Sparse Fisher’s discriminant analysis with thresholded linear constraints

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Abstract
Various regularized linear discriminant analysis (LDA) methods have been proposed to address the problems of the classic methods in high-dimensional settings. Asymptotic optimality has been established for some of these methods in high dimension when there are only two classes. A major difficulty in proving asymptotic optimality for multiclass classification is that the classification boundary is typically complicated and no explicit formula for classification error generally exists when the number of classes is greater than two. For the Fisher’s LDA, one additional difficulty is that the covariance matrix is also involved in the linear constraints. The main purpose of this paper is to establish asymptotic consistency and asymptotic optimality for our sparse Fisher’s LDA with thresholded linear constraints in the high-dimensional settings for arbitrary number of classes. To address the first difficulty above, we provide asymptotic optimality and the corresponding convergence rates in high-dimensional settings for a large family of linear classification rules with arbitrary number of classes, and apply them to our method. To overcome the second difficulty, we propose a thresholding approach to avoid the estimate of the covariance matrix. We apply the method to the classification problems for multivariate functional data through the wavelet transformations.

Key Words: Sparse Fisher’s discriminant analysis; linear discriminant analysis; thresholded linear constraints; asymptotic consistency; asymptotic optimality, convergence rate.

Short title: Sparse FDA with thresholded linear constraints

1 Introduction

The linear discriminant analysis (LDA) has been a favored tool for classification in the settings of small $p$ and large $n$. The Fisher’s discriminant analysis is one of its important
special cases. However, these classic methods face major problems for high-dimensional data. In theory, Bickel and Levina (2004) and Shao et al. (2011) showed that the usual LDA can be as bad as the random guessing when \( p > n \). In practice, the classic methods have poor predictive performance in high-dimensional settings. To address these problems, various regularized discriminant analysis methods have been proposed, including Friedman (1989), Krzanowski et al. (1995), Dudoit et al. (2001), Bickel and Levina (2004), Guo et al. (2007), Xu et al. (2009), Tibshirani et al. (2002), Witten and Tibshirani (2011), Clemmensen et al. (2011), Shao et al. (2011), Cai and Liu (2011), Fan et al. (2012), Qi et al. (2015) and many others.

Asymptotic optimality has been established in some of these papers when there are two classes. Shao et al. (2011) made sparsity assumptions on both the difference \( \delta = \mu_2 - \mu_1 \), where \( \mu_1 \) and \( \mu_2 \) are the population means of the two classes, and the within-class covariance matrix \( \Sigma \). Then they applied thresholding procedures to both the sample estimates of \( \delta \) and \( \Sigma \), and obtained the asymptotic optimality and the corresponding convergence rate for their classification rule. Cai and Liu (2011) observed that in the case of two classes, the optimal classification rule depends on \( \Sigma \) only through \( \Sigma^{-1}\delta \). Hence, they assumed \( l_1 \) sparsity for \( \Sigma^{-1}\delta \), proposed a sparse estimate of it through minimizing its \( l_1 \) norm with an \( l_{\infty} \) constraint, and provided asymptotic optimality of their classification rule. Fan et al. (2012) imposed \( l_0 \) sparsity assumption on \( \Sigma^{-1}\delta \), estimated it through a minimization problem with an \( l_1 \) constraint and derived the asymptotic optimality. A difficulty preventing the derivation of asymptotic optimality of the linear classification rules for multiple classes is that for the two-class classification, the classification boundary of LDA is a hyperplane and an explicit formula for the classification error exists, however, for the multiclass classification, the classification boundary is usually complicated and no explicit formula for the classification error generally exist. The Fisher’s LDA projects the original variables \( X \) to a low dimensional subspace to generate new predictor variables, \( X\alpha_1, X\alpha_2, \ldots, X\alpha_{K-1} \), where the coefficient vectors \( \alpha_1, \alpha_2, \ldots, \alpha_{K-1} \) satisfy the linear constraints \( \alpha_i^T\Sigma\alpha_j = 0 \) for any \( 1 \leq j < i < K \), and \( K \) is the number of classes. These constraints imply that \( \alpha_i \) is orthogonal to the subspace spanned by \( \{\Sigma\alpha_1, \cdots, \Sigma\alpha_{i-1}\} \).

The motivation of this paper is to establish the asymptotic consistency and the asymp-
otic optimality of the sparse Fisher’s LDA method proposed in Qi, Luo, Carroll and Zhao (2015) in the high-dimensional settings for arbitrary number of classes. However, in order to obtain the asymptotic consistency, we revise the original method because it is hard to obtain a consistent estimate for a general $\Sigma$ in the high-dimensional settings without sparsity or other assumptions imposed on $\Sigma$. Instead of aiming to estimate $\Sigma$, we propose a soft-thresholding procedure and add it into the original method to get a consistent estimate of the subspace $\{\Sigma \alpha_1, \cdots, \Sigma \alpha_{i-1}\}$. We establish the asymptotic consistency of the estimates of $\alpha_i$ and the subspace $\{\Sigma \alpha_1, \cdots, \Sigma \alpha_{i-1}\}$ for the revised method. To prove the asymptotic optimality for this method, we establish the asymptotic optimality and the corresponding convergence rates in high-dimensional settings for a large family of linear classification rules with arbitrary number of classes under the situation of multivariate normal distribution. To assess the real performance of the revised method, we compare it with the original method and other sparse LDA methods through simulation studies. The revised method has good predictive performance as the original method and at the same time, it enjoys nice theoretical properties. We also apply the revised method to the classification problems for multivariate functional data through the wavelet transformations.

