_k$ . Then  $x_k \in S$  for each  $k = 1, 2, \ldots$ . Also,  $\|x - x_k\|^2 = \sum_{j=k+1}^{\infty} a_j^2 \to 0$  as  $k \to \infty$ . This implies that for any k > 0, the open ball B(x; h) with center at  $k = 1, 2, \ldots$  This shows that  $k = 1, 2, \ldots$  This shows t

To show part 2., note that  $H_k = \bigcup_{j=1}^k S_j$  and hence  $S = \bigcup_{k=1}^\infty S_k = \bigcup_{k=1}^\infty \bigcup_{j=1}^k S_j = \bigcup_{k=1}^\infty H_k$ . Since each  $H_k$  is a closed subset of H, and hence  $H_k \in \mathcal{B}(H)$ , we conclude that  $S = \bigcup_{k=1}^\infty H_k$  is in  $\mathcal{B}(H)$ . To see  $\mathcal{B}(S) \subset \mathcal{B}(H)$ , we first note that, since the metric  $d_S$  on S, defined by  $d_S(x, y) = \|x - y\|_H$  for all  $x, y \in S \subset H$ , is the restriction of the metric  $d_H$  on H, the subspace topology of S coincides with the topology induced by the metric  $d_S$ . This implies that for any open set A of S there exists an open subset B of H such that  $A = B \cap S$ . As both B and S are in  $\mathcal{B}(H)$ , we have  $A \in \mathcal{B}(H)$ . In other words, the collection  $\tau_S$  of all open sets of S is a subset of  $\mathcal{B}(H)$ . This implies  $\mathcal{B}(S) \subset \mathcal{B}(H)$ , recalling that  $\mathcal{B}(S)$  is the smallest  $\sigma$ -algebra containing  $\tau_S$ .

For part 3., we first note that  $\mathscr{B}(S) = \{B \cap S : B \in \mathscr{B}(H)\}$ , by Lemma 3 in Chapter II of Shiryayev (1984). Now, if  $B \in \mathscr{B}(H)$ , then  $B \cap S \in \mathscr{B}(S)$ , and hence  $X_S^{-1}(B) = X_S^{-1}(B \cap S) \in \mathscr{E}$ . Therefore,  $X_S$  is also  $\mathscr{E}$ - $\mathscr{B}(H)$  measurable, and hence an H-valued random element.  $\square$ 

PROOF OF PROPOSITION 2. We prove the claim by explicitly constructing such an S-valued random element Y, as follows. Let  $\varepsilon_1 = \{E(\|X - X_k\|_H^p)\}^{1/p}$  and  $\delta = (\varepsilon - \varepsilon_1)/2 > 0$ . Since  $f_k(0) > 0$  and  $f_k$  is continuous at 0, if  $\Omega_\delta = \{\omega \in \Omega : \xi_k(\omega) \in (-\delta/2, \delta/2)\}$ , then  $P(\Omega_\delta) > 0$ . Define  $Y(\omega) = X_k(\omega)$  if  $\omega \notin \Omega_\delta$  and  $Y(\omega) = X_{k-1}(\omega)$  otherwise. If we define  $Z(\omega) = \xi_k(\omega)\phi_k 1_{\Omega_\delta}$ , then  $Y = X_k - Z$ . Since  $\{E(\|Z\|_H^p)\}^{1/p}$  defines a norm on all H-valued random elements Z such that  $\{E(\|Z\|_H^p)\}^{1/p} < \infty$  [Vakhania, Tarieladze and Chobanyan (1987)], this implies that  $\{E(\|X - Y\|_H^p)\}^{1/p} = \{E(\|X - X_k + Z\|_H^p)\}^{1/p} \le \{E(\|X - X_k\|_H^p)\}^{1/p} + \{E(\|Z\|_H^p)\}^{1/p} < \varepsilon_1 + \delta P(\Omega_\delta) < \varepsilon$ . On the other hand, the continuity of  $f_k$  at 0 implies that  $P(\xi_k = 0) = 0$ , and hence we have  $\mathcal{K}(Y) = \mathcal{K}(X_k) - P(\Omega_\delta) < \mathcal{K}(X_k)$ .  $\square$ 

PROOF OF THEOREM 2. Note that each Lebesgue measure  $\tau_k$  is  $\sigma$ -finite. This means that for each k there is a countable partition  $S_{k1}, S_{k2}, \ldots$  of  $S_k$  such that  $S_{kj} \in \mathcal{B}(S)$  and  $\tau_k(S_{kj}) < \infty$  for all  $j = 1, 2, \ldots$  Since  $S = \bigcup_k \bigcup_j S_{kj}$ , we know that  $\{S_{kj} : j = 1, \ldots, k = 1, \ldots\}$  forms a countable partition of S, where each  $S_{kj}$  has finite measure  $\tau(S_{kj}) = \tau_k(S_{kj}) < \infty$ . This shows that  $\tau$  is  $\sigma$ -finite.

