Sensible Functional Linear Discriminant Analysis

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Summary

The focus of this paper is to extend Fisher’s linear discriminant analysis (LDA) to both densely recorded functional data and sparsely observed longitudinal data for general c-category classification problems. We propose an efficient approach to identify the optimal LDA projections in addition to managing the noninvertibility issue of the covariance operator emerging from this extension. A conditional expectation technique is employed to tackle the challenge of projecting sparse data to the LDA directions. We study the asymptotic properties of the proposed estimators and show that asymptotically perfect classification can be achieved in certain circumstances. The performance of this new approach is further demonstrated with numerical examples.

Keywords: classification, functional data, linear discriminant analysis, longitudinal data, smoothing.

1 Introduction

Classification identifies the class, from a set of classes, to which a new observation belongs, based on the training data containing observations whose class labels are known. Due to its importance in many applications, statistical approaches have been extensively developed. To name but a few, principal component analysis (PCA, Turk and Pentland (1991)), Fisher’s linear discriminant analysis (LDA, Fisher (1936), Rao (1948)), partial least square approaches (PLS, Barker and Rayens (2003)), etc. have all been explored for classification. The common essence of these approaches is to find optimal projections based on a particular criterion for subsequent classification. While the data dimension is moderate, these

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approaches or their variants often work nicely. With the advent of modern technology and devices for collecting data, the dimension of data can become very high and may be intrinsically infinite, such as functional data; this requires the aforementioned approaches to be adapted. Motivated by the Fisher’s LDA, we propose “sensible” functional LDA (sFLDA) to search the optimal projections for subsequent classification.

LDA aims at finding ideal linear projections and performs classification on the projected subspace. Ideal projections are those maximizing the projected distances between classes while keeping the projected distances among subjects in the same class minimized. Take a $p$-dimensional case for example; mathematically the ideal projections are the eigenvector $b$ in

$$\Sigma_W^{-1}\Sigma_B b = \lambda b,$$

where $\Sigma_W^{-1}$ denotes the inverse of the within-subject covariance matrix $\Sigma_W$, and $\Sigma_B$ is the between covariance matrix that characterizes the variation of class means. Under classical multivariate settings, $\Sigma_W$ is invertible. Please refer to Mardia et al. (1980) for the details of LDA. Due to its simplicity, LDA has been widely employed in many applications.

Extending (1.1) directly to functional data is tricky due to the noninvertible covariance operator. Specifically, the inverse of the covariance operator is unbounded if the functional data is in $L_2$, which is commonly assumed in the functional data analysis literature (e.g., Hall et al. 2003, Li and Hsing 2010, Delaigle and Hall 2012, etc.). To elucidate our idea, let us introduce notations first. Suppose the data consists of $c$ classes. Let $X_k$ be an $L_2$ stochastic process, defined on a finite compact interval $\mathcal{T}$, in class $k$ with mean function $\mu_k$ and a common covariance function $\Gamma_W$. Mercer’s theorem implies that the covariance function can be further decomposed as $\Gamma_W(s,t) = \sum_{j=1}^\infty \lambda_j \phi_j(s)\phi_j(t)$, where the eigenvalue $\lambda_j > 0$ is in descending order with corresponding eigenfunction $\phi_j$ and $\sum_{j=1}^\infty \lambda_j < \infty$.

Functional principal component analysis (FPCA) corresponds to a spectral decomposition of the covariance and leads to the well-known Karhunen-Loéve decomposition of the random function,

$$X_k(t) = \mu_k(t) + \sum_{j=1}^\infty A_{k,j} \phi_j(t),$$

where $A_{k,j}$ is the $j$th principal component score (PCS) with mean zero, variance $\lambda_j$ and $t \in \mathcal{T}$. Let $S_B$ (resp. $S_W$) be the space spanned by $\{\mu_k\}_{k=1}^c$ (resp. $\{\phi_j\}_{j=1}^\infty$). Since we do not assume completeness on $\{\phi_j\}_{j=1}^\infty$, $S_B \subset S_W$ is not always true (Hsing and Eubank 2015). We also do not impose any parametric assumptions on $X_k$ other than smoothness conditions on $\mu_k$ and $\Gamma_W$, which are quite common in functional data analysis (e.g., Rice and Silverman 1991, Chiou et al. 2003, Hall et al. 2004, etc.)

To handle the unbounded $\Gamma_W^{-1}$, basis-based approaches can be used to express the functional data with certain basis functions and turn the functional problem into a multivariate one. For example, Hall et al. 2001, Glendinning and Herbert 2003, Müller 2005, Leng and Müller 2006, and Song et al. 2008 performed classification based on FPCA; Preda et al. 2007 classified functional data by means of PLS; Berlinski et al. 2008, Rincón and Ruiz-Medina 2012, and Chang et al. 2014 developed approaches based on wavelets. However, doing so might lose crucial information for subsequent classification if the differences among classes are not well preserved due to inappropriate basis functions. For example, when
$S_B \not\subseteq S_W$ (e.g., a binary case where $\mu_1(t) = \sin(2\pi t)$, $\mu_2(t) = -\mu_1(t)$, $\phi_k(t) = \sqrt{2} \cos(2k\pi t)$ for $k = 1, \ldots, \infty$ and $t \in [0, 1]$), at least some $\mu_k$’s can not be well described by $\{\phi_j\}_{j=1}^{\infty}$ and thus FPCA based approaches might not be a good choice. This argument is substantiated with simulated data in section 6.

There exist other functional classification approaches under different considerations. To name a few, Ferraty and Vieu (2003) and Galeano et al. (2014) investigated distance-based approaches, Hastie et al. (1995) and Araki et al. (2009) developed regularized approaches, Epifanio (2008) proposed an approach to classify functional shapes, and Delaigle and Hall (2013) developed a functional classification framework when the observations were fragments of curves.

In a general $c$-category classification problem, at most $(c-1)$ projections in $S_B$ are useful for functional LDA. Merely considering the information in $S_B$ is insufficient, as reducing the within-class variation is equivalently important. With this in mind and to properly handle the noninvertibility issue of $\Gamma_W$, we propose a sensible classification approach to find projections in $P_W(S_B)$ and in $P_W(S_B)$ sequentially, where $P_W(S_B)$ (resp. $P_W(S_B)$) is the projection of $S_B$ on $S_W$ (resp. $S_W$, the orthogonal complement of $S_W$). Most existing approaches do not appear to appreciate that the optimal linear projections could be a set of the projections obtained in $P_W(S_B)$ and in $P_W(S_B)$; this may be because it suffices to consider projections in either $P_W(S_B)$ or $P_W(S_B)$ for binary classification problems. Accordingly, our procedure is more general.

Despite the difference in sampling schemes, functional data and longitudinal data come from similar sources. Therefore, it is practical to develop unified approaches for them (e.g., Müller (2005), Hall et al. (2006), Jiang and Wang (2010), etc.). James and Hastie (2001) employed natural cubic splines to tackle the problem of sparsity. Wu and Liu (2013) applied the FPCA approach proposed in Yao et al. (2005) to reconstruct sparsely observed longitudinal data and performed robust support vector machine (SVM) on the reconstructed curves. This strategy leads to the same predicament as other FPCA based approaches mentioned earlier. The major challenge in extending Fisher’s LDA to longitudinal data is to perform classification on a new subject with longitudinal observations. The sparsity and irregularity of the observations make the projections difficult. We propose an imputation approach based on a conditional expectation technique (in section 5) to resolve the sparsity issue without losing the subtle information about the mean functions.