The rest of this paper is organized as follows. In Section 2, we introduce notations and briefly review the classic Fisher’s discriminant analysis. Our sparse Fisher’s LDA method with thresholded linear constraints is introduced in Section 3. In Section 4, we present the main theoretical results. Sections 5 and 6 are simulation studies and applications, respectively. The proofs of all theorems are provided in supplementary material.

2 Fisher’s discriminant analysis

We first introduce the notations used throughout the paper. For any vector $\mathbf{v} = (v_1, \cdots, v_p)^T$, let $\|\mathbf{v}\|_1$, $\|\mathbf{v}\|_2$, and $\|\mathbf{v}\|_\infty = \max_{1 \leq i \leq p} |v_i|$ denote the $l_1$, $l_2$, and $l_\infty$ norms of $\mathbf{v}$, respectively. For any $p \times p$ symmetric matrix $\mathbf{M}$, we use $\lambda_{max}(\mathbf{M})$, $\lambda_{min}(\mathbf{M})$ and $\lambda_{min}^+(\mathbf{M})$ to denote the largest eigenvalue, the smallest eigenvalue and the smallest positive eigenvalue of $\mathbf{M}$, respectively. Now suppose that $\mathbf{M}$ is symmetric and nonnegative definite. We define two norms
for $\mathbf{M}$,

$$
\|\mathbf{M}\| = \sup_{\mathbf{v} \in \mathbb{R}^p, \|\mathbf{v}\|_2 = 1} \|\mathbf{M}\mathbf{v}\|_2 = \lambda_{\text{max}}(\mathbf{M}), \quad \text{and} \quad \|\mathbf{M}\|_\infty = \max_{1 \leq k, l \leq p} |M_{kl}|,
$$

(2.1)

where $M_{kl}$ is the $(k, l)$-th entry of $\mathbf{M}$. The first norm is the usual operator norm and is also called the spectral norm. The second is the max norm.

Throughout this paper, we assume that the number $K$ of classes is fixed and can be any positive integer. Suppose that the population in the $i$-th class has a multivariate normal distribution $N_p(\mu_i, \Sigma)$, where $\mu_i$ is the true class mean of the $i$-th class, $1 \leq i \leq K$, and $\Sigma$ is the true common within-class covariance matrix for all classes. We assume that the prior probabilities for all the classes are the same and equal to $1/K$. It will be seen that when we add a constant vector to all the observations, the classification results do not change for all the classification rules involved in this paper. Therefore, without loss of generality, we assume that the overall mean of the whole population is zero, that is,

$$
\mu_1 + \mu_2 + \cdots + \mu_K = 0.
$$

(2.2)

Define a $p \times K$ matrix $\mathbf{U} = [\mu_1, \mu_2, \cdots, \mu_K]$, which is the collection of class means. Under the assumption (2.2), the between-class covariance matrix is

$$
\mathbf{B} = \sum_{i=1}^{K} \alpha_i \alpha_i^T / K = \mathbf{U} \mathbf{U}^T / K.
$$

(2.3)

The Fisher’s discriminant analysis method (when the true class means and the true covariance matrix are known) sequentially finds linear combinations $\mathbf{X} \alpha_1, \cdots, \mathbf{X} \alpha_{K-1}$ by solving the following generalized eigenvalue problem. Suppose that we have obtained $\alpha_1, \cdots, \alpha_{i-1}$, where $1 \leq i \leq K - 1$, then $\alpha_i$ is the solution to

$$
\max_{\alpha \in \mathbb{R}^p} \alpha^T \mathbf{B} \alpha, \quad \text{subject to} \quad \alpha^T \Sigma \alpha = 1, \quad \alpha^T \Sigma \alpha_j = 0, \quad 1 \leq j \leq i - 1.
$$

(2.4)

The Fisher’s classification rule is to assign a new observation $\mathbf{x}$ to class $i$ if

$$
(\mathbf{x} - \mu_i)^T \mathbf{D} (\mathbf{x} - \mu_i) < (\mathbf{x} - \mu_j)^T \mathbf{D} (\mathbf{x} - \mu_j)
$$

(2.5)

for all $1 \leq j \neq i \leq K$, where $\mathbf{D} = \sum_{k=1}^{K-1} \alpha_k \alpha_k^T$. 
It is well known that under our setting (that is, the population in each class has a normal distribution with the same covariance matrix and the prior probabilities for all classes are the same), the optimal classification rule is to assign a new observation $\mathbf{x}$ to class $i$ if

$$(\mathbf{x} - \mathbf{\mu}_i)^T \Sigma^{-1} (\mathbf{x} - \mathbf{\mu}_i) < (\mathbf{x} - \mathbf{\mu}_j)^T \Sigma^{-1} (\mathbf{x} - \mathbf{\mu}_j)$$

(2.6)

for all $1 \leq j \neq i \leq K$ (Theorem 6.8.1 in Anderson (2003) or Theorem 13.2 in Härdle and Simar (2012)). Moreover, the optimal rule (2.6) is equivalent to the Fisher’s discriminant rule (2.5).