To show that  $P_X$  is absolutely continuous to  $\tau$ , suppose  $A \in \mathcal{B}(S)$  and  $\tau(A) = 0$ , and define  $A_k = A \cap S_k$ . Then  $\tau_k(A_k) = 0$  for all k. Note that  $P_X(A) = \sum_{k=1}^{\infty} P_X(A_k)$ . Define  $\eta_k(x) = (\langle x, \phi_1 \rangle, \langle x, \phi_2 \rangle, \ldots, \langle x, \phi_k \rangle) \in \mathbb{R}^k$  for each  $x \in H_k$ . Note that each  $\eta_k$  is a canonical isomorphic mapping between  $H_k$  and  $\mathbb{R}^k$ . Thus, the Lebesgue measure of  $\eta_k(A_k)$  is equal to  $\tau_k(A_k)$  and is zero. Now,  $P_X(A_k) = P\{(\xi_1, \xi_2, \ldots, \xi_k) \in \eta_k(A_k), X = k\} = P\{(\xi_1, \xi_2, \ldots, \xi_k) \in \eta_k(A_k) \mid X = k\}P(X = k) = \pi_k \int_{\eta_k(A_k)} f_k(t_1, t_2, \ldots, t_k) dt_1 dt_2 \cdots dt_k = 0$ , where the last equality is due the fact that the Lebesgue measure of  $\eta_k(A_k)$  is zero and the fact that  $f_k$  is a density function by assumption. Therefore,  $P_X(A) = 0$ , and we conclude that  $P_X$  is absolutely continuous w.r.t.  $\tau$ .

By the Radon–Nykodym theorem, there is a density f of  $P_X$  on S with respect to  $\tau$ . Now we show that f defined in (1) is such a density. Let  $A \in \mathcal{B}(S)$ . As above we define  $A_k = A \cap S_k$ . Then  $A_1, A_2, \ldots$  form a partition of A, and hence

(14) 
$$\int_A f d\tau = \sum_k \int_{A_k} f d\tau = \sum_k \pi_k \int_{A_k} f_k d\tau_k.$$

Now, for each k,

(15) 
$$P_X(A_k) = \Pr\{(\xi_1, \xi_2, \dots, \xi_k) \in \eta(A_k), K = k\}$$
$$= \pi_k \Pr\{(\xi_1, \xi_2, \dots, \xi_k) \in \eta(A_k) \mid K = k\}$$
$$= \pi_k \int_{\eta(A_k)} f_k(t_1, t_2, \dots, t_k) dt_1 dt_2 \cdots dt_k = \pi_k \int_{A_k} f_k d\tau_k.$$

Given (14) and (15), we conclude that  $\int_A f d\tau = \sum_k P_X(A_k) = P_X(A)$ , and hence f is a probability density function of  $P_X$  w.r.t.  $\tau$ .  $\square$ 

To simplify notation, we simply use r from now on, while one should be aware that r grows to infinity as sample size  $n \to \infty$ . The proof of Theorem 3 requires several lemmas.

Let  $\hat{G}(s,t) = n^{-1} \sum_{i=1}^{n} X_i(s) X_i(t)$  denote the empirical version of G(s,t) and  $\hat{\phi}_k$  be the kth eigenfunction of  $\hat{G}$ . When it is clear from the context, we use G and  $\hat{G}$  to denote the corresponding covariance operator. Define  $\hat{\Delta} = \{ \int_{D \times D} (\hat{G}(s,t) - G(s,t))^2 ds dt \}^{1/2}$  and for a constant  $C_4 > 0$ ,

(16) 
$$J' = \{j-1 : \lambda_j - \lambda_{j+1} \ge 2\hat{\Delta}\}, \text{ and } J = \{j \in J' : j \le C_4 n^{1/(2b+2)}\}.$$

From  $\hat{\Delta} = O_p(n^{-1/2})$  [Hall and Hosseini-Nasab (2006)] and assumption (A3), we have

$$P(C_5n^{1/(2b+2)} \le \sup J \le C_4n^{1/(2b+2)}) \to 1$$

for a positive constant  $C_5 \leq C_4$ . The following lemma quantifies the estimation quality of the eigenfunctions  $\hat{\phi}_k$  and the principal component scores  $\hat{\xi}_{ik}$ . Let  $\hat{\xi}_{i,(k)} = (\hat{\xi}_{i,1}, \hat{\xi}_{i,2}, \dots, \hat{\xi}_{i,k})$  where  $\hat{\xi}_{ij} = \langle X_i, \hat{\phi}_j \rangle$ .

