A survey of functional principal component analysis

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Abstract

Advances in data collection and storage have tremendously increased the presence of functional data, whose graphical representations are curves, images or shapes. As a new area of statistics, functional data analysis extends existing methodologies and theories from the realms of functional analysis, generalized linear model, multivariate data analysis, nonparametric statistics, regression models and many others. From both methodological and practical viewpoints, this paper provides a review of functional principal component analysis, and its use in explanatory analysis, modeling and forecasting, and classification of functional data.

Keywords: dimension reduction, explanatory analysis, functional data clustering, functional data modeling, functional data forecasting

1 Introduction

Due to recent advances in computing and the opportunity to collect and store high-dimensional data, statisticians can now study models for high-dimensional data. In many practical applications ranging from genomics to finance, analyzing high-dimensional or functional data has had a significant impact on statistical methods and thinking, changing forever the way in which we display, model and forecast high-dimensional data. In a broader term, functional data analysis (FDA) refers to the statistical analysis of data consisting of random functions, where each function is considered as a sample from a stochastic process. FDA methodology provides a new statistical approach to the analysis of independent or time series of random functions generated from one or more stochastic process(es).

Since the first edition of the book by Ramsay & Silverman (1997), FDA has become increasingly popular for analyzing high-dimensional data in the last two decades, and it has received widespread attention in the statistical community. The attention paid to FDA has contributed a rapidly increasing body of published research. In 2002, a joint summer research conference on "Emerging Issues in Longitudinal Analysis" provided a platform for emerging ideas from longitudinal data analysis and FDA. Based on that conference, *Statistics Sinica* published a special issue (vol 14, issue 3) in 2004, which dealt exclusively with the close connection between longitudinal and functional data, along with two review articles by Rice (2004) and Davidian et al. (2004). In 2007, *Computational Statistics & Data Analysis* published a special issue (vol 51, issue 10) on FDA, along with a review article by González-Manteiga & Vieu (2007). *Computational Statistics* also published a special issue (vol 22, issue 3) on modeling functional data, along with a review article by Valderrama (2007). In 2008, a workshop on "Functional and Operatorial Statistics" at Université Paul Sabatier in Toulouse provided a platform for emerging ideas from FDA and operatorial statistics. Based on that conference, the *Journal of Multivariate Analysis* published a special issue (vol 101, issue 2), which drew a close connection between FDA and nonparametric function estimation.

Despite the close connection among FDA, multivariate data analysis and longitudinal data analysis, FDA is unique in its own right. Different from multivariate data analysis, FDA can extract additional information contained in the smooth functions and their derivatives, not normally available through multivariate and longitudinal data analysis methods. For example, Ramsay (2000) used a differential equation to model some exceedingly complex handwriting data. Mas & Pumo (2009) considered a functional linear regression, where the covariates are functions and their first derivative. Through a well-known spectroscopy data set, they demonstrated that the functional linear regression with first derivative gives a more accurate prediction than the one without derivative. Moreover, Mas & Pumo (2007) extended the functional autoregressive of order 1 by adding the first derivative as an additional covariate. Apart from the ability of capturing underlying dynamics through derivatives, FDA is unique in the types of data design. Similar to longitudinal data analysis, FDA is able to analyze data observed at a set of sparse grid points with noise (James & Hastie 2001, Yao et al. 2005*a*). Different from longitudinal data analysis, FDA can also analyze functions observed with or without noise at an arbitrarily dense grid.

However, despite the fast development in theoretical and practical aspects of functional data analysis, there are only few survey papers on functional data analysis and its techniques. A notable exception is the survey paper of Geenens (2011), who provided a detailed overview on nonparametric functional regression and its relationship with the so-called "curse of dimensionality" (Bellman 1961). Another notable exception is a recent review paper by Hall (2011), who provided a detailed overview on the roles of FPCA in functional linear regression and density estimation for functional data. Differing from Hall (2011), this survey paper aims to describe the roles of FPCA in functional data exploratory analysis, modeling and forecasting functional data, and classification of functional data.

This paper consists of six sections, and revisits the research on FPCA undertaken, mainly in statistics. Section 2 provides the methodological background of FPCA. In Section 3, we review FPCA for explanatory analysis. Section 4 revisits FPCA for modeling and forecasting functional data. In Section 5, we review FPCA for clustering functional data. A conclusion is presented in Section 6.

2 Functional principal component analysis (FPCA)

2.1 Some literature

The advances of FPCA date back to the early 1940s when Karhunen (1946) and Loève (1946) independently developed a theory on the optimal series expansion of a continuous stochastic process, and extended eigenanalysis from a symmetric matrix to integral operators with symmetric kernels. Later, Rao (1958) and Tucker (1958) provided applications of the Karhunen-Loève (KL) expansion to functional data, by applying multivariate PCA to observed function values. They also include an outlook for statistical inference including functional data. Important asymptotic properties of FPCA estimators for the infinite-dimensional case were studied by Dauxois et al. (1982) for a vector of random functions. Since then, many theoretical development of FPCA came from the linear operator viewpoint, including the work by Besse (1992), Cardot et al. (1999), Cardot et al. (2007), Ferraty & Vieu (2006), Mas (2002), Mas (2008), Bosq (2000), among many others. In contrast to the linear operator viewpoint, practical motivations led to more recent work which view FPCA from the kernel aspect, see for example, Yao et al. (2005*b*), Hall & Horowitz (2007), Hall & Hosseini-Nasab (2006), Hall & Vial (2006), Hall et al. (2006), and Shen (2009). This viewpoint is advantage in certain applications, for instance, in the calculation of the kernel operator or incorporating local smoothing ideas such as those used in Hall et al. (2006), Yao et al. (2005*b*) and Horváth & Kokoszka (2012).

Some extensions and modifications of FPCA have been put forward in statistical literature. These include

(1) smoothed FPCA: As pointed out by Ramsay & Silverman (2005), principal component analysis (PCA) of functional data is more appealing if some type of smoothness is incorporated into the principal components themselves. In statistical literature, there are at least two ways of performing smoothed FPCA. The first is to smooth the functional data before applying FPCA (Ramsay & Dalzell 1991, Foutz & Jank 2010). The second is to directly define smoothed principal components by adding a roughness penalty term to the sample covariance and maximizing the sample covariance (Pezzulli & Silverman 1993, Silverman 1996).