The rest of this paper proceeds as follows. In the next section, the motivation and the framework of sFLDA are introduced. The proposed estimators and their asymptotic properties are provided in sections 3 and 4, respectively. We propose an imputation approach for longitudinal data while performing projections in section 5. In section 6, simulation studies under three data configurations are conducted. In section 7, our approach, along with some competitors, is applied to two real data examples. Conclusions are given in the last section. Appendices include the assumptions made for the asymptotics, the leave-one-curve-out cross-validation (CV) formulae of bandwidth selections, and some details for Section 2.1. All the proofs are contained in the supplementary material.
2 Method

Let us elucidate our idea through the following example, where we aim to find the optimal projections, \( \beta \)'s, for subsequent classification. For convenience, we denote \( \langle \beta, X \rangle = \int_{T} \beta(t)X(t)dt \).

**Example 2.1** Suppose the data in class \( k \) is generated from

\[
X_{k,i}(t) = \mu_{k}(t) + \sum_{j=1}^{\infty} A_{k,i,j}\phi_{j}(t),
\]

where \( \phi_{j}(t) = \sqrt{2}\sin(2\pi j t), t \in [0, 1], A_{k,i,j} \sim N(0, 1/j^2), \) and \( i = 1, \ldots, n_{k} \).

**Case (a):** \( \mu_{1}(t) = \sqrt{2}\sin(2\pi t), \mu_{2}(t) = 0; \)

**Case (b):** \( \mu_{1}(t) = \sqrt{2}\cos(2\pi t), \mu_{2}(t) = 0; \)

**Case (c):** \( \mu_{1}(t) = \sqrt{2}\sin(2\pi t), \mu_{2}(t) = \sqrt{2}\cos(2\pi t), \mu_{3}(t) = 0. \)

The first two cases are simple binary problems. Case (a) corresponds to the situation where \( S_{B} \subseteq S_{W} \), and \( \beta(t) = \sqrt{2}\sin(2\pi t) \) is the optimal projection for functional LDA. Case (b) is a typical instance where \( S_{W} \perp S_{B} \). The optimal projection is \( \beta^{\ast}(t) = \sqrt{2}\cos(2\pi t) \in S_{B} \) as perfect classification can be achieved. Specifically, \( \langle \beta^{\ast}, X_{1,i} \rangle = 1 \) and \( \langle \beta^{\ast}, X_{2,i} \rangle = 0 \) for all \( i = 1, \ldots, n_{k} \), where \( n_{k} \) is the number of functions in class \( k \). Case (c) combines the situations considered in cases (a) and (b). \( \beta \in \mathcal{P}_{W}(S_{B}) \) (resp. \( \beta^{\ast} \in \mathcal{P}_{W}^{\perp}(S_{B}) \)) can be used to separate the curves in class 2 (resp. 1) from those in the other two classes. Between these two projections, \( \beta^{\ast} \) is more informative for classification as \( \beta^{\ast} \) can completely separate the curves in class 2 from those of the other two classes. Specifically, \( \langle \beta^{\ast}, X_{2,i} \rangle = 0 \) for all \( i = 1, \ldots, n_{k} \). This example shows that both \( S_{W} \) and \( S_{W}^{\perp} \) are helpful for classification and \( \beta \) in \( \mathcal{P}_{W}^{\perp}(S_{B}) \) is more informative.

Since the information in both \( S_{B} \) and \( S_{W} \) is essential to identify \( \beta \)'s and generally \( S_{B} \not\subseteq S_{W} \), we consider finding \( \beta \)'s in \( \mathcal{P}_{W}(S_{B}) \) and in \( \mathcal{P}_{W}(S_{B}) \) sequentially. We first consider \( \beta \)'s in \( \mathcal{P}_{W}(S_{B}) \) because they can lead to asymptotically perfect classification (see Theorem 4.4 for details). Without loss of generality, we let the global mean \( \mu = \sum_{k=1}^{c} \pi_{k} \mu_{k} = 0 \), where \( \pi_{k} \) is the probability that a randomly selected function \( X \) is from class \( k \) and \( \sum_{k=1}^{c} \pi_{k} = 1 \). So, the between covariance

\[
\Gamma_{B}(s, t) = \sum_{k=1}^{c} \pi_{k} \{ \mu_{k}(s) - \mu(s) \} \{ \mu_{k}(t) - \mu(t) \}
\]

\[
= \sum_{k=1}^{c} \pi_{k} \mu_{k}(s) \mu_{k}(t),
\]

for \( s, t \in T \). In practice, \( \pi_{k} \) is unknown and we estimate it with \( n_{k}/\sum_{i=1}^{c} n_{i} \). For convenience, we denote \( \Gamma_{B} = \int_{T} \Gamma(s, t)\beta(t)dt \).
2.1 sFLDA

Specifically, sFLDA is defined as finding the optimal projections,

\[ \beta_1 = \arg \max_{\beta \in \mathcal{P}_W(S_B)} \langle \beta, \Gamma_B \beta \rangle, \]

\[ \beta_j = \arg \max_{\beta \in \mathcal{P}_W(S_B), \langle \beta, \beta_i \rangle = 0 \text{ for } i < j} \langle \beta, \Gamma_B \beta \rangle \quad \text{for } j = 2, \ldots, c'; \]

\[ \beta_{c' + 1} = \arg \max_{\beta \in \mathcal{P}_W(S_B)} \langle \beta, \Gamma_W \beta \rangle, \]

\[ \beta_{c' + j} = \arg \max_{\beta \in \mathcal{P}_W(S_B), \langle \beta, \beta_{c' + i} \rangle = 0 \text{ for } i < j} \langle \beta, \Gamma_W \beta \rangle \quad \text{for } j = 2, \ldots, c'', \]

(2.1)

where \( \| \beta \| = 1 \), \( c' \) (resp. \( c'' \)) is the dimension of \( \mathcal{P}_W(S_B) \) (resp. \( \mathcal{P}_W(S_B) \)), and both \( c' \) and \( c'' \) are unknown in practice. These \( \beta \)'s are optimal in the sense that (i) when \( S_B \perp S_W \), asymptotically perfect classification can be achieved, and (ii) when \( S_B \subset S_W \), they are the optimal projections of functional LDA. To identify \( \{ \beta_i \}_{i=1}^{c'} \), we introduce a symmetric non-negative definite kernel

\[ \Gamma_B \setminus W(s, t) = \sum_{k=1}^{c} \pi_k r_k(s) r_k(t), \]

(2.3)

where \( r_k(t) = \mu_k(t) - \sum_{j=1}^{\infty} \langle \mu_k, \phi_j \rangle \phi_j(t) \). \( r_k \) is the projection of \( \mu_k \) on \( S_W \) and \( r_k \in \mathcal{P}_W(S_B) \). By Mercer’s Theorem,

\[ \Gamma_B \setminus W(s, t) = \sum_{j=1}^{c'} \eta_j \psi_j(s) \psi_j(t), \]

(2.4)

where \( \psi_j \) is the \( j \)th eigenfunction of \( \Gamma_B \setminus W \) with corresponding eigenvalue \( \eta_j > 0 \) in descending order. Simple calculations (see Appendix C for detail) lead to \( \beta_j = \psi_j \) for \( j = 1, \ldots, c' \), where \( c' \leq c - 1 \).