LEMMA 1. If assumptions (A0), (A2) and (A3) hold,

(17) 
$$\sup_{n \ge 1} \sup_{k \in J} n^2 k^{-4(b+1)} E \| \hat{\phi}_k - \phi_k \|^4 < \infty;$$

(18) 
$$\sup_{n \ge 1} \sup_{k \in J} nk^{-2b-3} E \|\xi_{i,(k)} - \hat{\xi}_{i,(k)}\|^2 < \infty.$$

PROOF. The bound in (17) directly follows from Lemma 3.4 of Hall and Hosseini-Nasab (2009),  $E(\hat{\Delta}^4) = O(n^{-2})$  [Lemma 3.3 of Hall and Hosseini-Nasab (2009)] and (A3). To show (18),

$$E \|\hat{\xi}_{i,(k)} - \xi_{i,(k)}\|^{2} = \sum_{j=1}^{k} E(|\hat{\xi}_{i,j} - \xi_{i,j}|^{2}) = \sum_{j=1}^{k} E(\langle X_{i}, \hat{\phi}_{j} - \phi_{j} \rangle^{2})$$

$$\leq \sum_{j=1}^{k} E(\|X_{i}\|^{2} \|\hat{\phi}_{j} - \phi_{j}\|^{2})$$

$$\leq \sum_{j=1}^{k} \{E(\|X_{i}\|^{4}) E(\|\hat{\phi}_{j} - \phi_{j}\|^{4})\}^{1/2}$$

$$= \{E(\|X\|^{4})\}^{1/2} \sum_{j=1}^{k} \{E(\|\hat{\phi}_{j} - \phi_{j}\|^{4})\}^{1/2}.$$

Then (18) follows with the fact  $E(||X||^4) < \infty$  and (17).  $\square$ 

We next examine the discrepancy between true and estimated likelihood functions. Recall that  $Q_r = \min(K, r)$ ,  $Z = \sum_{j=1}^{Q_r} \langle X, \phi_j \rangle \phi_j$ , the log-likelihood of Z with  $\pi_r^* = 1 - \sum_{k=1}^{r-1} \pi_k$ ,

$$L_{r,1}(Z \mid \theta_{[r]}) = \log \left\{ \pi_r^* f_r(Z \mid \theta_{(r)}) 1_{Z \in S_r} + \sum_{k=1}^{r-1} \pi_k f_k(Z \mid \theta_{(k)}) 1_{Z \in S_k} \right\},\,$$

and  $L_r(\theta_{[r]}) = E\{L_{r,1}(z \mid \theta_{[r]})\}$ . Define the log-likelihood function of  $\theta$  given  $Z_1, \ldots, Z_n$  by  $L_{r,n}(\theta_{[r]}) = \frac{1}{n} \sum_{i=1}^n L_{r,1}(Z_i \mid \theta_{[r]})$ . The following lemma quantifies the discrepancy between  $L_{r,n}(\theta_{[r]})$  and  $L_r(\theta_{[r]})$ .

LEMMA 2. If the assumptions in Theorem 3 hold, then for each  $\theta_{[r]}$ ,

$$r^a |L_{r,n}(\theta_{[r]}) - L_r(\theta_{[r]})| \stackrel{p}{\longrightarrow} 0.$$

PROOF. We first express  $L_r(\theta_{[r]}) = E\{L_{r,1}(z \mid \theta_{[r]})\}$  as follows:

$$L_{r}(\theta_{[r]}) = E \log \left\{ \pi_{r}^{*} f_{r}(Z \mid \theta_{(r)}) 1_{Z \in S_{r}} + \sum_{k=1}^{r-1} \pi_{k} f_{k}(Z_{i} \mid \theta_{(k)}) 1_{Z \in S_{k}} \right\}$$

$$= E E \left[ \log \left\{ \pi_{r}^{*} f_{r}(Z \mid \theta_{(r)}) 1_{Z \in S_{r}} + \sum_{k=1}^{r-1} \pi_{k} f_{k}(Z \mid \theta_{(k)}) 1_{Z \in S_{k}} \right\} \mid Q_{r} \right]$$

$$= \pi_{r}^{*} E \left[ \log \left\{ \pi_{r}^{*} f_{r}(Z \mid \theta_{(r)}) \right\} \mid K \geq r \right]$$

$$(19)$$

$$+ \sum_{k=1}^{r-1} \pi_k E[\log\{\pi_k f_k(Z \mid \theta_{(k)})\} \mid K = k]$$

$$= \pi_r^* \log \pi_r^* + \sum_{k=1}^{r-1} \pi_k \log \pi_k + \pi_r^* E\{g_r(\tilde{\xi}_1, \tilde{\xi}_2, \dots, \tilde{\xi}_r)\}$$

$$+ \sum_{k=1}^{r-1} \pi_k E\{g_k(\tilde{\xi}_1, \tilde{\xi}_2, \dots, \tilde{\xi}_k)\},$$