(2) robust FPCA: A serious drawback to the estimators of principal components is their sensitivity to outliers. Locantore et al. (1999) proposed robust estimators for the principal components by adapting a bounded influence approach. Gervini (2008) proposed a fully functional robust estimators which are functional versions of the multivariate median and spherical principal components (see also Locantore et al. 1999). Hyndman & Ullah (2007) proposed a robust estimator based on a robust projection-pursuit approach to forecast age-specific mortality and fertility rates observed over time. The asymptotic properties of a robust projection-pursuit approach were studied by Bali et al. (2011). As an alternative to the robust estimators of mean function and principal components, we can identify and remove outliers. Following this idea, Fraiman & Muniz (2001) proposed the trimmed means using the notion of functional depth. Subsequently, Cuevas et al. (2007), López-Pintado & Romo (2007, 2009), Cuevas & Fraiman (2009), Cuesta-Albertos & Nieto-Reyes (2010) and Gervini (2012) also proposed a series of depth-based estimators.

(3) sparse FPCA: When there are only a few and much irregularly spaced data points, the estimation of FPCA must be adjusted (Castro et al. 1986). Rice & Wu (2001) proposed the use of mixed effects model to estimate functional principal components. These models address the sparsity issue, where each functional data denoted by X_i can be estimated by all functions not only the ith function. However, the high-dimensional variance-covariance matrix of the random vectors may be numerically unstable, which may lead to ill-posed problems. James et al. (2000) and James &

Sugar (2003) proposed the reduced rank model that avoids the potential ill-posed problems from the mixed effects model. Zhou et al. (2008) extended the reduced rank model to two-dimensional sparse principal component model via a penalized estimation and splines. Kayano & Konishi (2010) extended the reduced rank model to multidimensional sparse functional data. In a different approach, Yao et al. (2005*a*) proposed a FPCA through conditional expectation to solve the issue of sparse and irregular functional data, provided that the number of subjects increases and the pooled time points from the entire sample become dense in the domain of the data.

(4) common FPCA: For a group of functional data samples, Benko et al. (2009) proposed common functional principal component estimation and presented a bootstrap test for examining the equality of the eigenvalues, eigenfunctions and mean functions of two functional data samples. Boente et al. (2010) studied statistical inference under common functional principal components. While Coffey et al. (2011) applied the idea of common functional principal components to the study of human movement, Fengler et al. (2003) and Benko & Härdle (2005) applied the common functional principal component to model implied volatility surface dynamics.

(5) multilevel FPCA: FPCA is commonly applied to functional data generated from one stochastic process. However, sometimes we observe functional data generated from at least two stochastic processes, for example, a patient's health status is monitoring by his/her intraday blood pressure and heart beat over a time period. In such a case, Di et al. (2009) introduced multilevel FPCA, which is designed to extract the intra- and inter-subject geometric components of multilevel functional data. Crainiceanu et al. (2009) extended the idea of multilevel FPCA to functional regression, while Zipunnikov et al. (2011) proposed fast and scalable multilevel FPCA for analyzing hundreds and thousands brain images scanned using Magnetic Resonance Imaging.

2.2 Methodology

PCA was one of the first multivariate data analysis methods to be adapted to functional data (Dauxois et al. 1982). The main idea of this extension is simply to replace vectors by functions, matrices by compact linear operators, covariance matrices by covariance operators, and scalar products in vector space by scalar products in L^2 space. Below we state some notations and definitions used in this paper.

1) (Ω, A, P): a probability space with sigma operator A and measure P.

2) $L^2_{\mathcal{I}}$: the space of square-integrable functions on the compact set $\mathcal{I}$, $f : \mathcal{I} \rightarrow R, (\int_{\mathcal{I}} f^2)^{1/2} < \infty$. This space is a separable Hilbert space, with inner product $< f, g >= \int_{\mathcal{I}} fg$ and norm $\|f\|^2 = (\int_{\mathcal{I}} f^2)^{1/2}$.

3) H: a separable Hilbert space endowed with inner product and associated norm.

4) Let H^* denote the dual space of H, consisting of all continuous linear functionals from H into the field of real or complex number. If x is an element of H, then the function ψ_x, defined by

$$\psi_x(y) =< y, x >, \qquad \forall y \in H, \tag{1}$$

is an element of H^*. The Riesz representation theorem states that every element of H^* can be expressed uniquely by (1) (see Akhiezer & Glazman 1981, pp.61-63 for its proof).

2.2.1 FPCA from the kernel viewpoint

Let X be a random variable $X : \Omega \rightarrow L^2(\mathcal{I})$, such that $X \in L^2(\Omega)$. X can also be seen as a stochastic process defined on a compact set $\mathcal{I}$, with finite variance $\int_{\mathcal{I}} \mathrm{E}(X^2) < \infty$. Let μ be the mean function of X, without lose of generality, let $X^c = X - \mu$ be a centered stochastic process. In what follows, we state without proof the underlying concepts of FPCA. For detailed proofs, readers can refer to Tran (2008) and above references on theoretical development of FPCA.

Definition 1 (Covariance Operator) *The covariance function of X is defined to be the function $K : \mathcal{I} \times \mathcal{I} \rightarrow R$, such that*

$$\begin{aligned} K(u, v) &= Cov(X(\mu), X(v)) \\ &= E\{[X(\mu) - \mu(\mu)][X(v) - \mu(v)]\}. \end{aligned}$$

By assuming X is a continuous and square-integrable covariance function, the function K

induces the kernel operator $L^2(\mathcal{I}) \to L^2(\mathcal{I}), \phi \to K\phi$, given by

$$(K\phi)(\mu) = \int_{\mathcal{I}} K(u, v)\phi(v)dv.$$

Lemma 1 (Mercer's Lemma) *Assume that K is continuous over $\mathcal{I}^2$, there exists an orthonormal sequence (ϕ_k) of continuous function in $L^2(\mathcal{I})$ and a non-increasing sequence (λ_k) of positive numbers, such that*

$$K(u, v) = \sum_{k=1}^{\infty} \lambda_k \phi_k(u)\phi_k(v), \quad u, v \in \mathcal{I}.$$

Theorem 1 (Karhunen-Loève expansion) *With Mercer's Lemma, a stochastic process X can be expressed as*

$$X(u) = \mu(u) + \sum_{k=1}^{\infty} \sqrt{\lambda_k}\xi_k\phi_k(u), \tag{2}$$

where $\xi_k = 1/\sqrt{\lambda_k}\int_{\mathcal{I}} X^c(v)\phi_k(v)dv$ is an uncorrelated random variable with zero mean and unit variance. It is noteworthy that the equality in (2) generally holds in quadratic mean (for random variables in Hilbert space) and almost surely for Gaussian random variables. The principal component scores $\beta_k = \sqrt{\lambda_k}\xi_k$ are given by the projection of X^c in the direction of the kth eigenfunction ϕ_k, i.e., $\beta_k =< X^c, \phi_k >$. The scores constitute an uncorrelated sequence of random variables with zero mean and variance λ_k. They can be interpreted as the weights of the contribution of the functional principal components ϕ_k to X.