In practice, the true class means and $\Sigma$ are unknown. Consider a training data set, $\mathbf{X} = \{\mathbf{x}_{ij} : 1 \leq i \leq K, 1 \leq j \leq n_i\}$, where $\mathbf{x}_{ij}$ is the $j$th observation from the $i$th class and $n_i$ is the number of the observations of the $i$th class. The numbers $(n_1, n_2, \ldots, n_K)$ can be either random or nonrandom. Let $n = \sum_{i=1}^{K} n_i$ be the total number of observations in the data. Throughout this paper, we use

$$\bar{\mathbf{x}}_i = \frac{1}{n_i} \sum_{j=1}^{n_i} \mathbf{x}_{ij}, \quad \bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^{K} \sum_{j=1}^{n_i} \mathbf{x}_{ij}, \quad \hat{\Sigma} = \frac{1}{n-K} \sum_{i=1}^{K} \sum_{j=1}^{n_i} (\mathbf{x}_{ij} - \bar{\mathbf{x}}_i)(\mathbf{x}_{ij} - \bar{\mathbf{x}}_i)^T,$$

$$\hat{\mathbf{B}} = \frac{1}{n} \sum_{i=1}^{K} n_i (\bar{\mathbf{x}}_i - \bar{\mathbf{x}})(\bar{\mathbf{x}}_i - \bar{\mathbf{x}})^T, \quad 1 \leq i \leq K,$$

(2.7)

to denote the sample class means, the sample overall mean, the sample within-class covariance matrix and the sample between-class covariance matrix, respectively. Then the classic Fisher’s discriminant analysis is to sequentially obtain the estimates $\hat{\alpha}_1, \ldots, \hat{\alpha}_{K-1}$ of $\alpha_1, \ldots, \alpha_{K-1}$ by solving

$$\max_{\mathbf{\alpha} \in \mathbb{R}^p} \mathbf{\alpha}^T \hat{\mathbf{B}} \mathbf{\alpha}, \quad \text{subject to} \quad \mathbf{\alpha}^T \hat{\Sigma} \mathbf{\alpha} = 1, \quad \mathbf{\alpha}^T \hat{\Sigma} \hat{\alpha}_j = 0, \quad 1 \leq j < i,$$

(2.8)

where $1 \leq i \leq K - 1$. The classification rule is to assign a new observation $\mathbf{x}$ to class $i$ if

$$(\mathbf{x} - \bar{\mathbf{x}}_i)^T \tilde{\mathbf{D}} (\mathbf{x} - \bar{\mathbf{x}}_i) < (\mathbf{x} - \bar{\mathbf{x}}_j)^T \tilde{\mathbf{D}} (\mathbf{x} - \bar{\mathbf{x}}_j),$$

(2.9)

for all $1 \leq j \neq i \leq K$, where $\tilde{\mathbf{D}} = \sum_{k=1}^{K-1} \hat{\alpha}_k \hat{\alpha}_k^T$. 

3 Sparse Fisher’s discriminant analysis with thresholded linear constraints

In the high-dimensional setting, the classic Fisher’s discriminant analysis has several drawbacks. First, $\hat{\Sigma}$ is not full rank, so the solution to (2.8) does not exist. Second, $\hat{B}$ and $\hat{\Sigma}$ as given in (2.7) are not consistent estimates in terms of the operator norm. Hence, the estimates of $\alpha_k$, $1 \leq k \leq K - 1$, obtained by classic Fisher’s discriminant analysis are not consistent. Third, suppose that we have obtained an estimate $\tilde{\alpha}_1$ of $\alpha_1$, in order to estimate $\alpha_2$, we have to estimate the coefficient vector of the linear constraint in (2.4), $\Sigma \alpha_1$. However, even if $\tilde{\alpha}_1$ is consistent, $\hat{\Sigma} \tilde{\alpha}_1$ is not a consistent estimate of $\Sigma \alpha_1$ due to the inconsistency of $\hat{\Sigma}$. To address these drawbacks, we describe a revised method of the sparse Fisher’s discriminant analysis in Qi et al. (2015).

3.1 The case of $K = 2$

When there are two classes, there is only one component $\alpha_1$ and $B = (\mu_1 \mu_1^T + \mu_2 \mu_2^T)/2 = \mu_1 \mu_1^T$ because $\mu_1 = -\mu_2$. It is easily seen that $\alpha_1 = \Sigma^{-1} \delta / \sqrt{\delta^T \Sigma^{-1} \delta}$, where $\delta = \mu_2 - \mu_1$. Cai and Liu (2011) and Fan et al. (2012) imposed $l_1$ and $l_0$ sparsity assumptions on $\Sigma^{-1} \delta$, respectively. Equivalently, we assume that $\alpha_1$ is sparse in terms of $l_1$ norm as in Cai and Liu (2011). In the case of $K = 2$, it is not necessary to revise the original method in Qi et al. (2015). The estimate $\hat{\alpha}_1$ of $\alpha_1$ is the solution to

$$\max_{\alpha \in \mathbb{R}^p} \alpha^T \hat{B} \alpha, \quad \text{subject to} \quad \alpha^T \hat{\Sigma} \alpha + \tau \|\alpha\|_1^2 = 1,$$

where $\|\alpha\|_2^2 = (1 - \lambda)\|\alpha\|_2^2 + \lambda \|\alpha\|_1^2$ and both $\tau \geq 0$ and $0 \leq \lambda \leq 1$ are tuning parameters. The introduction of $\|\alpha\|_2^2$ overcomes the issue that $\hat{\Sigma}$ is not full rank in high-dimensional setting, and the term $\|\alpha\|_1^2$ encourages the sparsity of the solution. A difference between our penalty and the usual lasso or elastic-net penalty is that we use the squared $l_1$-norm. This particular form of our penalty leads to the property that $\hat{\alpha}_1$ is also the solution to

$$\max_{\alpha \in \mathbb{R}^p, \alpha \neq 0} \frac{\alpha^T \hat{B} \alpha}{\alpha^T \hat{\Sigma} \alpha + \tau \|\alpha\|_1^2},$$
where the objective function is scale-invariant. That is, for any nonzero number $t$, the vector $t\hat{\alpha}_1$ is also a solution to (3.2). This scale-invariant property is intensively used in our theoretical development. Once we obtain $\hat{\alpha}_1$, our classification rule is to assign a new observation $x$ to class $i$ if $(x - \bar{x}_i)^T\hat{D}(x - \bar{x}_i) < (x - \bar{x}_j)^T\hat{D}(x - \bar{x}_j)$ for $1 \leq j \neq i \leq 2$, where $\hat{D} = \hat{\alpha}_1\hat{\alpha}_1^T$.