Next, we look for \( \{ \beta_i \}_{i=1}^{c' + c''} \) in \( \mathcal{P}_W(S_B) \). Similar to (2.3)–(2.4), we define another symmetric non-negative definite kernel

\[ \Gamma_B W(s, t) = \sum_{k=1}^{c} \pi_k r_k(s) r_k(t), \]

(2.5)

where \( r_k(t) = \mu_k(t) - r_k(t) \). \( r_k \) is the projection of \( \mu_k \) on \( S_W \), and \( r_k \in \mathcal{P}_W(S_B) \). Again, by Mercer’s Theorem,

\[ \Gamma_B W(s, t) = \sum_{j=1}^{c''} \eta_j \psi_j(s) \psi_j(t), \]

(2.6)
where $\eta_j^* > 0$ is the $j$th eigenvalue in descending order with corresponding eigenfunction $\psi_j^*(t)$ and $c'' \leq c - 1$. Since $\beta(t) = \sum_{i=1}^{c''} a_i \psi_i^*(t)$ for some constant $a = (a_1, \ldots, a_{c''})^T$, obtaining $\{\beta_j\}_{j=c'+1}^{c+c''}$ in (2.2) becomes equivalent to solving the eigenequation

$$\Omega_W^{-1} \Omega_B a = \zeta a,$$

(2.7)

where $\|a\| = 1$, $\Omega_B = \text{diag}(\eta_1^*, \ldots, \eta_{c'}^*)$, and the element in $i$th row and $j$th column of $\Omega_W$ is $\langle \psi_j^*, \Gamma_W \psi_i^* \rangle$. The equivalence is detailed in Appendix C. Consequently, the noninvertibility issue of $\Gamma_W$ is avoided and finding $\{\beta_i\}_{i=c'+1}^{c+c''}$ is streamlined to a multivariate problem (2.7).

When $\{\beta_i\}_{i=1}^{c+c''}$ are available, one could apply any classifiers on the projections to perform classification. For illustration purposes and simplicity, we employ the nearest centroid classifier in our analysis.

### 2.2 Special Cases

When $S_B \perp S_W$, only $\beta_i$’s in (2.1) are considered and asymptotically perfect discrimination can be achieved (shown in Theorem 1.4), and case (b) in Example 2.1 is an artificial example with $c = 2$.

When $S_B \subseteq S_W$, only $\beta_i$’s in (2.2) are considered and most existing functional LDA approaches were developed under this specific situation. For example, (2.3) in Delaigle and Hall (2012) implies that $S_B \subseteq S_W$ is considered, and the authors showed that these $\beta_i$’s can lead to asymptotically perfect classification for binary classification problems under some conditions. However, (2.7) is computationally not only easier but more efficient as the eigenfunctions of $\Gamma_W$ irrelevant to $S_B$ are filtered out in (2.7). A typical example of $S_B \subseteq S_W$ is the multiplicative random effect model, where the mean function is proportional to one of the eigenfunctions, e.g., Jiang et al. (2009). Further, Case (a) in Example 2.1 is an artificial example with $c = 2$.

Note that when $S_B \not\subseteq S_W$ and $c = 2$, only one $\beta$ in $\mathcal{P}_W(S_B)$ is considered. Specifically, sFLDA identifies $\beta$ via (2.1) with $c' = 1$ and asymptotically perfect classification is expected.

### 3 Estimation

Let $y_{k,ij}$ be the $j$-th observation of subject $i$ in class $k$ made at $t_{k,ij}$, for $j = 1, \ldots, m_{k,i}$, $i = 1, \ldots, n_k$, and $k = 1, \ldots, c$. Specifically,

$$y_{k,ij} = X_{k,i}(t_{k,ij}) + \epsilon_{k,ij},$$

where $X_{k,i}$ is defined as in (1.2), and $\epsilon_{k,ij}$ is the measurement error with mean zero and variance $\sigma^2$ and is independent from all other random variables. The mean function for class $k$ can be estimated by applying any one dimensional smoother to $\{(y_{k,ij}, t_{k,ij}) | 1 \leq j \leq m_{k,i}\}$.
\( m_{k,i}, 1 \leq i \leq n_k \). Take the local linear smoother for example,

\[
\hat{\mu}_k(t) = \hat{b}_0, \text{ where for } \hat{b} = (\hat{b}_0, \hat{b}_1),
\]

\[
\hat{b} = \arg \min_b \sum_{i=1}^{n_k} \frac{1}{m_{k,i}h_k} \sum_{j=1}^{m_{k,i}} K(\frac{t-t_{k,ij}}{h_k}) \times \{Y_{k,ij} - b_0 - b_1(t_{k,ij} - t)\}^2,
\]

\( h_k \) is the bandwidth and \( K(\cdot) \) is the kernel function. The within covariance function \( \Gamma_W \) can be estimated by applying a two dimensional smoother to \( \{(R_{k,i,j,\ell}, t_{k,i,\ell}, t_{k,j,\ell})|k = 1, \ldots, c; i = 1, \ldots, n_k; 1 \leq j \neq \ell \leq m_{k,i}\} \), where \( R_{k,i,j,\ell} = y_{k,ij} y_{k,i\ell} \) and \( y_{k,ij} = y_{k,ij} - \hat{\mu}_k(t_{k,ij}) \). Take the two dimensional local linear smoother for example,

\[
\hat{\Gamma}_W(s,t) = \hat{b}_0, \text{ where for } \hat{b} = (\hat{b}_0, \hat{b}_1, \hat{b}_2),
\]

\[
\hat{b} = \arg \min_b \sum_{k=1}^{c} \sum_{i=1}^{n_k} \frac{1}{m_{k,i}(m_{k,i} - 1)h_W^2} \times \sum_{1 \leq j \neq \ell \leq m_{k,i}} K(\frac{s-t_{k,ij}}{h_W})K(\frac{t-t_{k,i\ell}}{h_W}) \times \{R_{k,i,j,\ell} - b_0 - b_1(t_{k,ij} - s) - b_2(t_{k,i\ell} - t)\}^2.
\]

The bandwidths of \( \hat{\mu}_k \)'s and that of \( \hat{\Gamma}_W \) in our numerical analyses are selected via leave-one-curve-out CV, and the formulae are provided in Appendix B. To estimate \( \sigma^2 \), we employ the approach in Yao et al. (2005) and denote it as \( \hat{\sigma}^2 \). Details are omitted to save space. We obtain \( \lambda_i \)'s and \( \phi_i \)'s by applying an eigendecomposition to \( \hat{\Gamma}_W \).

### 3.1 Estimating \( \beta_1, \ldots, \beta_{c'} \)

To estimate \( \{\beta_i\}'s \), we suggest performing an eigendecomposition on

\[
\hat{\Gamma}_{B\setminus W}(s,t) = \sum_{k=1}^{c} \frac{n_k}{n} \hat{r}_k(s)\hat{r}_k(t),
\]

where \( \hat{r}_k(t) = \hat{\mu}_k(t) - \sum_{j=1}^{L} \langle \hat{\mu}_k, \hat{\phi}_j \rangle \hat{\phi}_j(t) \), for \( \{\hat{\psi}_i\}'s \) as well as \( \{\hat{\beta}_i\}'s \). Both \( L \) and \( c' \) are selected by fraction of variation explained (FVE). Specifically,

\[
L = \arg \min_{1 \leq \ell < \infty} \frac{\sum_{i=1}^{\ell} \lambda_i}{\sum_{i=1}^{n_k} \lambda_i} \geq \mathcal{P}_1, \text{ and}
\]

\[
c' = \arg \min_{1 \leq \ell' < c-1} \frac{\sum_{i=1}^{\ell'} \hat{\eta}_i}{\sum_{i=1}^{n_k} \hat{\eta}_i} \geq \mathcal{P}_2,
\]

where \( \hat{\lambda}_i \) (resp. \( \hat{\eta}_i \)) is the \( i \)-th eigenvalue of \( \hat{\Gamma}_W \) (resp. \( \hat{\Gamma}_{B\setminus W} \)), and \( 0 < \mathcal{P}_1, \mathcal{P}_2 \leq 1 \).