2.2.2 FPCA from the linear operator viewpoint

The theoretical covariance operator Γ and its empirical counterpart $\widehat{\Gamma}$, based on the independent and identically distributed samples $X_1, \ldots, X_n$ are symmetric positive trace class operators from H to H defined by

$$\Gamma = \mathrm{E}[(X_1 - \mathrm{E}X_1) \otimes (X_1 - \mathrm{E}X_1)],$$
$$\widehat{\Gamma} = \frac{1}{n}\sum_{s=1}^{n}(X_s - \overline{X}_n) \otimes (X_s - \overline{X}_n),$$

where $\overline{X}_n = \frac{1}{n}\sum_{s=1}^{n} X_s$ and $\otimes$ represents the tensor product. The tensor product of two vector spaces $\boldsymbol{U}$ and $\boldsymbol{V}$, denoted by $\boldsymbol{U} \otimes \boldsymbol{V}$, is a way of creating a new vector space similar to multiplication of integer. For example,

$$\boldsymbol{U} \otimes \boldsymbol{V} = \begin{pmatrix} u_{1,1}\boldsymbol{V} & u_{1,2}\boldsymbol{V} & \cdots \\ u_{2,1}\boldsymbol{V} & u_{2,2}\boldsymbol{V} & \cdots \\ \vdots & \cdots & \ddots \end{pmatrix}.$$

Theorem 2 (Riesz representation theorem) *Since $L^2(\mathcal{I})$ is a Hilbert space, by the Riesz representation theorem, the covariance operator can be viewed as*

$$\Gamma_X : L^2(\mathcal{I}) \to L^2(\mathcal{I}), \qquad \Gamma_X(t) = E[< X^c, t > X^c], \quad t \in L^2(\mathcal{I}).$$

Tran (2008) showed the equivalent relationship between covariance operator K and linear operator Γ. Furthermore, the covariance operator Γ is a linear, self-adjoint, positive semidefinite operator (Weidmann 1980, p.166).

Theorem 3 (Spectral theorem) *Let T be a compact self-adjoint bounded linear operator on a separable Hilbert space H. There exists a sequence of real eigenvalues of T: $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq 0$. Let Π_k be the orthogonal projections onto the kth eigenspace, and*

$$T = \sum_{k=1}^{\infty} \lambda_k \Pi_k.$$

Remark 1 *A number of properties associated with the FPCA is listed below.*

(a) FPCA minimizes the mean integrated squared error of the reconstruction error function over the whole functional data set. This is given by

$$\begin{aligned} &E\int_{\mathcal{I}} \Big[X^c(t) - \sum_{k=1}^{K} < X^c, \phi_k > \phi_k(t)\Big]^2 dt \\ =&E\int_{\mathcal{I}} \Big[X^c(t) - \sum_{k=1}^{K} \beta_k \phi_k(t)\Big]^2 dt, \qquad K < \infty. \end{aligned}$$

(b) *FPCA provides a way of extracting a large amount of variance.*

$$Var[X^c(t)] = \sum_{k=1}^{\infty} Var(\beta_k)\phi_k^2(t) = \sum_{k=1}^{\infty} \lambda_k \phi_k^2(t),$$

where $\lambda_1 \geq \lambda_2, \dots, \geq 0$ *is a decreasing sequence of eigenvalues and* $\phi_k(t)$ *is orthonormal. The cumulative percentage of the overall variation explained by the first* K *components is given by the ratio* $\sum_{k=1}^{K} \lambda_k / \sum_{k=1}^{\infty} \lambda_k$*. Based on the ratio, the optimal number of components can be determined by passing a certain threshold level.*

(c) *The principal component scores are uncorrelated, that is* $cov(\beta_i, \beta_j) =< \Gamma\phi_i, \phi_j >= \lambda_i \delta_{ij}$*, where* $\delta_{ij} = 1$ *if* $i = j$ *and 0 otherwise.*

Because the centered stochastic process X^c is unknown in practice, the population eigenvalues and eigenfunctions can only be approximated through realizations of $\{X_1(t), X_2(t), \dots, X_n(t)\}$. The sample mean and sample covariance are given by

$$\bar{X}(t) = \frac{1}{n}\sum_{s=1}^{n} X_s(t),$$
$$\widehat{\Delta}(t) = \sum_{k=1}^{\infty} \widehat{\lambda}_k \widehat{\phi}_k(t)\widehat{\phi}_k(t),$$

where $\widehat{\lambda}_1 > \widehat{\lambda}_2 > \cdots \geq 0$ are the sample eigenvalues of $\widehat{\Delta}(t)$, and $\widehat{\phi}_1(t), \widehat{\phi}_2(t), \dots$ are the corresponding orthogonal sample eigenfunctions. Dauxois et al. (1982), Yao et al. (2005*b*, Section 3), Hall & Hosseini-Nasab (2006) and Poskitt & Sengarapillai (2013, Lemmas 1-3) showed that $\bar{X}$ is a uniformly consistent estimate of μ; $\widehat{\lambda}_k$ provides a uniformly consistent estimate of λ_k; and $\widehat{\phi}_k$ provides a uniformly consistent estimate of ϕ_k.

2.3 Computation

In order to compute functional principal components and their scores, there exist at least three computation approaches. These include

(a) Discretization: FPCA is carried out in a similar fashion as PCA, except that it is necessary to renormalize the eigenvectors and interpolate them with a suitable smoother (Rao 1958). This discretization approach was the earliest method to compute functional principal components.

(b) Basis function expansion: The second approach involves expressing a stochastic process as a linear combination of basis functions, that is $X^c(t) = \sum_{k=1}^{\infty} \beta_k \phi_k(t)$. The advantage of the basis function expansion over the previous discretization approach is that the smoothness of $\phi_k(t)$ can be imposed by the roughness penalty approaches (see for example Rice & Silverman 1991, Pezzulli & Silverman 1993, Silverman 1996, Aguilera et al. 1996, Yao & Lee 2006). Among all possible basis functions, the widely used ones are polynomial basis functions (which are constructed from the monomials $\phi_k(t) = t^{k-1}$), Bernstein polynomial basis functions (which are constructed from $1, 1-t, t, (1-t)^2, 2t(1-t), t^2, \dots$), Fourier basis functions (which are constructed from $1, \sin(wt), \cos(wt), \sin(2wt), \cos(2wt), \dots$), radial basis functions, wavelet basis functions, and orthogonal basis functions (such as the functional principal components).