### 3.2 The case of $K > 2$

If $K > 2$, more than one components need to be estimated. $\alpha_1$ is estimated in the same way as $K = 2$. Since the higher order component $\alpha_i$, $1 < i \leq K - 1$, satisfies the constraints in (2.4), $\alpha_i$ is actually orthogonal to the subspace spanned by $\{\Sigma\alpha_1, \ldots, \Sigma\alpha_{i-1}\}$ in $\mathbb{R}^p$. Because $\alpha_i$ is the eigenvector of the generalized eigenvalue problem (2.4), for any $1 \leq j < K - 1$, $B\alpha_j$ and $\Sigma\alpha_j$ have the same directions and only differ by a scale factor, which is the $j$-th eigenvalue. Hence, the subspace spanned by $\{B\alpha_1, \ldots, B\alpha_{i-1}\}$ is the same as that of $\{\Sigma\alpha_1, \ldots, \Sigma\alpha_{i-1}\}$.

Because in the high-dimensional settings, $\hat{\Sigma}$ and $\hat{B}$ are not consistent estimates of $\Sigma$ and $B$ in terms of the operator norm, respectively, neither of the subspaces spanned by $\{\hat{\Sigma}\hat{\alpha}_1, \ldots, \hat{\Sigma}\hat{\alpha}_{i-1}\}$ and $\{\hat{B}\hat{\alpha}_1, \ldots, \hat{B}\hat{\alpha}_{i-1}\}$ is a consistent estimate of the subspace spanned by $\{\Sigma\alpha_1, \ldots, \Sigma\alpha_{i-1}\}$ (or by $\{B\alpha_1, \ldots, B\alpha_{i-1}\}$), even if $\hat{\alpha}_j$, $1 \leq j \leq i - 1$, are consistent estimates. Therefore, in order to estimate these subspaces, in addition to the sparsity assumption on $\{\alpha_1, \ldots, \alpha_{K-1}\}$, we also make sparsity assumptions on the vectors, $\Sigma\alpha_1, \ldots, \Sigma\alpha_{K-1}$, in terms of $l_1$ norm. Lemma 2 in Section 4 shows that making sparsity assumptions on $\Sigma\alpha_1, \ldots, \Sigma\alpha_{K-1}$ is equivalent to or weaker than assuming the sparsity of $\{\mu_i - \mu_j, 1 \leq i \neq j \leq K\}$ in terms of $l_1$ norm. The latter assumption has been made in Shao et al. (2011). Bickel and Levina (2004) assumes that $\mu_1$ and $\mu_2$ are sparse when $K = 2$, which implies that $\mu_1 - \mu_2$ is sparse.

Under the above assumptions, suppose that we have obtained the estimate $\hat{\alpha}_j$ of $\alpha_j$, $1 \leq j \leq i - 1$, then we obtain the estimate $\hat{\xi}_j$ of $B\alpha_j$ as the solution to

$$\min_{\xi \in \mathbb{R}^p} \left[ \|\xi - \hat{B}\hat{\alpha}_j\|_2^2 + \kappa\|\xi\|_1 \right],$$

(3.3)
where $\kappa \geq 0$ is a tuning parameter. It can be shown that the $l$-th coordinate of $\hat{\xi}_j$ is
\[
(\hat{\xi}_j)_l = \text{sign}((\hat{B}\hat{\alpha}_j)_l) \left[ \left| (\hat{B}\hat{\alpha}_j)_l \right| - \kappa/2 \right] I_{\left| (\hat{B}\hat{\alpha}_j)_l \right| \geq \kappa/2}; \quad 1 \leq l \leq p,
\]
(3.4)
where $I_{\left| (\hat{B}\hat{\alpha}_j)_l \right| \geq \kappa/2}$ is the indicator function of $\left| (\hat{B}\hat{\alpha}_j)_l \right| \geq \kappa/2$. So we actually estimate $B\alpha_j$ by applying the soft-thresholding to $\hat{B}\hat{\alpha}_j$. We will show that the subspace spanned by $\{\hat{\xi}_1, \ldots, \hat{\xi}_{i-1}\}$ is a consistent estimate of the subspace spanned by $\{B\alpha_1, \ldots, B\alpha_{i-1}\}$ and provide the convergence rate in Section 4. An alternative way to obtain a consistent estimate of the subspace is to apply the soft-thresholding to $\hat{\Sigma}\hat{\alpha}_1, \ldots, \hat{\Sigma}\hat{\alpha}_{i-1}$. However, it turns out that the real predictive performance of this alternative is inferior to the proposed, so we do not consider it in this paper. Now suppose that we have obtained the estimates $\hat{\alpha}_1, \ldots, \hat{\alpha}_{i-1}$ and $\hat{\xi}_1, \ldots, \hat{\xi}_{i-1}$, then $\hat{\alpha}_i$ is the solution to
\[
\max_{\alpha \in \mathbb{R}^p} \alpha^T \hat{B}\alpha, \quad \text{subject to} \quad \alpha^T \hat{\Sigma}\alpha + \tau \|\alpha\|_\lambda^2 = 1, \quad \alpha^T \hat{\xi}_j = 0, \quad j < i.
\]
(3.5)
The optimization problems (3.1) and (3.5) are both special cases of the following general problem:
\[
\max_{\alpha \in \mathbb{R}^p} \alpha^T \Pi\alpha, \quad \text{subject to} \quad \alpha^T C\alpha + \tau \|\alpha\|_\lambda^2 \leq 1, \quad L\alpha = 0,
\]
(3.6)
where $\Pi$ and $C$ are any two $p \times p$ nonnegative definite symmetric matrices, and $L$ is either equal to zero or any matrix with $p$ columns. $L\alpha = 0$ can be viewed as linear constraints imposed on $\alpha$. For example, (3.5) is the special case of (3.6) with $\Pi = \hat{B}$, $C = \hat{\Sigma}$ and $L = (\hat{\xi}_1, \ldots, \hat{\xi}_{i-1})^T$. In Qi et al. (2015), we solve (3.6) by the following algorithm.