In general, the threshold \( \mathcal{P} \) is chosen to be 80% or 85% in FPCA; however, we choose 95% to select both \( L \) and \( c' \) in our analyses to prevent accidentally excluding the information about \( S_B \) in \( \mathcal{P}_W(S_B) \) or including the information about \( S_W \) in \( \mathcal{P}_W(S_B) \). Consider a general
case where $S_B \not\subseteq S_W$. Empirically, the estimated $S_W$, denoted as $\hat{S}_W$, is spanned by $\{\hat{\phi}_i\}_{i=1}^L$. When the selected $L$ is too large, some unreliable $\hat{\phi}_i$’s are used to estimate $S_W$. Let $\{\hat{\phi}_i\}_{i=L-d+1}^L$ be these unreliable estimates, where $d$ is some positive integer. If $\{\hat{\phi}_i\}_{i=L-d+1}^L$ is orthogonal to $S_B$, the subsequent classification remains unchanged as $\hat{r}_k$’s are not affected due to $\langle \hat{\mu}_k, \hat{\phi}_j \rangle = O(h_k^2 + \delta_{nk1}(h_k))$ for $L - d < j \leq L$ by (4.1). However, if $\{\hat{\phi}_i\}_{i=L-d+1}^L$ is not orthogonal to $S_B$, which certainly is possible, the subsequent classification tends to be corrupted as some of the information about $\beta$’s in the $\hat{r}_k$’s might be removed due to $\langle \hat{\mu}_k, \hat{\phi}_j \rangle = \langle \mu_k, \phi_j \rangle + O(h_k^2 + \delta_{nk1}(h_k))$ and $\langle \mu_k, \phi_j \rangle \neq 0$ for $L - d < j \leq L$. When the selected $L$ is too small, $\hat{r}_k$’s tend not to be orthogonal to $S_W$. However, since the number of $\beta$’s can be smaller than the dimension of $\Gamma_{BW}$, it is possible that $\hat{\beta}$’s are orthogonal to $S_W$. When this happens, asymptotically perfect classification can still be achieved. However, if those $\beta$’s are not orthogonal to $S_W$, asymptotically perfect classification might not be achieved as the projections of different classes might not be well separated from each other.

So, we need a criterion to select $L$ properly and our empirical experience indicates that FVE is a good choice. Furthermore, FVE is computationally simple and fast and free of model assumptions.

### 3.2 Estimating $\beta_{c'+1}, \ldots, \beta_{c'+c''}$

Similarly to estimating $\{\hat{\beta}_i\}_{i=1}^c$, we first estimate $\Gamma_{BW}$ by

$$\hat{\Gamma}_{BW}(s, t) = \sum_{k=1}^c \frac{n_k}{n} \hat{r}_k(s)\hat{r}_k^*(t), \quad (3.4)$$

where $\hat{r}_k^*(t) = \hat{F}_k(t) - \hat{r}_k(t)$. The estimated eigenfunctions $\hat{\psi}_i^*(t)$’s and estimated eigenvalues $\hat{\eta}_i^*$’s are obtained by applying an eigendecomposition to $\hat{\Gamma}_{BW}$. Again, $c''$ is selected by FVE with threshold 95%.

$\Omega_B = \text{diag}(\hat{\eta}_1^*, \ldots, \hat{\eta}_{c''}^*)$ and the element in $i$th row and $j$th column of $\Omega_W$ is $\langle \hat{\psi}_i^*, \hat{\Gamma}_W \hat{\psi}_j^* \rangle$. Therefore, $\hat{\beta}(t) = \sum_{i=1}^{c''} \hat{a}_i \hat{\psi}_i^*(t)$, where $(\hat{a}_1, \ldots, \hat{a}_{c''})^T$ is obtained by solving (2.7), where $\Omega_W$ and $\Omega_B$ are replaced with $\hat{\Omega}_W$ and $\hat{\Omega}_B$, respectively. Given $c'' \leq (c - 1)$, letting $c' = c - 1$ may not be particularly detrimental to results; however, it is not necessary to include those $\hat{\psi}_j^*$’s corresponding to very small $\hat{\eta}_j^*$’s as they are not reliable when performing classification. That is the main reason that only a truncated number of estimated eigenfunctions are used.

### 3.3 Cases where $c' = c - 1$

When $S_B \not\subseteq S_W$ and $S_B \not\subseteq S_W$, our procedure estimates the optimal set $\{\beta_j\}_{j=1}^{c'+c''}$ by both (2.1) and (2.2). However, $\hat{\Gamma}_{BW}$ is theoretically zero when $S_B \subseteq S_W$, but in practice $\hat{\Gamma}_{BW}$ is a random matrix and has $(c - 1)$ non-zero eigenvalues due to random noise. Consequently, when $c' = (c - 1)$, the true case ($S_B \subseteq S_W$ or $S_B \perp S_W$) needs to be further clarified. Our empirical experience indicates that $q$-fold CV works well. Specifically, we first randomly divide the training sample into $q$ groups. Each time one group is used as the testing sample while the remaining $(q - 1)$ groups are applied to perform sLDA under both cases. The procedure is repeated $q$ times and the decision is made by comparing the
overall misclassification rates. The choice of $q$ depends on the sample size, the number of observations per subject and available time for computation. Our experience indicates that $q = 5$ is acceptable in our analysis. However, a larger $q$ definitely can help reduce the model misspecification rate and thus the misclassification rate as more samples are used. Please see the supplement for details.

3.4 Algorithm

The sFLDA procedures can be summarized as Algorithm 1 and the MATLAB code of sFLDA is available at https://github.com/chenlu-hung/SFLDA

**Algorithm 1** Steps to perform sFLDA.

**Input:** \((y_{k,ij}, t_{k,ij}) : 1 \leq i \leq n_k, 1 \leq j \leq m_{k,i}\) for \(k = 1, \ldots, c\).

**Output:** \(\hat{\beta}_1, \ldots, \hat{\beta}_{c'+c''}\).

1. Perform an eigendecomposition to \(\hat{\Gamma}_{B\setminus W} (3.3)\) to obtain \(\hat{\beta}_1, \ldots, \hat{\beta}_{c'}\), where \(c'\) is decided by FVE. (Section 3.1)
2. if \(c' < c - 1\) (i.e. \(S_B \not\subset S_W\) and \(S_B \not\subset S_W^\perp\)) then
   3. Perform an eigendecomposition to \(\hat{\Gamma}_{BW} (3.4)\) to obtain \(\hat{\beta}_{c'+1}, \ldots, \hat{\beta}_{c'+c''}\), where \(c''\) is decided by FVE. (Section 3.2)
4. else
   5. Use \(q\)-fold CV to determine whether \(S_B \perp S_W\) or \(S_B \subseteq S_W\). (Section 3.3)
   6. if \(S_B \perp S_W\) then
      7. Set \(c'' = 0\).
   8. else
      9. Set \(c' = 0\) and Perform an eigendecomposition to \(\hat{\Gamma}_{BW} (3.4)\) to obtain \(\hat{\beta}_1, \ldots, \hat{\beta}_{c''}\), where \(c''\) is decided by FVE. (Section 3.2)
10. end if
11. end if