(c) Numerical approximation: To address the problem of unequally spaced functional data, this approach consists in approximating functional principal components by quadrature rules (see for example, Castro et al. 1986). Furthermore, Castro et al. (1986) studied the computational issue of functional principal components, and emphasized that the multivariate PCA fails to explicitly incorporate information about the spacing of the observation points.

3 FPCA in explanatory analysis

To motivate the discussion, Figure 1 shows annual smoothed age-specific log mortality curves for French males between 1816 and 2009. The data were taken from the Human Mortality Database (2012). The age-specific mortality rates are the ratios of death counts to population exposure in the relevant year for a given age.

The observed log mortality rates were smoothed using penalized splines with the partial monotonic constraint, as described in Ramsay (1988) and Hyndman & Ullah (2007). It is assumed that there is an underlying continuous and smooth function $f_s(t)$ that is observed with error at discrete ages. Then, we can express

$$X_s(t_i) = f_s(t_i) + \sigma_s(t_i)\varepsilon_{s,i}, \quad i = 1, 2, \dots, p, \quad s = 1, 2, \dots, n, \tag{3}$$

where $X_s(t_i)$ denotes the log of observed mortality rates for age t_i at year s; $\sigma_s(t_i)$ allows the amount of noise to vary with t_i in year s; and $\varepsilon_{s,i}$ is an independent and identically distributed standard normal random variable.

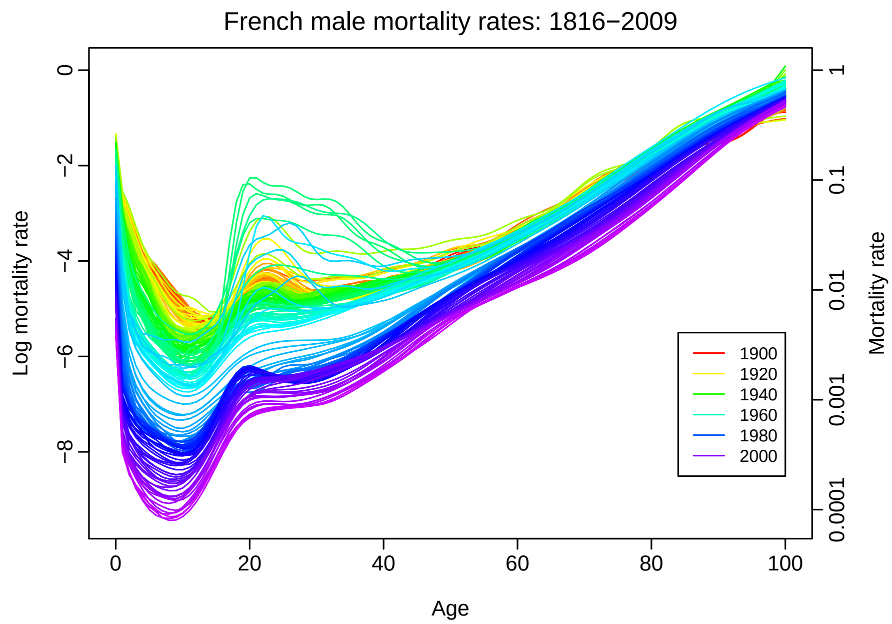


Figure 1: French male age-specific log mortality rates (1816-2009). The oldest years are shown in red, with the most recent years in violet. Curves are ordered chronologically according to the colors of the rainbow. The left vertical axis measures log mortality rates, whereas the right vertical axis adds non-log units to ease interpretation. Log mortality rates dip in early childhood, climb in the teen years, stablize in the early 20s, and then steadily increase with age. Some years exhibit sharp increases in the mortality rates between the late teens and early 20s.

As can be seen from Figure 1, log mortality rates dip in early childhood, climb in the teen years, stablize in the early 20s, and then steadily increase with age. Some years exhibit sharp increases in mortality rates between the late teens and early 20s. Some of the mortality curves shown in yellow and green indicate sudden increases to mortality rates between the ages of 20 and 40 for a number of years.

Using FPCA, we decompose a set of smoothed functions $\{f_1(t), \dots, f_n(t)\}$ into a set of functional principal components and principal component scores presented in Figure 2. Let $\phi_k(t)$ represent the kth functional principal component (also known as basis function), and let $\beta_{s,k}$ denote the principal component scores (also known as basis function coefficient) for the kth component at the sth observation. Much of the information inherent in the original data is captured by the first few functional principal components and their associated scores (Jones & Rice 1992, Sood et al. 2009, Hyndman & Shang 2010). Thus, we will take the first two score vectors $(\beta_{1,1}, \dots, \beta_{n,1})$ and $(\beta_{1,2}, \dots, \beta_{n,2})$, and consider methods of bivariate depth and bivariate density that could be applied to these vectors. For simplicity, we denote the bivariate point $(\beta_{s,1}, \beta_{s,2})$ as $\boldsymbol{z}_s$.