where (19) is obtained by noting that  $1_{Z \in S_k} = 0$  if  $Q_r \neq k$ , and  $1_{Z \in S_k} = 1$  if  $Q_r = k$ . Let  $W_{n,i} = L_{r,1}(Z_i \mid \theta_{[r]}) - L_r(\theta_{[r]})$ . Then  $E(W_{n,i}) = 0$  and  $L_{r,n}(\theta_{[r]}) - L_r(\theta_{[r]}) = n^{-1} \sum_{i=1}^n W_{n,i}$ . We shall show that  $r^a W_{n,i}$  satisfies the Cesàro-type uniform integrability defined in Sung (1999), and hence admits a weak law of large numbers. First, we show that  $\sup_{n\geq 1} n^{-1} \sum_{i=1}^n r^a E |W_{n,i}| = O(1)$ . For sufficiently large n, given (A6), with definition  $\tilde{\xi}_{(k)} = (\tilde{\xi}_1, \tilde{\xi}_2, \dots, \tilde{\xi}_k)$ , we have

$$E|W_{n,i}| \leq E|g_{r}(Z)1_{Z \in S_{r}} - \pi_{r}^{*}E(g_{r}(\tilde{\xi}_{(r)}))|$$

$$+ \sum_{k=1}^{r-1} E|g_{k}(Z)1_{Z \in S_{k}} - \pi_{k}E(g_{k}(\tilde{\xi}_{(k)}))|$$

$$= E|g_{r}(\tilde{\xi}_{(r)})1_{K \geq r} - \pi_{r}^{*}E(g_{r}(\tilde{\xi}_{(r)}))|$$

$$+ \sum_{k=1}^{r-1} E|g_{k}(\tilde{\xi}_{(k)})1_{K = k} - \pi_{k}E(g_{k}(\tilde{\xi}_{(k)}))|$$

$$\leq 2\pi_{r}^{*}E|g_{r}(\tilde{\xi}_{(r)})| + 2\sum_{k=1}^{r-1} \pi_{k}E|g_{k}(\tilde{\xi}_{(k)})|$$

$$\leq r^{-a+c-\beta+1} + c_{2}\sum_{k=1}^{r-1} k^{-a+c-\beta} \leq c_{3}r^{-a},$$

where  $c_3$  is a constant that does not depend on n and i, and the last inequality is due to the condition  $\beta > c+1$  in (A6). Thus,  $\sup_{n\geq 1} n^{-1} \sum_{i=1}^n E\{r^a|W_{n,i}|\} = O(1)$ . Since for any n, the random variables  $W_{n,1}, W_{n,2}, \ldots, W_{n,n}$  are i.i.d.,

(21) 
$$\lim_{u \to \infty} \sup_{n \ge 1} n^{-1} \sum_{i=1}^{n} E\{r^{a} | W_{n,i} | 1_{|W_{n,i}| > u}\} = \lim_{u \to \infty} \sup_{n \ge 1} E\{r^{a} | W_{n,1} | 1_{|W_{n,1}| > u}\} = 0.$$

as  $E\{r^a|W_{n,1}|\}<\infty$  by (20). Then  $r^aW_{n,i}$  satisfies the Cesàro-type uniform integrability, and the conclusion of the lemma follows from a weak law of large numbers for triangular arrays [Sung (1999)].  $\square$ 

We are now ready to quantify the discrepancy from the estimated likelihood function  $\hat{L}_{r,n}$  by plugging in the estimated quantities  $\hat{\phi}_k$  and  $\hat{\xi}_{ik}$ .

LEMMA 3. If the assumptions in Theorem 3 hold, then for each  $\theta_{[r]}$ ,

$$r^a |\hat{L}_{r,n}(\theta_{[r]}) - L_r(\theta_{[r]})| \stackrel{p}{\longrightarrow} 0.$$

PROOF. Recall  $\hat{\xi}_{i,(k)} = (\hat{\xi}_{i,1}, \hat{\xi}_{i,2}, \dots, \hat{\xi}_{i,k})$ , and define

$$\begin{split} Y_{n,i} &= \pi_r^* \big\{ C_1 H_r(\xi_{i,(r)}) \| \hat{\xi}_{i,(r)} - \xi_{i,(r)} \|^{\nu_1} \mathbf{1}_{Z_i \in S_r} + C_2 r^{\alpha_2} \| \hat{\xi}_{i,(r)} - \xi_{i,(r)} \|^{\nu_2} \mathbf{1}_{Z_i \in S_r} \big\} \\ &+ \sum_{k=1}^{r-1} \pi_k \big\{ C_1 H_k(\xi_{i,(k)}) \| \hat{\xi}_{i,(k)} - \xi_{i,(k)} \|^{\nu_1} \mathbf{1}_{Z_i \in S_k} \\ &+ C_2 k^{\alpha_2} \| \hat{\xi}_{i,(k)} - \xi_{i,(k)} \|^{\nu_2} \mathbf{1}_{Z_i \in S_k} \big\}. \end{split}$$

By (A4), we have

$$|\hat{L}_{r,n}(\theta_{[r]}) - L_r(\theta_{[r]})| \le |L_{r,n}(\theta_{[r]}) - L_r(\theta_{[r]})| + n^{-1} \sum_{i=1}^n Y_{n,i}.$$