4 Asymptotics

Before deriving the theoretical results of \(\{\hat{\beta}_i\}_{i=1}^{c'+c''}\), we list some useful results from Li and Hsing (2010). First, we define the \(j\)th harmonic mean of \(m_{k,i}\) as \(\gamma_{n_{k,i}} = (n_k^{-1} \sum_{i=1}^{n_k} 1/m_{k,i})^{-1}\),

\[
\delta_{n,1}(h) = \max_{1 \leq k \leq c} \left\{ \left\{ 1 + 1/(h_k \gamma_{n_{k,1}}) \right\} \log n_k/n_k \right\}^{1/2}, \text{ and}
\delta_{n,2}(h) = \max_{1 \leq k \leq c} \left\{ \left\{ 1 + 1/(h_k \gamma_{n_{k,1}}) + 1/(h_k^2 \gamma_{n_{k,2}}) \right\} \log n_k/n_k \right\}^{1/2}.
\]

Li and Hsing (2010) showed that under Assumptions A.1–A.4,

\[
\sup_{t \in T} |\hat{\mu}_k(t) - \mu_k(t)| = O(h_k^2 + \delta_{n,1}(h_k)) \quad \text{a.s.} \quad (4.1)
\]
for \( k = 1, \ldots, c \) and that under Assumptions A.1–A.6,

\[
\sup_{s, t \in T} |\hat{\Gamma}_W(s, t) - \Gamma_W(s, t)| = O(h^2 + \delta_{n,1}(h) + h_W^2 + \delta_{n,2}(h_W)) \text{ a.s.}\]

We assume that \( n_k \)'s are of the same order, and thus it is reasonable to have \( h_k \)'s of the same order, \( h \). If the order of \( h_1 \) is smaller or equal to that of \( h_2 \), we denote it as \( h_1 \preceq h_2 \).

Note that \( \lambda_j - \lambda_{j+1} \geq C^{-1} J^{-(a_1+1)} \) for \( a_1 \geq 1 \),

\[
\Delta_n = L^{2a_1+3} \{ h^4 + \delta_{n,1}^2(h) + h_W^4 + \delta_{n,2}^2(h_W) \} + L^{-2(a-1)}.
\]

First, we can obtain the following theorem about \( \hat{r}_k \) and \( \hat{\Gamma}_{B \setminus W} \).

**Theorem 4.1** Under Assumptions A.1–A.7,

\[
\| \hat{r}_k - r_k \|^2 = O(\Delta_n) \text{ a.s. for } k = 1, \ldots, c;
\]

\[
\| \hat{\Gamma}_{B \setminus W} - \Gamma_{B \setminus W} \|^2 = O(\Delta_n) \text{ a.s.}
\]

Similarly, we can have the following theorem about \( \hat{r}_k^* \) and \( \hat{\Gamma}_{BW} \).

**Theorem 4.2** Under Assumptions A.1–A.7,

\[
\| \hat{r}_k^* - r_k^* \|^2 = O(\Delta_n) \text{ a.s. for } k = 1, \ldots, c;
\]

\[
\| \hat{\Gamma}_{BW} - \Gamma_{BW} \|^2 = O(\Delta_n) \text{ a.s.}
\]

Simple calculations and Theorem 4.2 lead to

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Theorem 4.3 Under Assumptions A.1–A.7,
\[
\|\hat{\Omega}_W - \Omega_W\|^2 = O(\Delta_n) \text{ a.s., and}
\|\hat{\Omega}_B - \Omega_B\|^2 = O(\Delta_n) \text{ a.s.}
\]

The asymptotic properties of \(\{\hat{\beta}_j\}_{j=1}^{c'}\) and \(\{\hat{\beta}_j\}_{j=c'+1}^{c''}\) can be obtained by applying perturbation theory to Theorems 4.1 and 4.3, respectively. Thus, the corollary follows.

Corollary 4.1 Under Assumptions A.1–A.7 and that nonzero \(\eta_j\)’s are distinct, for \(1 \leq j \leq (c' + c'')\),
\[
\sup_{t \in T} |\hat{\beta}_j(t) - \beta_j(t)| = O(\sqrt{\Delta_n}) \text{ a.s.} \tag{4.4}
\]

Under different sampling schemes, for \(1 \leq j \leq (c' + c'')\),

- **longitudinal data** (i.e., \(m_{k,i} < \infty\)),
  \[
  \sup_{t \in T} |\hat{\beta}_j(t) - \beta_j(t)| = O(L_{n+3/2}\{h^2 + (\log n/nh^2)\} + h_W^2 + (\log n/nh_W)^2) + L^{-(\alpha - 1/2)} \text{ a.s.}
  \]

- **functional data** (i.e., \(m_{k,i} \geq \frac{1}{T} \to \infty\)),
  \[
  \sup_{t \in T} |\hat{\beta}_j(t) - \beta_j(t)| = O(L_{n+3/2}\{h^2 + h_W^2 + (\log n/nh_W^2)\} + L^{-(\alpha - 1/2)} \text{ a.s.}
  \]

4.2 Asymptotically Perfect Discrimination

To show the asymptotically perfect classification property, we consider the case where \(c'' = 0\), i.e., all \(\beta_i\)'s are in \(P_{W}(S_B)\), for illustration purposes as [Delaigle and Hall (2012)] has shown that when \(S_B \subset S_W\), asymptotically perfect classification can be achieved for binary problems under certain conditions. Suppose the function \(Y\) to be classified is observed at \((t_1, \ldots, t_m)\) with unknown class label \(\kappa\) and \(Y\) is further contaminated with measurement error. Specifically, \(Y(t_i) = X_k(t_i) + \epsilon\) for \(i = 1, \ldots, m\), and \(\epsilon\) is i.i.d. measurement error with mean zero and finite variance \(\sigma^2\). Denote \(\nu_k = (\langle \beta_1, \mu_k \rangle, \ldots, \langle \beta_c, \mu_k \rangle)^T\) for \(1 \leq k \leq c\) and \(\hat{\nu} = (\langle \hat{\beta}_1, Y \rangle, \ldots, \langle \hat{\beta}_c, Y \rangle)^T\).

Theorem 4.4 Under conditions listed in Theorem 4.1, we have
\[
\|\hat{\nu} - \nu_\kappa\|^2 = O \left(\Delta_n + \frac{\log m}{m}\right) \text{ a.s.,}
\]

and if further \(\min_{1 \leq i \leq c, i \neq \kappa} \|\nu_k - \nu_i\|^2 > C(\Delta_n + \log m/m)\) for some \(C > 0\),
\[
\kappa = \arg\min_{1 \leq i \leq c} \|\hat{\nu} - \nu_i\| \text{ a.s..} \tag{4.5}
\]

Theorem 4.4 indicates that when all \(\beta_i\)'s are in \(P_{W}(S_B)\), the projection of \(Y\), \(\hat{\nu}\), will converge to \(\nu_\kappa\) when \(n\) and \(m\) are large enough. Moreover, if \(\nu_\kappa\) and the other \(\nu_i\)'s are not very close, the class label of \(Y\) can be correctly classified by employing any nearest centroid based classifier.
5 Imputation Approach for Longitudinal Data

The above mentioned estimators are applicable to both functional and longitudinal data. With \( \{\hat{\beta}_j\}_{j=1}^c \), having LDA projections for a subject with dense observations for subsequent classification is not difficult. However, the projection is nontrivial for a new subject with sparse observations. One might consider employing the FPCA approach in Yao et al. (2005) to first reconstruct the curve and perform projections later. However, doing so causes some potential risks. When the magnitude of mean functions is relatively small compared to the first few eigenvalues of \( \Gamma_W \) and \( S_B \perp S_W \), the true mean function will never be well preserved through the FPCA reconstruction. Take a binary classification problem for example: for \( t \in [0, 1] \), \( \mu_1(t) = \sin(2\pi t)/10, \mu_2(t) = -\sin(2\pi t)/10 \), and \( \phi_k(t) = \sqrt{2}\cos(2\pi kt) \) and \( \lambda_k = 2/k \) for \( k = 1, \ldots, 10 \). In the pooled covariance function, \( \sin(2\pi t) \) corresponds to the smallest eigenvalue, which is too small to be picked up in practice. Thus, the information about the mean function is lost in the FPCA reconstruction. Therefore, we propose an imputation approach to predict the projections.