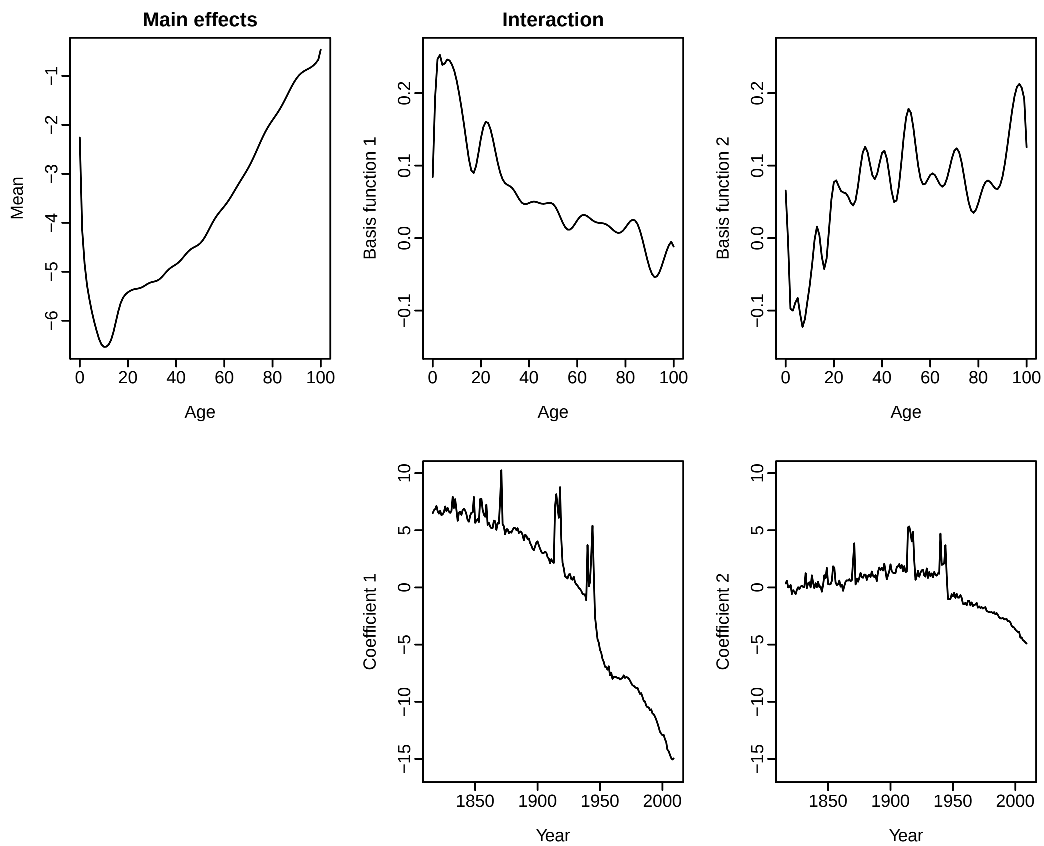
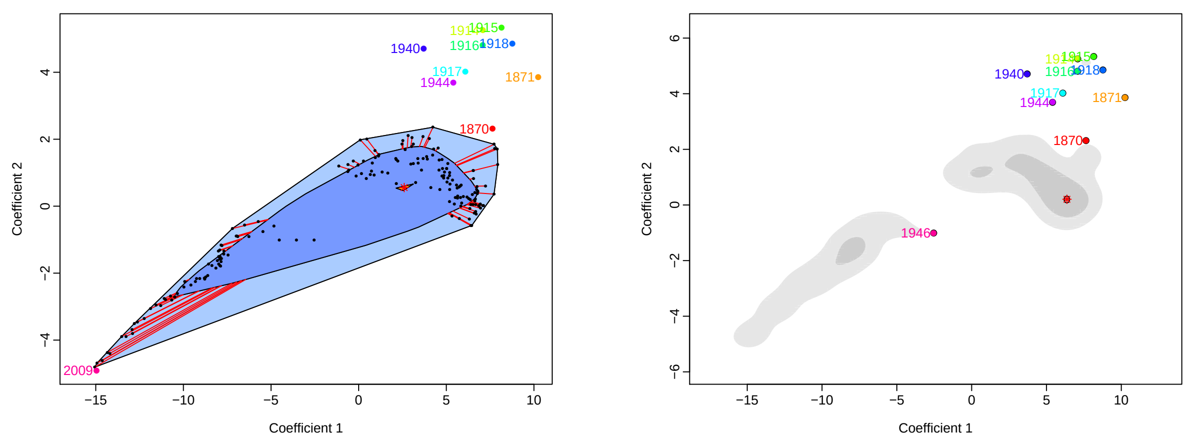


Figure 2: Functional principal component decomposition. The first two functional principal components and their associated scores for the French male log mortality rates between ages 0 and 100 for years from 1816 to 2009.

The bivariate scores can be ordered by using Tukey's halfspace location depth (Tukey 1975). The observations can be ordered by the distances $o_s = d(\boldsymbol{z}_s, \boldsymbol{Z})$ in an increasing order, where $\boldsymbol{Z} = \{\boldsymbol{z}_s; s = 1, \dots, n\}$. The first observation by this ordering can be considered as the median, whereas the last observation can be considered as the outermost observation. This leads to the development of bivariate bagplot of Rousseeuw et al. (1999). Similar to a univariate boxplot, the bivariate bagplot has a central point (the Tukey median), an inner region (the "bag"), and an outer region (the "fence"), beyond which outliers are shown as individual points. As shown in Figure 3a, the bag is defined as the smallest depth region containing at least 50% of the total number of observations. The outer region of the bagplot is the convex hull of the points containing the region obtained by inflating the bag by a factor of ρ. When the projected bivariate principal component scores follow a standard bivariate normal distribution, $\rho = 1.96$ indicates that 95% of the observations are in the fence.



(a) Bivariate bagplot. The dark and light blue regions show the bag and fence regions. The red asterisk denotes the Tukey median. The points outside the fence region are outliers.

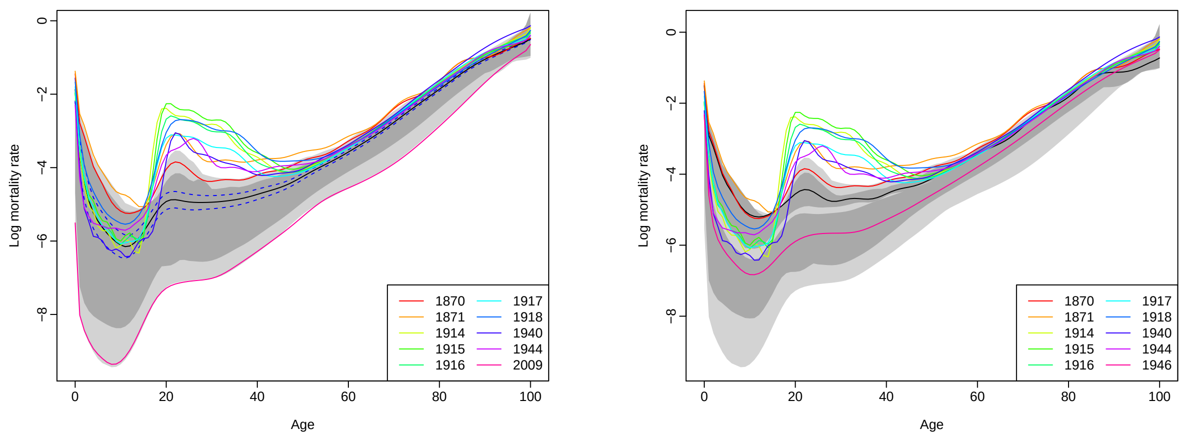
(b) Bivariate HDR boxplot. The dark and light gray regions show the 50% HDR and 95% HDR. The red asterisk is the mode. The points outside the outer HDR are outliers.

Figure 3: Bivariate data display based on the first two principal component scores.