Algorithm 3.1.

1. Choose an initial vector $\alpha^{(0)}$ with $\Pi\alpha^{(0)} \neq 0$.
2. Iteratively compute a sequence $\alpha^{(1)}, \alpha^{(2)}, \ldots, \alpha^{(i)}, \ldots$ until convergence as follows: for any $i \geq 1$, compute $\alpha^{(i)}$ by solving
\[
\max_{\alpha \in \mathbb{R}^p} (\Pi\alpha^{(i-1)})^T \alpha, \quad \text{subject to} \quad \alpha^T C\alpha + \tau \|\alpha\|_\lambda^2 \leq 1, \quad L\alpha = 0.
\]
(3.7)
The key step (3.7) of Algorithm 3.1 is a special case of the following problem with \( c = \Pi\alpha^{(i-1)} \):

\[
\max_{\alpha} c^T \alpha, \quad \text{subject to} \quad \alpha^T C \alpha + \tau \|\alpha\|_2^2 \leq 1, \quad L \alpha = 0,
\]

(3.8)

where \( c \) is any nonzero vector. The algorithm and the related theory to solve (3.8) have been developed and described in details in Qi et al. (2015).

Once we obtain all the estimates \( \hat{\alpha}_1, \ldots, \hat{\alpha}_{K-1} \), we build the classification rule which assigns a new observation \( x \) to class \( i \) if

\[
(x - \bar{x}_i)^T \hat{D}(x - \bar{x}_i) < (x - \bar{x}_j)^T \hat{D}(x - \bar{x}_j),
\]

(3.9)

for all \( 1 \leq j \neq i \leq K \), where

\[
\hat{D} = (\hat{\alpha}_1, \ldots, \hat{\alpha}_{K-1}) \hat{K}^{-1} (\hat{\alpha}_1, \ldots, \hat{\alpha}_{K-1})^T,
\]

(3.10)

and \( \hat{K} \) is a symmetric \((K-1) \times (K-1)\) matrix with the \((i, j)\)-th entry equal to \( \hat{\alpha}_i^T \hat{\Sigma} \hat{\alpha}_j \). This choice of \( \hat{D} \) allows us to achieve a better convergence rate than \( \tilde{D} \) used in the classic Fishers discriminant analysis rule (2.9).

In Qi et al. (2015), we proposed to estimate \( \alpha_i \) by solving

\[
\max_{\alpha \in \mathbb{R}^p} \alpha^T \hat{B} \alpha, \quad \text{subject to} \quad \alpha^T \hat{\Sigma} \alpha + \tau \|\alpha\|_2^2 = 1, \quad \alpha^T \hat{B} \hat{\alpha}_j = 0, \quad j < i,
\]

(3.11)

where we used the unthresholded vector \( \hat{B} \hat{\alpha}_j \) in the linear constraints. That method has a good empirical performance, but we cannot provide the theoretical results due to the difficulty mentioned at the beginning of Section 3.

4 Asymptotic consistency and asymptotic optimality

In this section, we will provide the asymptotic results of the method described in Section 3. We first consider two mechanisms of class label generation. The first is a random mechanism in which sample observations are randomly drawn from any of \( K \) classes with equal probability \( 1/K \). Hence, \((n_1, n_2, \ldots, n_K)\) follows a multinomial distribution with parameters \( n \) and \((1/K, \ldots, 1/K)\). In this case, we have the following result.
**Lemma 1.** Suppose that \((n_1, n_2, \cdots, n_K)\) follows a multinomial distribution with parameters \(n\) and \((1/K, \cdots, 1/K)\). Given any \((K, n, p)\) satisfying that \(p \geq 2\), \(K \leq p + 1\) and \(\sqrt{K \log p/n}\) is bounded by some constant \(d_0\), for any \(M > 0\), we have

\[
P \left( \max_{1 \leq i \leq K} \left| \frac{n_i}{n} - \frac{1}{K} \right| > C \sqrt{\frac{\log p}{Kn}} \right) \leq p^{-M} \tag{4.1} \]

for any \(C \geq (M + 3)(d_0 + 1)\).

The second mechanism is nonrandom, that is, \((n_1, n_2, \cdots, n_K)\) are nonrandom numbers. In this case, we will impose the following Condition 1 (a) on these numbers.

**Condition 1.**

(a). If \((n_1, n_2, \cdots, n_K)\) are nonrandom, then there exists a constant \(C_0\) (independent of \(n, p\) and \(K\)), such that we have \(\max_{1 \leq i \leq K} |n_i/n - 1/K| \leq C_0 \sqrt{\log p/(Kn)}\) for all large enough \(n\).