For the projection of a new subject \( i \) from unknown class \( k \), we consider

\[
E(\langle \beta, X_{k,i}\rangle | y_{k,i}^N) = \langle \beta, E(X_{k,i}|y_{k,i}^N) \rangle,
\]

(5.1)

where \( y_{k,i}^N = (y_{k,i1}, \ldots, y_{k,im_i})^T \) and

\[
E(X_{k,i}|y_{k,i}^N) = \sum_{j=1}^c E(1_{(j=k)}|y_{k,i}^N) \left\{ \mu_j(t) + \sum_{\ell=1}^{\infty} A_{j,\ell} \phi_\ell(t) \right\}.
\]

The estimators of \( \mu_j \) and \( \phi_\ell \) have been detailed earlier. Given the class label \( j \), the PCS \( A_{j,\ell} \) can be predicted by PACE (Yao et al., 2005) and denoted as \( \hat{A}_{j,\ell} \). We estimate \( E(1_{(j=k)}|y_{k,i}^N) \) by a pseudo-likelihood approach, which may seem a little ad hoc; however, it works well in general because it can preserve the mean functions that may not be represented through the FPCA reconstruction, as we mentioned earlier. Specifically,

\[
\hat{E}(1_{(k=j)}|y_{k,i}^N) = \frac{(n_j/n)f_j(y_{k,i}^N)}{\sum_{j=1}^c (n_j/n)f_j(y_{k,i}^N)};
\]

(5.2)

where \( f_k(y_{i,j}^N) \propto \exp\{- (y_{i,j}^N - \hat{\mu}_k)^T \hat{\Gamma}_{k,i}^{-1} (y_{i,j}^N - \hat{\mu}_k) \} \), \( \hat{\mu}_k = \hat{\mu}_k(T_{k,i}), T_{k,i} = (t_{k,i1}, \ldots, t_{k,im_i})^T \), and \( \hat{\Gamma}_{W,k,i} = \sum_{\ell=1}^L \hat{\lambda}_\ell \hat{\phi}_\ell(T_{k,i}) \hat{\phi}_\ell(T_{k,i})^T + \hat{\sigma}^2 I_{m_i \times m_i} \).

To sum up, the projection is predicted by

\[
\langle \hat{\beta}, \hat{E}(X_{k,i}|y_{k,i}^N) \rangle = \sum_{j=1}^c \hat{E}(1_{(j=k)}|y_{k,i}^N) \left\{ \langle \hat{\beta}, \hat{\mu}_j \rangle + \sum_{\ell=1}^L \hat{A}_{j,\ell} \langle \hat{\beta}, \hat{\phi}_\ell \rangle \right\}.
\]

6 Simulation Studies

Here we investigate the empirical performance of sFLDA by conducting simulation studies with three different cases on the structure of the mean function. The data is generated
from
\[ y_{k,i}(t) = \mu_k(t) + \sum_{j=1}^{10} A_{k,i,j}\phi_j(t) + \epsilon, \] for \( k = 1, 2, 3, \)

where \( \phi_j(t) = \sin(2\pi j t), t \in [0,1], A_{k,i,j} \sim N(0, 1/j^2), \) and \( \epsilon \sim N(0, 1/11^2) \). We still consider the same mean structures as follows:

(a) \( \mu_1(t) = \sin(2\pi t), \mu_2(t) = \sin(4\pi t), \) and \( \mu_3(t) = 0; \)

(b) \( \mu_1(t) = \sin(2\pi t), \mu_2(t) = \sin(2\pi t) + \frac{1}{4}\cos(2\pi t), \) and \( \mu_3(t) = 0; \)

(c) \( \mu_1(t) = \frac{1}{5}\cos(2\pi t), \mu_2(t) = \frac{1}{5}\cos(4\pi t), \) and \( \mu_3(t) = 0. \)

For each case, we generate 300 random trajectories (100 per \( k \)) as a training set and an additional 300 random trajectories (100 per \( k \)) as the testing sample for both functional and longitudinal cases. The functional observations are made on a grid of 200 equispaced points on \([0,1]\) for each subject. For longitudinal data, we randomly select 2 to 10 different observation times from the 200 equispaced points with equal probabilities for each subject. The sFLDA is compared with several widely used methods, including spline-based LDA (FLDA, James and Hastie (2001)), FPCA+LDA (Müller, 2005), and penalized PLS (PPLS, Krämer et al. (2008)). Note that the PLS proposed in Delaigle and Hall (2012) is for binary classification and is not directly applicable for a general \( c \)-category problem. Thus, we compare sFLDA with PPLS instead. The R code for FLDA is adapted from the author’s website; the MATLAB package “PACE” (Yao et al., 2005) and the R package “ppls” (Krämer et al., 2008) are employed to perform FPCA and PPLS, respectively. Each experiment consists of 100 runs. All the tuning parameters of the compared approaches (if any) are selected via leave-one-curve-out CV.

Next, we elaborate why these three cases are considered. Case (a) considers the situation where \( S_B \subseteq S_W \), in which \( S_B \) can be well-represented by the first two eigenfunctions, and thus both FPCA+LDA and sFLDA are expected to perform relatively well. In case (b), the mean functions can not be fully represented by the eigenfunctions. This implies that both \( S_W \) and \( S_W^\perp \) are informative, but not sufficient, for discrimination. Case (c) is a typical example where \( S_W \perp S_B \). Since the variation between the mean functions is much smaller than the first few eigenvalues, performing FPCA results in the loss of considerable information for discrimination; thus, FPCA+LDA acts similarly to a random guess in this case.

| Case | FLDA   | FPCA+LDA | PPLS   | sFLDA   |
|------|--------|----------|--------|---------|
| (a)  | 46.1 ± 4.0 | 33.3 ± 3.1 | 53.1 ± 3.5 | 33.0 ± 3.1 |
| (b)  | 42.2 ± 4.9 | 53.5 ± 2.6 | 55.5 ± 2.8 | 23.3 ± 3.0 |
| (c)  | 12.5 ± 13.0 | 66.0 ± 3.1 | 3.3 ± 10.0 | 0 ± 0.0 |

The results of the simulated functional data are summarized in Table 1, indicating sFLDA works very well for all three cases. As expected, FPCA+LDA performs similarly.
to sFLDA and both outperform the other two methods in case (a). In case (b), sFLDA significantly outperforms all the other approaches. In case (c), sFLDA does achieve asymptotically perfect classification as expected. PPLS and FLDA perform much better than FPCA+LDA. As mentioned earlier, FPCA+LDA acts like a random guess as crucial information is lost for discrimination in the FPCA step.