Another way to order the points is by the value of a bivariate kernel density estimate (Scott 1992) at each observation. Let $o_s = \widehat{f}(\boldsymbol{z}_s)$, where $\widehat{f}(\boldsymbol{z})$ is a bivariate kernel density estimate calculated from all of the bivariate principal component scores. The functional data can then be ordered by values of o_s in a decreasing order. So the observation with the highest density is the first observation (also known as the mode), and the last observation has the lowest density value, considered as the outermost observation. This leads to the development of bivariate highest density region (HDR) boxplot (Hyndman 1996). As shown in Figure 3b, the bivariate HDR boxplot displays the mode, defined as $\arg\sup \widehat{f}(\boldsymbol{z})$, along with the 50% inner and customarily 95% outer highest density regions.

The functional bagplot and functional HDR boxplot are mappings of the bagplot and HDR boxplot of the first two principal component scores to the functional curves. As shown in Figure 4, the functional bagplot displays the median curve, the inner and outer regions.

The inner and outer regions are defined as the region bounded by all curves corresponding to the points in the bivariate bag and bivariate fence regions. The functional HDR boxplot displays the modal curve, and the inner and outer regions. The inner region is defined as the region bounded by all curves corresponding to points inside the 50% bivariate HDR. The outer region is similarly defined as the region bounded by all curves corresponding to the points within the outer bivariate HDR.



(a) Functional bagplot. The black line is the median curve, surrounded by 95% pointwise confidence intervals. The curves outside the fence region are shown as outliers of different colors.

(b) Functional HDR boxplot. The black line is the modal curve. The curves outside the outer HDR are shown as outliers of different colors.

Figure 4: Functional data display based on the first two principal component scores.

As illustrated by the French male log mortality rates, FPCA plays an essential role in exploratory analysis of functional data, and it can be used to extract possible non-linear features in the data. In this example, it reduces infinite-dimensional functional curves to finite-dimensions. Based on the bivariate principal component scores, we can rank the bivariate scores by depth and density, match the depth and density indexes back to the corresponding functional curves. This allows us to obtain a ranking of functional data, from which outliers can be detected.

4 FPCA in modeling and forecasting

As a powerful dimension reduction tool (as shown in Section 3), FPCA has been extensively used to regularize ill-conditioned estimators in functional regression models (see for example, Reiss & Ogden 2007). A characteristic of functional regression model typically consists of functional predictors and/or responses, where the functional objects are realizations of a stochastic process. For instance, Foutz & Jank (2010) utilized FPCA to decompose investment curves into shapes that capture features such as "longevity" or "sudden change", and used these quantitative characterizations in a forecasting model, and they showed that their data-driven characterizations via FPCA lead to significant improvements in terms of forecast accuracy compared to a parametric model with polynomial features. Similarly, Jank & Yahav (2010) used FPCA to extract features of online auction networks. For more details on functional regression, see Ramsay & Silverman (2002, 2005) for a collection of parametric functional regression models, and Ferraty & Vieu (2006) for a range of nonparametric functional regression models. Some recent advances in the field are collected in Ferraty & Romain (2011).

Among all possible functional regression models, the functional linear regression model is a commonly used parametric tool for investigating the relationship between the predictors and responses, where at least one variable is functional in nature. Numerous examples of using functional linear regression models can be found in a various range of fields, such as atmospheric radiation (Hlubinka & Prchal 2007), chemometrics (Yao & Müller 2010), climate variation forecasting (Shang & Hyndman 2011), demographic forecasting (Hyndman & Shang 2009), gene expression (Yao et al. 2005*a*), health science (Harezlak et al. 2007), linguistic (Hastie et al. 1995, Aston et al. 2010), medical research (Yao et al. 2005*b*), and many others.

Apart from the functional linear regression models, there exist other regression models for analyzing the relationship between predictor and response variables, where at least one of them is functional. Some popular functional regression models include:

1) generalized functional linear models, where the response is scalar and predictor is function (see for example, Cardot et al. 1999, Cardot, Ferraty, Mas & Sarda 2003, James 2002, James & Silverman 2005, Müller & Stadtmüller 2005, Reiss & Ogden 2007, Krämer et al. 2008, Araki et al. 2009).

2) functional quadratic regression models, where the response is scalar and predictor is function (see for example, Yao & Müller 2010, Horváth & Reeder 2011).

3) functional additive models, where the response is scalar and predictor is function (see

for example, Müller & Yao 2008, 2010, Febrero-Bande & González-Manteiga 2011, Ferraty et al. 2011, Fan & James 2013).

4) functional mixture regression models, where the response is scalar and predictor is function (see for example, Yao et al. 2011)

5) functional regression models, where both predictor and response are functions (see for example, Ramsay & Dalzell 1991, Cardot et al. 1999, Cuevas et al. 2002, Cardot, Faivre & Goulard 2003, Chiou & Müller 2009).

6) functional response models, where the response is function and predictor is multivariate (see for example, Faraway 1997, Chiou, Müller & Wang 2003, Chiou, Müller, Wang & Carey 2003, Chiou et al. 2004).

7) functional multivariate regression models, where the response is multivariate and predictor is function (see for example, Matsui et al. 2008).

Regardless of the type of functional regression model, there are two difficulties in using them for analyzing the relationship between predictor and response variables. These are the inverse problem of covariance structure and the so-called "curse of dimensionality" (Bellman 1961), arising from the sparsity of data in high-dimensional space. While the inverse problem of covariance structure can lead to numerically unstable estimates of regression coefficients, the "curse of dimensionality" problem is troublesome in nonparametric statistics for which the asymptotic behavior of the estimates decays exponentially with the increasing number of explanatory variables (Aneiros-Pérez & Vieu 2008).

As pointed out by James & Sugar (2003), there are two general strategies for overcoming these problems, namely regularization and dimension reduction. Regularization can be implemented in various ways, such as a ridge estimator (Hoerl 1962), a smoothing spline estimator (Wahba 1990), a penalized regression spline estimator (Eilers & Marx 1996), and a penalized least squares estimator (Green & Silverman 1994), to name only a few. The aim of regularization is to stablize the singular covariance structure, and obtain accurate estimates of the regression coefficients. By contrast, dimension reduction techniques, such as the functional principal component regression (Reiss & Ogden 2007), and functional partial least squares (Preda & Saporta 2005), reduce the dimensionality of the data to a few latent components, in order to effectively summarize the main features of the data.