From the condition  $r = n^{\gamma - \varepsilon}$  in Theorem 3 and the definition of J in (16), we have  $P\{r \in J\} \to 1$  as  $n \to \infty$ . Thus, we may assume  $r \in J$  in the sequel. With Lemma 1, if  $\nu' \le 2$ , then  $E \|\hat{\xi}_{i,(k)} - \xi_{i,(k)}\|^{\nu'} \le \{E \|\hat{\xi}_{i,(k)} - \xi_{i,(k)}\|^2\}^{\nu'/2} = O(k^{(2b+3)\nu'/2}n^{-\nu'/2})$  uniformly for  $k \le r$  and n. Since  $2\nu_1 \le 2$ ,  $\nu_2 \le 2$ ,  $\alpha = \max(\alpha_1, \alpha_2)$  and  $\nu = \min(2\nu_1, \nu_2)$ , for some  $c_0 > 0$ ,

$$\begin{split} E\big\{\big|H_{k}(\xi_{i,(k)})\big|\|\hat{\xi}_{i,(k)} - \xi_{i,(k)}\|^{\nu_{1}}\big\} &\leq \big[E\big\{H_{k}(\xi_{i,(k)})\big\}^{2}\big]^{1/2} \big(E\|\hat{\xi}_{i,(k)} - \xi_{i,(k)}\|^{2\nu_{1}}\big)^{1/2} \\ &= O\big(k^{(2b+3)\nu/2+\alpha}n^{-\nu/2}\big), \\ E\big\{k^{\alpha_{2}}\|\hat{\xi}_{i,(k)} - \xi_{i,(k)}\|^{\nu_{2}}\big\} &= O\big(k^{(2b+3)\nu/2+\alpha}n^{-\nu/2}\big). \end{split}$$

Recall  $\gamma_1 = (2b+3)\nu/2 + \alpha - 2\beta$ ,  $\gamma_2 = a + (\gamma_1 + 2)1_{\gamma_1 > -2}$ ,  $\gamma = \min\{\nu/(2\gamma_2), 1/(2b+2)\}$  in Theorem 3, implying  $\gamma \gamma_2 \le \nu/2$ , and hence,

$$E|Y_{n,i}| \leq (\pi_r^*)^2 E\{C_1 | H_r(\xi_{i,(r)}) | \|\hat{\xi}_{i,(r)} - \xi_{i,(r)}\|^{\nu_1} + C_2 r^{\alpha_2} \|\hat{\xi}_{i,(r)} - \xi_{i,(r)}\|^{\nu_2} \}$$

$$+ \sum_{k=1}^{r-1} \pi_k^2 E\{C_1 | H_k(\xi_{i,(k)}) | \|\hat{\xi}_{i,(k)} - \xi_{i,(k)}\|^{\nu_1} + C_2 k^{\alpha_2} \|\hat{\xi}_{i,(k)} - \xi_{i,(k)}\|^{\nu_2} \}$$

$$\leq c_1 r^{-2\beta+2} r^{(2b+3)\nu/2+\alpha} n^{-\nu/2} + c_2 \sum_{k=1}^{r-1} k^{-2\beta+(2b+3)\nu/2+\alpha} n^{-\nu/2}$$

$$= c_1 r^{\gamma_1+2} n^{-\nu/2} + c_2 \sum_{k=1}^{r-1} k^{\gamma_1} n^{-\nu/2} \leq c_3 n^{-\nu/2} r^{\gamma_2-a} \leq c_4 r^{-a} n^{-\varepsilon\gamma_2/2},$$

where the last inequality is due to  $r = O(n^{\gamma - \varepsilon})$ , and  $c_1, c_2, c_3, c_4$  are positive constants that do not depend on n. Setting  $\delta = 3/(3 + \varepsilon v/\gamma_2) < 1$ , by the Lyapunov inequality,  $r^{a\delta}E|Y_{n,i}|^{\delta} \le r^{a\delta}(E|Y_{n,i}|)^{\delta} \le c_4 r^{a\delta} r^{-a\delta} n^{-\delta\varepsilon v/(2\gamma_2)} = c_4 n^{-\delta\varepsilon v/(2\gamma_2)}$  uniformly for n and  $r = O(n^{\gamma - \varepsilon})$ . Although the  $Y_{n,i}$  are not independent of  $Y_{n,j}$ , they have the same distribution due to symmetry. Therefore, noting that  $1 - \delta\{1 + \varepsilon v/(2\gamma_2)\} < 0$ , we have

(23) 
$$\sup_{n\geq 1} n^{-\delta} \sum_{i=1}^{n} E\{r^{a\delta} |Y_{n,i}|^{\delta}\} \leq \sup_{n\geq 1} c_4 n^{-\delta} n n^{-\delta \varepsilon \nu/(2\gamma_2)}$$

$$= \sup_{n\geq 1} c_4 n^{1-\delta\{1+\varepsilon \nu/(2\gamma_2)\}} = O(1).$$

The result  $r^{a\delta}E|Y_{n,i}|^{\delta} = O(n^{-\delta \varepsilon \nu/(2\gamma_2)})$  also implies that