(b). There exists a constant \(c_0 > 0\) (independent of \(n, p\) and \(K\)) such that

\[
c_0^{-1} \leq \lambda_{\min}(\Sigma) \leq \lambda_{\max}(\Sigma) \leq c_0 \quad \text{and} \quad \max_{1 \leq i \leq K} \|\mu_i\|_{\infty} \leq c_0.
\]

Lemma 1 and Condition 1 (a) ensure that the number of observations in different classes do not differ greatly in each of the two mechanisms. The regularity condition for \(\Sigma\) in Condition 1 (b) has been used in Shao et al. (2011) and Cai and Liu (2011). The condition about \(\mu_i\) can be achieved by scaling each of the \(p\) variables. Under Condition 1, we have the following two probability inequalities about \(\|\hat{\Sigma} - \Sigma\|_{\infty}\) and \(\|\hat{B} - B\|_{\infty}\), which play basic roles in our theoretical development.

**Theorem 4.1.** Suppose that Condition 1 holds, \(p \geq 2\), \(K \leq p + 1\) and \(K \log p/n \to 0\) as \(n \to \infty\). Then for any \(M > 0\), we can find \(C\) large enough and independent of \(n, p\) and \(K\) such that

\[
P \left( \|\hat{\Sigma} - \Sigma\|_{\infty} > C \sqrt{\frac{K \log p}{n}} \right) \leq p^{-M}, \quad P \left( \|\hat{B} - B\|_{\infty} > C \sqrt{\frac{K \log p}{n}} \right) \leq p^{-M}
\]

for all large enough \(n\).
Remark 1. Theorem 4.1 holds even if $K \to \infty$ as $n \to \infty$. However, since we need the condition that $K$ is bounded in the following theorems, we fix $K$ in this paper.

Define a $p \times p$ nonnegative definite matrix

$$\Xi = \Sigma^{-1/2} \mathbf{B} \Sigma^{-1/2}. \quad (4.2)$$

Solving the generalized eigenvalue problem (2.4) is equivalent to computing the eigenvalues and eigenvectors of $\Xi$. In fact, because $\alpha_k$, $1 \leq k \leq K - 1$, are the generalized eigenvectors of the problem (2.4), we have

$$\mathbf{B} \alpha_k = \nu_k \Sigma \alpha_k, \quad \text{and hence,} \quad \Xi \Sigma^{1/2} \alpha_k = \nu_k \Sigma^{1/2} \alpha_k, \quad (4.3)$$

for any $1 \leq k \leq K - 1$, where $\nu_k$ is the corresponding generalized eigenvalue. Therefore,

$$\gamma_1 = \Sigma^{1/2} \alpha_1, \quad \gamma_2 = \Sigma^{1/2} \alpha_2, \quad \cdots, \quad \gamma_{K-1} = \Sigma^{1/2} \alpha_{K-1}, \quad (4.4)$$

are the eigenvectors of $\Xi$ with corresponding eigenvalues $\nu_1, \nu_2, \ldots, \nu_{K-1}$, respectively. So they are orthogonal to each other. In the following, we will use $\lambda_k(\Xi)$, $1 \leq k \leq K - 1$, to denote the eigenvalues of $\Xi$, which are just the above generalized eigenvalues and also equal to the maximum values of the optimization problems (2.4). Since $\Xi$ has the same rank as $\mathbf{B}$ which is not greater than $K - 1$ due to the constraint (2.2), $\Xi$ has at most $K - 1$ positive eigenvalues. By the conditions $\alpha_k^T \Sigma \alpha_k = 1$, $1 \leq k \leq K - 1$, we have

$$\|\gamma_1\|_2 = \|\gamma_2\|_2 = \cdots = \|\gamma_{K-1}\|_2 = 1. \quad (4.5)$$

which are estimates of $\gamma_1, \cdots, \gamma_{K-1}$, respectively. Since $-\hat{\mathbf{a}}_k$ is also the solution to the optimization problem in (3.1) or (3.5), without loss of generality, we choose the sign of $\hat{\mathbf{a}}_k$ such that $\hat{\gamma}_k^T \gamma_k \geq 0$, for $1 \leq k \leq K - 1$. We impose the following regularity conditions on the eigenvalues of $\Xi$.

**Condition 2.** There exist positive constants $c_1, c_2$ and $c_3$ which are all independent of $n$, $p$ and $K$ such that

(a). $\lambda_1(\Xi) \geq \lambda_2(\Xi) \geq \cdots \geq \lambda_{K-1}(\Xi) \geq c_1,$
(b). \( \min \left\{ \frac{\lambda_1(\Xi)}{\lambda_1(\Xi)} - \frac{\lambda_2(\Xi)}{\lambda_2(\Xi)}, \ldots, \frac{\lambda_{K-2}(\Xi)}{\lambda_{K-2}(\Xi)} - \frac{\lambda_{K-1}(\Xi)}{\lambda_{K-1}(\Xi)} \right\} \geq c_2, \)

(c). The ratio between the largest and the smallest eigenvalue satisfies \( \lambda_1(\Xi)/\lambda_{K-1}(\Xi) \leq c_3. \)

In the case of \( K = 2, \) we will show in Remark 2 (3) that \( \lambda_1(\Xi) \) has the same order as \( \| \mu_2 - \mu_1 \|^2. \) Therefore, roughly speaking, Condition 2 (a) implies that the class means are not too close to each other. Condition 2 (b) prevents the cases that the spacing between adjacent eigenvalues is too small. Condition 2 (c) excludes the situations where the effects of higher order components are dominated by those of lower order components and are negligible asymptotically.