In this section, I adopt the second approach and revisit the use of FPCA for modeling a time series of curves. To motivate the discussion, I revisit the French male log mortality rates described in Section 3. Using FPCA, a time series of smoothed curves is decomposed into a set of functional principal components and their associated principal component scores. This is given by

$$f_s(t) = a(t) + \sum_{k=1}^{K} \beta_{s,k}\phi_k(t) + e_s(t), \qquad s = 1, 2, \dots, n, \tag{4}$$

where $a(t)$ is the mean function estimated by $\widehat{a}(t) = \frac{1}{n}\sum_{s=1}^{n} f_s(t)$; $\{\phi_1(t), \dots, \phi_K(t)\}$ is a set of the first K functional principal components; $\{\beta_{s,1}, \dots, \beta_{s,K}\}$ is a set of uncorrelated principal component scores for year s; $e_s(t)$ is the residual function with mean zero, and $K < n$ is the number of functional principal components used. There are numerous ways of determining the optimal number of K, such as the bootstrap approach proposed by Hall & Vial (2006) and Bathia et al. (2010), description length approach proposed by Poskitt & Sengarapillai (2013), pseudo-AIC (Shibata 1981), scree plot (Cattell 1966), and eigenvector variability plot (Tu et al. 2009).

By conditioning on the past curves $\boldsymbol{\mathcal{I}} = \{X_1(t), \dots, X_n(t)\}$ and the fixed functional principal components $\boldsymbol{\mathcal{B}} = \{\phi_1(t), \dots, \phi_K(t)\}$, the h-step-ahead forecast of $X_{n+h}(t)$ can be obtained by

$$\widehat{X}_{n+h|n}(t) = \mathrm{E}[X_{n+h}(t)|\boldsymbol{\mathcal{I}}, \boldsymbol{\mathcal{B}}] = \widehat{a}(t) + \sum_{k=1}^{K} \widehat{\beta}_{n+h|n,k}\phi_k(t), \tag{5}$$

where $\widehat{\beta}_{n+h|n,k}$ denotes the h-step-ahead forecast of $\beta_{n+h,k}$ using a univariate time series, such as exponential smoothing (Hyndman et al. 2008).

While (5) produces the point forecasts, it is also important to construct prediction intervals in order to assess model uncertainty. The forecast variance follow from (4). Due to the orthogonality between functional principal components and the error term, the overall forecast variance can be approximated by the sum of four variances. By conditioning on $\boldsymbol{\mathcal{I}}$ and $\boldsymbol{\mathcal{B}}$, the overall forecast variance is obtained by

$$\mathrm{Var}[X_{n+h}(t)|\boldsymbol{\mathcal{I}}, \boldsymbol{\mathcal{B}}] \approx \widehat{\sigma}_a^2(t) + \sum_{k=1}^{K} u_{n+h|n,k}\phi_k^2(t) + v(t) + \sigma_{n+h}^2(t), \tag{6}$$

where $\phi_k^2(t)$ is the variance of the kth functional principal component; $u_{n+h|n,k}$ is the variance of the kth principal component scores; $v(t)$ is the variance of the model error; the variance of the mean function $\widehat{\sigma}_a^2(t)$ and the observational error variance $\sigma_{n+h}^2(t)$ are estimated from (3) (Hyndman & Ullah 2007). The $100(1-\alpha)\%$ pointwise prediction interval of $X_{n+h}(t)$ is given by

$$\widehat{X}_{n+h|n}(t) \pm z_\alpha \sqrt{\text{Var}[X_{n+h}(t)|\boldsymbol{\mathcal{I}}, \boldsymbol{\mathcal{B}}]},$$

where z_α is the $(1-\alpha/2)$ standard normal quantile.

As a demonstration, Figure 5 plots the one-step-ahead point forecast and 80% pointwise prediction interval for the age-specific French male log mortality rates in 2010. While the past data used for estimation are shown in gray, the point forecast is shown in solid black line along with the 80% pointwise prediction interval shown in dotted red lines.

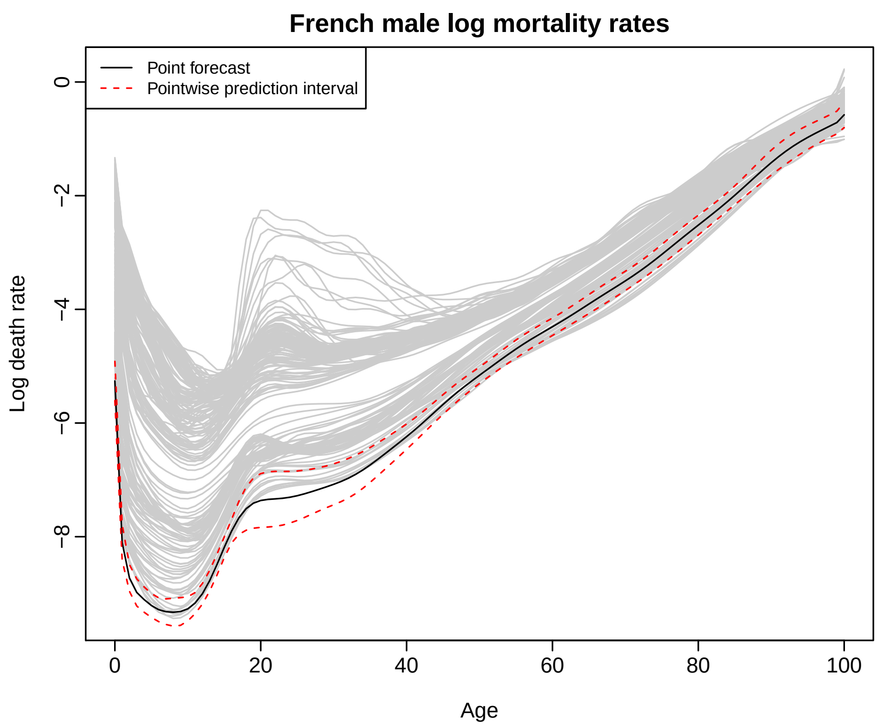


Figure 5: One-step-ahead point forecast and 80% pointwise prediction interval for the age-specific French male log mortality rates in 2010. The past observed data are shown in gray, the point forecast is shown in solid black line, along with the 80% pointwise prediction interval shown in dotted red lines.

As illustrated by the French male log mortality rates, FPCA plays an important role in reducing dimensionality of functional data. Without losing much information, FPCA allows us to model underlying features of functional data. Based on the forecasted principal component scores, point and interval forecasts can be obtained with fixed functional principal components and mean function.

5 FPCA in classification

As pointed out by Delaigle et al. (2012), problems of functional data clustering are hindered by difficulties associated with the intrinsic infinite dimension of functions. For the parametric classifiers, the difficulty lies in inverting the covariance operator. For the nonparametric classifiers, the difficulty is caused by the so-called "curse of dimensionality" (Bellman 1961) which creates problems with data analysis (Aggarwal et al. 2001). These difficulties motivated methods for dimension reduction.