Although one can always reconstruct longitudinal data, the classification results highly depend on the reconstruction quality and generally are not better than those based on functional data. So, we simply compare sFLDA with the approaches designed for longitudinal data, i.e., FLDA, FPCA+LDA and FPCA+SVM [Wu and Liu, 2013]. The results are summarized in Table 2. FPCA+LDA, FPCA+SVM and sFLDA have similar performance and all outperform FLDA in case (a). sFLDA significantly (resp. slightly) outperforms FPCA+LDA and FPCA+SVM in case (b) (resp. (c)). When the number of observations per subject increases, the performance of sFLDA improves dramatically. However, FPCA+LDA and FPCA+SVM do not perform significantly better with the increase in $m_{k,i}$. Please refer to Table 3 in the supplement and Table 1 for more details. Generally, FLDA does not perform well in all three cases. Comparing Table 2 with Table 1, FLDA, FPCA+LDA, and sFLDA perform similarly or worse due to fewer observations. Table 2 also provides the error rates under correctly specified scenario (Oracle) and the number of incorrect decisions made by $q$-fold CV. As expected, $q$-fold CV does not perform well in case (b) due to the mean functions only being partially represented by the eigenfunctions of $\Gamma_W$ while additional useful information is contained in $S_W^\perp$. This complex model structure makes the model selection quite challenging, especially for sparsely and irregularly observed longitudinal data. However, $q = 5$ appears to work nicely as the sFLDA misclassification rates are very close to those under Oracle.

![Table 2: Classification error rates (%) for longitudinal data under three simulation settings, where M/M stands for model misspecification rate out of 100 runs due to performing $q$-fold CV.](image)

| Case | FLDA  | FPCA+LDA | FPCA+SVM | sFLDA  | M/M     | Oracle |
|------|-------|----------|----------|--------|---------|--------|
| (a)  | 44.9 ± 2.9 | 38.4 ± 2.7 | 38.6 ± 2.7 | 37.5 ± 2.8 | 25      | 37.0 ± 2.8 |
| (b)  | 55.6 ± 2.6 | 57.3 ± 3.7 | 57.1 ± 3.6 | 46.1 ± 3.3 | 83      | 46.2 ± 3.9 |
| (c)  | 59.3 ± 3.9 | 60.7 ± 4.7 | 60.1 ± 4.8 | 54.0 ± 5.0 | 5       | 54.4 ± 4.5 |

### 7 Data Analysis

Two real data examples under different configurations are considered. For the functional dataset, we compare sFLDA with FLDA, FPCA+LDA and PPLS. For the longitudinal dataset, sFLDA is compared with FLDA, FPCA+LDA, FPCA+SVM and PPLS. As PPLS is not designed for longitudinal data, we reconstruct the latent trajectories by the imputation approach in Section 5 and perform PPLS to the reconstructed curves. All the tuning parameters for the existing approaches (if any) are selected by leave-one-curve-out CV.
Table 3: Misclassification rates (mean±std%) of Phoneme dataset.

| n   | FLDA   | FPCA+LDA | PPLS   | sFLDA  |
|-----|--------|----------|--------|--------|
| 50 | 13.8 ± 0.6 | 16.3 ± 0.7 | 10.0 ± 0.5 | 9.0 ± 0.5 |
| 100| 11.8 ± 0.4 | 16.3 ± 0.6 | 9.7 ± 0.5  | 7.8 ± 0.5  |

7.1 Functional Data

The phoneme dataset (available at [http://statweb.stanford.edu/~tibs/ElemStatLearn/](http://statweb.stanford.edu/~tibs/ElemStatLearn/)) is used here. The dataset consists of 4509 speech frames (transformed into log-periodogram of length 256) of five phonemes (872 frames for “she”, 757 frames for “dark”, 1163 frames for the vowel in “she”, 695 frames for the vowel in “dark”, and 1022 frames for the first vowel in “water”). To evaluate the performance of different approaches, we split the dataset into training and testing sets 100 times. In each split, we randomly select \( n \) log-periodogram samples per phoneme for training, and the remaining ones are for testing. The misclassification rates of different approaches with different training sample size \( n \) are summarized in Table 3, indicating sFLDA outperforms all the other approaches, and PPLS works better than FLDA and FPCA+LDA. Our algorithm selects three LDA directions from (2.1) and one from (2.2). This suggests that \( S_B \nsubseteq S_W \) may be more suitable for this data. This dataset further demonstrates the advantage of our approach for multi-category classification, where the LDA directions may be in a combination of (2.1) and (2.2).

7.2 Longitudinal Data

The relative spinal bone mineral density dataset ([Bachrach et al., 1999](http://statweb.stanford.edu/~tibs/ElemStatLearn)) is considered. The measurements were made on 154 North American adolescents with 70 male and 84 female children. The observation \( y_{k,i,j} \) represents the relative spinal bone mineral density for child \( i \) measured at age \( t_{k,i,j} \). The measured densities are shown in Figure 1 with females in red (dot-dashed) and males in blue (dashed). Even though females and males have different development patterns (e.g., females develop earlier than males), the development also varies from subject to subject, which makes the classification difficult.

The leave-one-out misclassification rates of sFLDA, FPCA+LDA, FPCA+SVM, PPLS and FLDA are 29.2%, 30.1%, 30.1%, 33.1% and 35.7%, respectively. The first three approaches perform similarly and all slightly outperform FLDA and PPLS. FPCA+LDA works better than PPLS, which suggests that the scenario \( S_B \nsubseteq S_W \) is more appropriate for this case. Our algorithm selects the LDA direction through (2.2) and has the lowest misclassification rate.

8 Conclusions

We have proposed sFLDA for both functional data and longitudinal data to find the optimal LDA projections \( \beta's \) in \( P_T(S_B) \) and \( P_W(S_B) \) sequentially. Theoretically, one could follow the technique in [He et al., 2003](http://statweb.stanford.edu/~tibs/ElemStatLearn) to tackle the noninvertibility issue of \( \Gamma_W \) while extending...
LDA to functional data directly. However, our strategy through (2.7) is more appealing in
that not only is the noninvertibility issue avoided but it is computationally easier. We have
also investigated the asymptotic properties of the proposed estimators. When all the \( \beta \)'s are
in \( P_{W}(S_B) \), we have shown that sFLDA can achieve asymptotically perfect discrimination
when a nearest centroid classifier is applied to the projected data.

The framework of sFLDA was developed under the LDA settings, where the covariance
functions among classes are identical. When the covariance structures among groups are
different, a few functional approaches based on the idea of quadratic discriminant analysis
have been proposed, such as James and Hastie (2001), and Delaigle and Hall (2012). Ex-
tending sFLDA for such general cases requires a more sophisticated procedure as the space
spanned by the eigenfunctions becomes much more complicated. We have been working on
this general problem with a completely different strategy and this remains an interesting
direction for future work.

Although sFLDA originates from extending Fisher’s LDA to its functional version, it
also works well empirically on high dimensional (HD) multivariate data classification (please
see the supplement for details). Note that (3.1) and (3.2) can simply be replaced with other
empirical estimates as no smoothing is needed in HD data. SVM is one of the best classifi-
cation approaches and is also the most widely used for HD data classification; however, it
requires lots of computational effort due to its complex quadratic computational algorithm
and the need to select tuning parameters. The computational burden becomes serious as
the data dimension and the sample size increases, which has particular relevance in the big
data era. Our numerical investigations have shown that sFLDA with less computational
cost still yields comparable performance with SVM, especially when the sample size is moderately large. Therefore, the proposed approach seems quite competitive and promising in this era of big data.