(24) 
$$\lim_{M \to \infty} \sup_{n \ge 1} n^{-\delta} \sum_{i=1}^{n} E\{r^{a\delta} | Y_{n,i}|^{\delta} 1_{|Y_{n,i}|^{\delta} > M}\} = 0.$$

Then the Cesàro-type uniform integrability is satisfied by  $r^a Y_{n,i}$  with exponent  $\delta < 1$ , based on (23) and (24), and the weak law of large numbers [Sung (1999)] implies  $n^{-1} \sum_{i=1}^n r^a Y_{n,i} = o_p(1)$ . This result, in conjunction with the fact  $r^a | L_{r,n}(\theta_{[r]}) - L_r(\theta_{[r]})| = o_p(1)$  and  $r^a | \hat{L}_{r,n}(\theta_{[r]}) - L_r(\theta_{[r]})| \leq r^a | L_{r,n}(\theta_{[r]}) - L_r(\theta_{[r]})| + n^{-1} \sum_{i=1}^n r^a Y_{n,i}$ , as well as  $\Pr\{r \in J\} \to 1$ , yields the result.  $\square$ 

PROOF OF THEOREM 3. By (A5),  $\theta_{[r],0}$  is the maximizer of  $L_r(\theta_{[r]})$ . Let  $h_5 = \min\{h_1, h_2, h_3\}$  and  $U_r^a = \{\theta_{[r]} : L_r(\theta_{[r],0}) - L_r(\theta_{[r]}) < h_5 r^{-a}\}$ , whence  $U_r^a \subset U_r \subset \mathcal{B}_r$ , where  $a = \max(a_1, a_2)$ ,  $U_r$  and  $\mathcal{B}_r$  are defined in (A5). Moreover, for all  $\theta_{[r]} \in U_r^a$ , there exists  $h_4 > 0$  not depending on r and  $\theta_{[r]}$ , such that

(25) 
$$L_r(\theta_{[r],0}) - L_r(\theta_{[r]}) \ge h_4 r^{-a} \|\theta_{[r]} - \theta_{[r],0}\|^2.$$

From (A1),  $\Theta = \prod_{j=1}^{\infty} I_{[\infty],j}$  is compact due to Tychonoff's theorem, which implies that the convergence of  $r^a |\hat{L}_{r,n}(\theta_{[r]}) - L_r(\theta_{[r]})|$  in Lemma 3 is uniform over  $\Theta$ . Thus, for any  $0 < \varepsilon^2 < h_5$ , there exists  $N_{\varepsilon} > 0$  such that if  $n > N_{\varepsilon}$ , then

$$\Pr(\left\{r^{a} \left| \hat{L}_{r,n}(\theta_{[r],0}) - L_{r}(\theta_{[r],0}) \right| < \varepsilon^{2}/2\right\} \cap \left\{r^{a} \left| \hat{L}_{r,n}(\hat{\theta}_{[r]}) - L_{r}(\hat{\theta}_{[r]}) \right| < \varepsilon^{2}/2\right\})$$
(26)
$$> 1 - \varepsilon/2,$$

where  $\hat{\theta}_{[r]}$  is a global maximizer of  $\hat{L}_{r,n}$ . Next, we show that

(27) 
$$\Pr\{r^{a}|\hat{L}_{r,n}(\hat{\theta}_{[r]}) - L_{r}(\theta_{[r],0})| < \varepsilon^{2}/2\} > 1 - \varepsilon/2.$$

If  $\hat{L}_{r,n}(\hat{\theta}_{[r]}) \geq L_r(\theta_{[r],0})$ , then  $0 \leq \hat{L}_{r,n}(\hat{\theta}_{[r]}) - L_r(\theta_{[r],0}) \leq \hat{L}_{r,n}(\hat{\theta}_{[r]}) - L_r(\hat{\theta}_{[r]})$  since  $L_r(\hat{\theta}_{[r]}) \leq L_r(\theta_{[r],0})$ , due to the fact that  $\theta_{[r],0}$  is the global maximizer of  $L_r(\cdot)$ . Similarly, if  $\hat{L}_{r,n}(\hat{\theta}_{[r]}) \leq L_r(\theta_{[r],0})$ , then  $0 \leq L_r(\theta_{[r],0}) - \hat{L}_{r,n}(\hat{\theta}_{[r]}) \leq L_r(\theta_{[r],0})$ 

 $L_r(\theta_{[r],0}) - \hat{L}_{r,n}(\theta_{[r],0})$  since  $\hat{L}_{r,n}(\theta_{[r],0}) \leq \hat{L}_{r,n}(\hat{\theta}_{[r]})$  due to the fact that  $\hat{\theta}_{[r]}$  is a global maximizer of  $\hat{L}_{r,n}(\cdot)$ . Combining these two cases yields  $|\hat{L}_{r,n}(\hat{\theta}_{[r]}) - L_r(\theta_{[r],0})| \leq \max\{|\hat{L}_{r,n}(\hat{\theta}_{[r]}) - L_r(\hat{\theta}_{[r]})|, |L_r(\theta_{[r],0}) - \hat{L}_{r,n}(\theta_{[r],0})|\}$ . This result, in conjunction with (26), yields (27).