Now we consider the choice of the tuning parameters, \( \tau \) and \( \lambda, \) in the penalized optimization problems (3.1) and (3.5). We will show that the choice of \( \lambda \) is not essential for the asymptotic convergence rates as long as it is asymptotically bounded away from zero. In the following theorems, we will choose tuning parameters \( (\tau_n, \lambda_n) \), which depend on the sample size \( n, \) satisfying

\[
0 < \lambda_n < 1, \quad \lim \inf_{n \to \infty} \lambda_n > \lambda_0, \quad \tau_n = C s_n, \quad \text{where} \quad s_n = \sqrt{\frac{K \log p}{n}}, \tag{4.6}
\]

\( \lambda_0 > 0 \) and \( C \) are constants independent of \( n, p \) and \( K. \) The constant \( C \) is chosen based on Theorem 4.1 such that for all large enough \( n, \)

\[
P\left( \| \hat{\Sigma} - \Sigma \|_\infty > \frac{C}{C_2 s_n} \right) \leq p^{-1}, \quad P\left( \| \hat{B} - B \|_\infty > \frac{C}{C_2 s_n} \right) \leq p^{-1}, \tag{4.7}
\]

where \( C_2 = 2(1 + c_1^{-1})/\lambda_0 \) and \( c_1 \) is the constant in Condition 2 (a). Define the event

\[
\Omega_n = \left\{ \| \hat{\Sigma} - \Sigma \|_\infty \leq \tau_n/C_2, \quad \| \hat{B} - B \|_\infty \leq \tau_n/C_2 \right\}, \tag{4.8}
\]

then by (4.7) \( P(\Omega_n) \geq 1 - 2p^{-1}. \)

We mainly consider the elements in \( \Omega_n \) in proofs.

We adopt the same definition of asymptotic optimality for a linear classification rule as in Shao et al. (2011), Cai and Liu (2011), Fan et al. (2012) and other papers. Let \( T_{OPT} \) denote the optimal linear classification rule (2.5) or (2.6) and \( R_{OPT} \) represent its misclassification error rate. Let \( T \) be any linear classification rule based on \( X. \) The conditional
The misclassification rate of $T$ given $X$ is defined as

$$R_T(X) = \sum_{i=1}^{K} P \left( \{ x_{\text{new}} \text{ belongs to the } i\text{-th class but } T(x_{\text{new}}) \neq i \} \mid X \right)$$

where $x_{\text{new}}$ is a new observation independent of $X$. Therefore, $R_T(X)$ is a function of $X$.

**Definition 1.** Let $T$ be a linear classification rule with conditional misclassification rate $R_T(X)$. Then $T$ is asymptotically optimal if

$$\frac{R_T(X)}{R_{OPT}} - 1 = o_p(1).$$

(4.9)

Since $0 \leq R_{OPT} \leq R_T(X) \leq 1$ for any $X$, (4.9) implies that $0 \leq R_T(X) - R_{OPT} = o_p(1)$. Hence we have $R_T(X) \to R_{OPT}$ in probability and $E[R_T(X)] \to R_{OPT}$, which have been used to define the consistency of a classification rule by Devroye et al. (1996) and others. If $R_{OPT}$ is bounded away from 0, then $R_T(X) - R_{OPT} = o_p(1)$ also implies (4.9). However, if $R_{OPT} \to 0$, (4.9) is stronger than $R_T(X) - R_{OPT} = o_p(1)$.

In the following, we will consider the asymptotic properties of our method and assume that $K$ is fixed, $p \to \infty$ and $s_n = \sqrt{K \log p/n} \to 0$ as $n \to \infty$. The following theorem provides an upper bound for the $l_1$ sparsity and the consistency of the estimator $\hat{\alpha}_1$ obtained from (3.1).

**Theorem 4.2.** Suppose that Conditions 1 and 2 hold. If $\|\alpha_1\|_1^2 s_n \to 0$ as $n, p \to \infty$, then for all large enough $n$, we have, in $\Omega_n$,

$$\|\hat{\alpha}_1\|_1^2 \leq 6\|\alpha_1\|_1^2 / \lambda_0, \quad \|\hat{\gamma}_1 - \gamma_1\|_2^2 \leq C_5\|\alpha_1\|_1^2 s_n, \quad (4.10)$$

$$\|\hat{\alpha}_1 - \alpha_1\|_2^2 \leq c_0 C_5\|\alpha_1\|_1^2 s_n,$$

where $C_5$ is a constant independent of $n$ and $p$, $\lambda_0$ is the constant in (4.6), and $c_0$ is the constant in Condition 1 (b). Therefore, $\hat{\alpha}_1$ is a consistent estimate of $\alpha_1$.

By Theorem 4.2, the estimate $\hat{\alpha}_1$ has the same order of $l_1$ sparsity as $\alpha_1$ and in order that $\hat{\alpha}_1$ is consistent, we need $\|\alpha_1\|_1^2$ is $o(\sqrt{n/\log p})$. In the following, we will consider the cases of $K = 2$ and $K > 2$, separately.
4.1 The case of $K = 2$

When $K = 2$, there exists only one component $\alpha_1$ and $\Xi$ has one positive eigenvalue $\lambda_1(\Xi)$. Therefore, Conditions 2 (b)-(c) are not necessary. We provide explicit formulas for the misclassification errors of the optimal rule with $D = \alpha_1\alpha_1^T$ and our rule with $\hat{D} = \hat{\alpha}_1\hat{\alpha}_1^T$, and prove the asymptotic optimality of our method in the following theorem.