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A Assumptions

Since the estimators Ĥk(t) and ˆΓW(s, t) are estimated by local linear smoothers, it is natural to make the standard smoothness assumptions on the second derivatives of µk and ΓW. It is assumed that in class k, the data (T,i, Yk,i), i = 1, · · · , nk, have the same distribution, where T,k,i = (Tk,i1, · · · , Tk,imk,i) and Yk,i = (Yk,i1, · · · , Yk,imk,i). Notice that (Tk,ij, Yk,ij) and (Tk,it, Yk,it) are dependent but identically distributed. Assume the density of time at observation to be g(t). Suppose Yk,ij = µk(Tk,ij) + Uk,ij, where cov(Ui(s), Ui(t)) = ΓW(s, t) + σ2I(s = t) and ΓW(s, t) = ∑∞ℓ=1 λℓφℓ(s)φℓ(t). Additional assumptions and conditions are listed below and similar ones can be found in Li and Hsing (2010).

A.1 For some constant Δt > 0 and ΔT < ∞, Δt ≤ g(t) ≤ ΔT for all t ∈ T. Further, g(·) is differentiable with a bounded derivative.

A.2 The kernel function K(·) is a symmetric probability density function on [−1, 1] and is of bounded variation on [−1, 1]. Further, we denote ν2 = ∫−1 1 u2K(u)du.

A.3 The mean function µk’s are twice differentiable and their second derivatives are bounded.

A.4 E(|Uk,ij|^λ) < ∞ and E( supt∈T |Xk(t)|δ ) < ∞ for some δ ∈ (2, ∞); hk → 0 and (hk/γn)−1(log nk/nk)^1/2δ → 0 as nk → ∞.

A.5 All second-order partial derivatives of ΓW exist and are bounded on T × T.

A.6 E(|Uk,ij|2δφ) < ∞ and E( supt∈T |Xk(t)|2δφ ) < ∞ for some δφ ∈ (2, ∞); hW → 0 and (hW/γn1 + hW/γn2)^−1(log n/n)^1/2δφ → 0 as n → ∞.

A.7 ⟨µk, φi⟩ ≤ Di−α for some positive constant D, where α > 1.
B  Bandwidth Selection

The bandwidths of $\hat{\mu}_k$’s and that of $\hat{\Gamma}_W$ are chosen via leave-one-curve-out CV as suggested by Rice and Silverman (1991). Specifically,

$$h_k = \arg \min_{h \in \mathbb{R}^+} \sum_{j=1}^{n_k} \sum_{\ell=1}^{m_{k,j}} \frac{1}{m_{k,j}} \sum_{t=1}^{m_{k,j}} \left\{ Y_{k,jt} - \hat{\mu}_k^{(-j)}(t_{k,jt}) \right\}^2,$$

where $\hat{\mu}_k^{(-j)}(t_{k,jt})$ is the estimated $\mu_k(t_{k,jt})$ when $h$ is the bandwidth and the observations of the $j$-th curve are not used to estimate $\mu_k$. Similarly, the bandwidth for $\hat{\Gamma}_W$ is defined as

$$h_W = \arg \min_{h \in \mathbb{R}^+} \sum_{k=1}^{c} \sum_{j=1}^{n_k} \sum_{\ell=1}^{m_{k,j}} \frac{1}{m_{k,j}(m_{k,j} - 1)} \sum_{1 \leq \ell_1 \neq \ell_2 \leq m_{k,j}} \left\{ R_{k,jt_1,\ell_1} - \hat{\Gamma}_W^{(-j)}(t_{k,jt_1}, t_{k,j\ell_2}) \right\}^2,$$

where $\hat{\Gamma}_W^{(-j)}(t_{k,jt_1}, t_{k,j\ell_2})$ is the estimated $\Gamma_W(t_{k,jt_1}, t_{k,j\ell_2})$ when $h$ is the bandwidth and $R_{k,jt_1,\ell_1}$’s of the $j$-th curve are not used to estimate $\Gamma_W$.

C  Some Details for Section 2.1

C.1  $\{\beta_i\}_{i=1}^{c'} \in \mathcal{P}_W^{-}(S_B)$

To show: $\beta_j = \psi_j$ for $j = 1, \ldots, c'$

Note that $\mu_k(t) = r_k(t) + r_k^*(t)$ for $t \in T$, where $r_k \in \mathcal{P}_W^{-}(S_B)$ and $r_k^*(t) = \sum_{j=1}^{\infty} \langle \mu_k, \phi_j \rangle \phi_j(t)$ is in $\mathcal{P}_W(S_B)$. Simple calculations lead to $\Gamma_B = \Gamma_{B\setminus W} + R_e$, where

$$\Gamma_B(s,t) = \sum_{k=1}^{c'} \pi_k \mu_k(s) \mu_k(t),$$

and

$$\Gamma_{B\setminus W}(s,t) = \sum_{k=1}^{c} \pi_k r_k(s) r_k(t).$$

Clearly, $\langle \beta, \Gamma_B \beta \rangle = \langle \beta, \Gamma_{B\setminus W} \beta \rangle$ if $\beta \in \mathcal{P}_W^{-}(S_B)$. Therefore, $\beta_j = \psi_j$.

C.2  $\{\beta_i\}_{i=c'+1}^{c'+c''} \in \mathcal{P}_W(S_B)$

To show: $\beta(t) = \sum_{i=1}^{c''} a_i \psi_i^*(t)$

Since $\mathcal{P}_W(S_B)$ is the space spanned by $\{r_k^*\}_{k=1}^{c}$ and $\psi_i^*$’s are the eigenfunctions of $\Gamma_{BW}$, a given $\beta \in \mathcal{P}_W(S_B)$ can be represented as $\beta(t) = \sum_{i=1}^{c''} a_i \psi_i^*(t)$, where $a_i$’s are basis coefficients. Direct calculations lead to

$$\langle \beta, \Gamma_{BW} \beta \rangle = a^T \Omega_B a, \quad (C.1)$$

and

$$\langle \beta, \Gamma_W \beta \rangle = a^T \Omega_W a. \quad (C.2)$$
Combining (C.1) and (C.2), (2.2) becomes

\[
\max_{\beta \in \mathcal{P}_W(S_B), \|\beta\|=1} \frac{\langle \beta, \Gamma_B \beta \rangle}{\langle \beta, \Gamma_W \beta \rangle} = \max_{\beta=\sum_{i=1}^{m'} a_i \psi_i^*} \frac{\langle \beta, \Gamma_B \beta \rangle}{\langle \beta, \Gamma_W \beta \rangle} = \max_{\|a\|=1} \frac{a^T \Omega_B a}{a^T \Omega_W a}, \tag{C.3}
\]

because \(\langle \beta, \Gamma_B \beta \rangle = \langle \beta, \Gamma_W \beta \rangle\) when \(\beta \in \mathcal{P}_W(S_B)\), and \(\|\beta\|=1\) implies \(\|a\|=1\). Therefore, (2.2) is equivalent to (C.3). Since \(\mathcal{P}_W(S_B) \subseteq S_W\), \(\Omega_W\) is nonsingular and thus invertible. As a result, (C.3) is equivalent to (2.7). Once \(a\) is solved by (2.7), we have \(\beta(t) = \sum_{i=1}^{m'} a_i \psi_i^*(t)\).

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