Then applying the triangle inequality in conjunction with (26) and (27) leads to  $\Pr\{r^a|L_r(\hat{\theta}_{[r]})-L_r(\theta_{[r],0})|<\varepsilon^2\}>1-\varepsilon.$  Since  $\varepsilon^2< h_5$ , we have  $\hat{\theta}_{[r]}\in U_r^a$  with probability  $(1-\varepsilon)$ , and then apply (25) to conclude that  $\Pr\{\|\hat{\theta}_{[r]}-\theta_{[r],0}\|<2\varepsilon/\sqrt{h_4}\}>1-\varepsilon$ , which yields the consistency of  $\hat{\theta}_{[r]}$ .

It remains to show the consistency of  $f(x \mid \hat{\theta}_{[r]})$  for any  $x \in \bigcup_{k=1}^{\infty} S_k$ , which implies that there exists some  $k_0 < \infty$  such that  $x \in S_{k_0}$ . Then  $f(x) = \sum_{k=1}^{k_0} f_k(x \mid \theta_k) 1_{S_k}$ , as the indicator functions  $1_{S_j}$  are all zero if  $j > k_0$ . For sufficiently large n such that  $k_0 \le r_n$ ,  $\theta_{[r_n]}$ , and hence,  $\theta_1, \ldots, \theta_{k_0}$  are all consistently estimated. The continuity of each  $f_k$  with respect to  $\theta_k$  in (A4) then implies that  $|f(x \mid \hat{\theta}_{[r]}) - f(x \mid \theta_{[\infty],0})| \xrightarrow{p} 0$ .  $\square$ 

## **REFERENCES**

- BENAGLIA, T., CHAUVEAU, D. and HUNTER, D. R. (2009). An EM-like algorithm for semiand nonparametric estimation in multivariate mixtures. *J. Comput. Graph. Statist.* **18** 505–526. MR2749842
- BESSE, P. and RAMSAY, J. O. (1986). Principal components analysis of sampled functions. Psychometrika 51 285–311. MR0848110
- BOENTE, G. and FRAIMAN, R. (2000). Kernel-based functional principal components. *Statist. Probab. Lett.* **48** 335–345. MR1771495
- BONGIORNO, E. G. and GOIA, A. (2016). Some insights about the small ball probability factorization for Hilbert random elements. Preprint. Available at arXiv:1501.04308v2.
- CAREY, J. R., LIEDO, P., MÜLLER, H.-G., WANG, J.-L. and CHIOU, J.-M. (1998). Relationship of age patterns of fecundity to mortality, longevity, and lifetime reproduction in a large, cohort of Mediterranean fruit fly females. *J. Gerontol.*, Ser. A, Biol. Sci. Med. Sci. 53 B245–B251.
- CASTRO, P. E., LAWTON, W. H. and SYLVESTRE, E. A. (1986). Principal modes of variation for processes with continuous sample curves. *Technometrics* **28** 329–337.
- CHEN, K. and LEI, J. (2015). Localized functional principal component analysis. J. Amer. Statist. Assoc. 110 1266–1275. MR3420700
- CHIOU, J.-M. and LI, P.-L. (2007). Functional clustering and identifying substructures of longitudinal data. J. R. Stat. Soc. Ser. B. Stat. Methodol. 69 679–699. MR2370075
- DABO-NIANG, S. (2002). Estimation de la densité dans un espace de dimension infinie: Application aux diffusions. C. R. Math. Acad. Sci. Paris 334 213–216. MR1891061
- DAUXOIS, J., POUSSE, A. and ROMAIN, Y. (1982). Asymptotic theory for the principal component analysis of a vector random function: Some applications to statistical inference. *J. Multivariate Anal.* **12** 136–154. MR0650934
- DELAIGLE, A. and HALL, P. (2010). Defining probability density for a distribution of random functions. *Ann. Statist.* **38** 1171–1193. MR2604709
- GASSER, T., HALL, P. and PRESNELL, B. (1998). Nonparametric estimation of the mode of a distribution of random curves. *J. R. Stat. Soc. Ser. B. Stat. Methodol.* **60** 681–691. MR1649539
- GIKHMAN, I. I. and SKOROKHOD, A. V. (1969). *Introduction to the Theory of Random Processes*. W. B. Saunders Co., Philadelphia, PA. MR0247660