In supervised functional data clustering, classifiers are constructed from the functional curves and their correct membership labels. In unsupervised functional data clustering, classifiers are constructed solely from the functional curves. The objective is to obtain a rule for a sample to classify a new curve by estimating its membership label. In the literature, dimension reduction is often performed by projecting functional data onto a set of lower-dimension basis functions, such as principal component basis functions (see for example, Hall et al. 2001, Glendinning & Herbert 2003, Huang & Zheng 2006, Song et al. 2008) or partial least squares basis functions (see for example, Preda et al. 2007, Delaigle & Hall 2012). The reduced space of functions spanned by a few eigenfunctions are thought of as a space, where most of the features of the functional data are constructed (Lee 2004). Cluster analysis is then performed on the first few principal component scores (see for example, Illian et al. 2009, Suyundykov et al. 2010). This two-step procedure is sometimes called tandem analysis by Arabie & Hubert (1994).

Apart from the two-step tandem clustering procedure, Hall et al. (2001) proposed a nonparametric procedure for signal discriminant, where dimension reduction is obtained by using the FPCA of covariance function, and then a new observation is assigned to the signal type with the highest posterior probability. Müller & Stadtmüller (2005) proposed a parametric procedure, and they used the FPCA to reduce dimensionality, prior to applying the machinery of the generalized linear model with logit link function. Bouveyron & Jacques (2011) developed the model-based clustering method of functional data to find cluster-specific functional subspaces. Tarpey (2007) developed a model-based clustering method using the K-means algorithm with canonical discriminant function, while Yamamoto (2012) also proposed a K-means criterion for functional data and seeks the subspace that is maximally informative about the clustering structure in the data. Furthermore, Rossi et al. (2004) proposed to classify functional data with self-organizing maps algorithm.

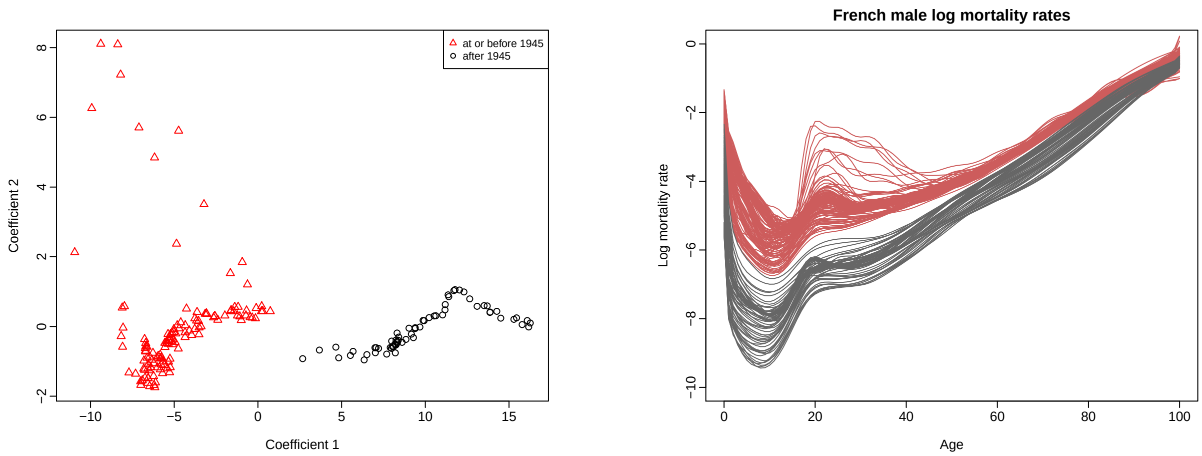
In this section, we present a simple demonstration on the use of tandem analysis for clustering a time series of functional curves. Although a more sophisticated algorithm can be used, I find that the tandem analysis performs well on the data considered. To motivate the discussion, I again revisit the French male log mortality rates described in Section 3. Using FPCA, a time series of functions is first decomposed into a set of functional principal components and their associated principal component scores. The principal component scores are considered as the surrogates of functional curves (see also Jones & Rice 1992, Sood et al. 2009), so that we can apply a multivariate clustering algorithm to the first two principal component scores, in order to reveal homogeneous subgroup of entities in a functional data set. Among all possible clustering algorithms, we consider the K-means algorithm because of its intuitive (see Hartigan & Wong 1979).

Given a set of principal component scores $(\boldsymbol{\beta}_1, \boldsymbol{\beta}_2, \dots, \boldsymbol{\beta}_n)$, the K-means algorithm partitions observations into K groups, so as to minimize the within-cluster sum of square, expressed as

$$\arg\min_{\mathrm{S}} \sum_{i=1}^{K} \sum_{\boldsymbol{\beta}_j \in S_i} \|\boldsymbol{\beta}_j - \boldsymbol{\mu}_i\|^2,$$

where $\|\cdot\|$ represents the Euclidean norm, and $\boldsymbol{\mu}_i$ is the mean vector for each group S_i for $i = 1, \dots, K$. Computationally, it uses the iterative updating scheme to refine its clustering membership. In the first step, we assign each observation to the cluster with the closest mean, then the mean value of each group is updated by the assigned observations in the second step. This iterative procedure is repeated until the assignment of membership labels does not change.

Figure 6a plots two clusters obtained by applying the K-means algorithms to the bivariate principal component scores. The red triangles represent the years at or before 1945, while the black circles represent the years after 1945. From this data set, it indicates a possible structural change in the French male log mortality rates before and after 1945. The corresponding indexes of the bivariate principal component scores are matched back to the functional curves in Figure 6b.



(a) Bivariate data display. (b) Functional data display.

Figure 6: The K-means algorithm applied to the first two principal component scores obtained from the FPCA.

6 Conclusion

Modern data analysis has had and will continue to benefit greatly from recent development of functional data analysis. Illustrated by the French male log mortality rates, this paper has broadly revisited FPCA mainly developed from the past three decades for analyzing ever increasingly high-dimensional data.

The application of FPCA is not exhaustive, as the emphasis is placed on its usage mainly in statistics. Even within the field of statistics, the citation in this paper is not exhaustive, as the emphasis is placed on the methodological and practical aspects of FPCA, instead of theoretical results of FPCA. However, this paper should be suffice for readers to quickly comprehend some existing literature on FPCA. As functional data analysis continues becoming popular in many scientific fields, the need for novel statistical developments of FPCA will only increase, promising an exciting future for statisticians in the field.

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