- GRENANDER, U. (1950). Stochastic processes and statistical inference. Ark. Mat. 1 195–277. MR0039202
- HALL, P. and HOROWITZ, J. L. (2007). Methodology and convergence rates for functional linear regression. Ann. Statist. 35 70–91. MR2332269
- HALL, P. and HOSSEINI-NASAB, M. (2006). On properties of functional principal components analysis. J. R. Stat. Soc. Ser. B. Stat. Methodol. 68 109–126. MR2212577
- HALL, P. and HOSSEINI-NASAB, M. (2009). Theory for high-order bounds in functional principal components analysis. *Math. Proc. Cambridge Philos. Soc.* **146** 225–256. MR2461880
- HALL, P., MÜLLER, H.-G. and WANG, J.-L. (2006). Properties of principal component methods for functional and longitudinal data analysis. *Ann. Statist.* **34** 1493–1517. MR2278365
- HALL, P. and VIAL, C. (2006). Assessing the finite dimensionality of functional data. J. R. Stat. Soc. Ser. B. Stat. Methodol. 68 689–705. MR2301015
- HSING, T. and EUBANK, R. (2015). Theoretical Foundations of Functional Data Analysis, with an Introduction to Linear Operators. Wiley, Chichester. MR3379106
- JACQUES, J. and PREDA, C. (2014). Model-based clustering for multivariate functional data. Comput. Statist. Data Anal. 71 92–106. MR3131956
- KNEIP, A. and UTIKAL, K. J. (2001). Inference for density families using functional principal component analysis. *J. Amer. Statist. Assoc.* **96** 519–542. MR1946423
- LEVINE, M., HUNTER, D. R. and CHAUVEAU, D. (2011). Maximum smoothed likelihood for multivariate mixtures. *Biometrika* **98** 403–416. MR2806437
- LI, Y. and GUAN, Y. (2014). Functional principal component analysis of spatiotemporal point processes with applications in disease surveillance. J. Amer. Statist. Assoc. 109 1205–1215. MR3265691
- LI, Y. and HSING, T. (2010). Uniform convergence rates for nonparametric regression and principal component analysis in functional/longitudinal data. Ann. Statist. 38 3321–3351. MR2766854
- LI, W. V. and LINDE, W. (1999). Approximation, metric entropy and small ball estimates for Gaussian measures. *Ann. Probab.* **27** 1556–1578. MR1733160
- LI, Y., WANG, N. and CARROLL, R. J. (2013). Selecting the number of principal components in functional data. *J. Amer. Statist. Assoc.* **108** 1284–1294. MR3174708
- LIU, X. and MÜLLER, H.-G. (2003). Modes and clustering for time-warped gene expression profile data. *Bioinformatics* **19** 1937–1944.
- RAMSAY, J. O. and SILVERMAN, B. W. (2005). Functional Data Analysis, 2nd ed. Springer, New York. MR2168993
- RAO, C. R. (1958). Some statistical methods for comparison of growth curves. *Biometrics* **14** 1–17. RICE, J. A. and SILVERMAN, B. W. (1991). Estimating the mean and covariance structure non-
- parametrically when the data are curves. J. R. Stat. Soc. Ser. B. Stat. Methodol. **53** 233–243. MR1094283
- SHIRYAYEV, A. N. (1984). *Probability. Graduate Texts in Mathematics* **95**. Springer, New York. MR0737192
- SILVERMAN, B. W. (1996). Smoothed functional principal components analysis by choice of norm. Ann. Statist. 24 1–24. MR1389877
- SLAETS, L., CLAESKENS, G. and HUBERT, M. (2012). Phase and amplitude-based clustering for functional data. Comput. Statist. Data Anal. 56 2360–2374. MR2897585
- SUNG, S. H. (1999). Weak law of large numbers for arrays of random variables. *Statist. Probab. Lett.* **42** 293–298. MR1688146
- VAKHANIA, N. N., TARIELADZE, V. I. and CHOBANYAN, S. A. (1987). Probability Distributions on Banach Spaces. Mathematics and Its Applications (Soviet Series) 14. D. Reidel, Dordrecht. MR1435288
- YAO, F., MÜLLER, H.-G. and WANG, J.-L. (2005). Functional data analysis for sparse longitudinal data. *J. Amer. Statist. Assoc.* **100** 577–590. MR2160561

ZHANG, X. and WANG, J.-L. (2016). From sparse to dense functional data and beyond. *Ann. Statist.* 44 2281–2321. MR3546451

Z. Lin

DEPARTMENT OF STATISTICAL SCIENCES UNIVERSITY OF TORONTO TORONTO, ONTARIO M5S 3G3

CANADA

E-MAIL: zhenhua@utstat.toronto.edu

H.-G. MÜLLER

DEPARTMENT OF STATISTICS UNIVERSITY OF CALIFORNIA, DAVIS DAVIS, CALIFORNIA 95616

USA

E-MAIL: hgmueller@ucdavis.edu

F. YAO

DEPARTMENT OF PROBABILITY AND STATISTICS SCHOOL OF MATHEMATICAL SCIENCES CENTER FOR STATISTICAL SCIENCE PEKING UNIVERSITY

**B**EIJING 10087

 $C \\ HINA$ 

AND

DEPARTMENT OF STATISTICAL SCIENCES

UNIVERSITY OF TORONTO TORONTO, ONTARIO M5S 3G3

CANADA

E-MAIL: fyao@math.pku.edu.cn