**Theorem 4.3.** Suppose that $K = 2$ and Conditions 1 and 2 (a) hold. Then the misclassification rate of the optimal rule (2.5) and the conditional misclassification rate of our sparse LDA rule in Section 3.1 are given by

$$R_{OPT} = \Phi \left( -\frac{\delta^T D \delta}{2 \|\delta^T D \Sigma^{1/2}\|_2} \right),$$

$$R(X) = \frac{1}{2} \Phi \left( -\frac{\delta^T \hat{D}(2\mu_2 - \bar{x}_1 - \bar{x}_2)}{2 \|\delta^T \hat{D} \Sigma^{1/2}\|_2} \right) + \frac{1}{2} \Phi \left( -\frac{\delta^T \hat{D}(\bar{x}_1 + \bar{x}_2 - 2\mu_1)}{2 \|\delta^T \hat{D} \Sigma^{1/2}\|_2} \right),$$

respectively, where $\Phi$ is the cumulative distribution function of the standard normal distribution, $\delta = \mu_2 - \mu_1$ and $\hat{\delta} = \bar{x}_2 - \bar{x}_1$. Moreover, if $\lambda_1(\Xi)\|\alpha_1\|^2 s_n \to 0$ as $n, p \to \infty$, our method is asymptotically optimal and we have

$$\frac{R(X)}{R_{OPT}} - 1 = O_p \left( \lambda_1(\Xi)\|\alpha_1\|^2 s_n \right).$$

**Remark 2.**

(1). The misclassification rate of the optimal rule is expressed as $R_{OPT} = \Phi \left( -\sqrt{\delta^T \Sigma^{-1} \delta}/2 \right)$ in Equation (1) in Shao et al. (2011) and Equation (5) in Cai and Liu (2011). Since by Lemma ?? (Supplementary Material), $\Sigma^{-1} \delta = D\delta$, the $R_{OPT}$ in (4.11) is the same as in those papers.

(2). Under the $l_1$ sparsity on $\Sigma^{-1} \delta$, Cai and Liu (2011) obtained the convergence rate

$$\frac{R(X)}{R_{OPT}} - 1 = O_p \left\{ \left( \|\Sigma^{-1} \delta\|_1 \sqrt{\Delta_p} + \|\Sigma^{-1} \delta\|_1^2 \right) \sqrt{\log p \over n} \right\},$$

in their Theorem 3, where $\Delta_p = \delta^T \Sigma^{-1} \delta$. When $K = 2$, $\alpha_1 = \Sigma^{-1} \delta/\sqrt{\delta^T \Sigma^{-1} \delta}$. By (??) (Supplementary Material) in the proof of Theorem 4.3, we have $\delta^T D \delta =$
\( \delta^T \Sigma^{-1} \delta = 4\lambda_1(\Xi) \). Hence, our convergence rate on the right hand side of (4.12) is

\[
O_p \left( \lambda_1(\Xi) \| \alpha_1 \|_1^2 / n \right) = O_p \left( (\delta^T \Sigma^{-1} \delta) \left( \frac{\Sigma^{-1} \delta}{\sqrt{\delta^T \Sigma^{-1} \delta}} \right) \right) = O_p \left( \| \Sigma^{-1} \delta \|_1^2 / \sqrt{\log p/n} \right).
\]

Compared to the convergence rate in (4.13), our convergence rate does not have the first term in (4.13).

### 4.2 The case of \( K > 2 \)

We first illustrate the relationship between sparsity assumptions on \( \Sigma \alpha_1, \ldots, \Sigma \alpha_{K-1} \) and \{\( \mu_i - \mu_j, 1 \leq i \neq j \leq K \}\} in the following lemma.

**Lemma 2.** Suppose that Conditions 1-2 hold. Then we have

\[
\frac{1}{(K-1)c_0 \sqrt{2K \lambda_1(\Xi)}} \left( \max_{1 \leq i \neq j \leq K} \| \mu_i - \mu_j \|_1 \right) \leq \frac{\max_{1 \leq i \leq K-1} \| \Sigma \alpha_i \|_1}{\sqrt{c_3 / \lambda_1(\Xi)}} \left( \max_{1 \leq i \neq j \leq K} \| \mu_i - \mu_j \|_1 \right).
\]

Since \( \lambda_1(\Xi) \geq c_1 \) by Condition 2 (a), Lemma 2 implies that if \( \lambda_1(\Xi) \) is bounded from the above, then \( \max_{1 \leq i \leq K-1} \| \Sigma \alpha_i \|_1 \) has the same order as \( \max_{1 \leq i \neq j \leq K} \| \mu_i - \mu_j \|_1 \). If \( \lambda_1(\Xi) \to \infty \), we have \( \max_{1 \leq i \leq K-1} \| \Sigma \alpha_i \|_1 / \max_{1 \leq i \neq j \leq K} \| \mu_i - \mu_j \|_1 \to 0 \). Therefore, making sparsity assumptions on \( \Sigma \alpha_1, \ldots, \Sigma \alpha_{K-1} \) is equivalent to or weaker than assuming the sparsity of \{\( \mu_i - \mu_j, 1 \leq i \neq j \leq K \}\} in \( l_1 \) norm.

We define the following measurement of sparsity on \( \alpha_i \) and \( \Sigma \alpha_i \), \( 1 \leq i \leq K-1 \):

\[
\Lambda_p = \max_{1 \leq i \leq K-1} \{ \| \alpha_i \|_1, \| \Sigma \alpha_i \|_1 \}.
\]

In the following theorem, we show that for each \( 1 \leq i \leq K-1 \), the \( l_1 \) sparsity of the estimate \( \hat{\alpha}_i \) is bounded by \( \Lambda_p \) multiplied by a constant which does not depend on \( n \) and \( p \), and \( \hat{\alpha}_i \) is a consistent estimate. Moreover, we show that the subspace spanned by \( \{ \hat{\xi}_1, \ldots, \hat{\xi}_i \} \) is a consistent estimate of the subspace spanned by \( \{ B\alpha_1, \ldots, B\alpha_i \} \) (or equivalently the subspace spanned by \( \{ \Sigma \alpha_1, \ldots, \Sigma \alpha_i \} \)) and provide the convergence rates, where \( \hat{\xi}_j \) is the solution.
to (3.3). In this paper, to measure whether two subspaces with the same dimensions in \( \mathbb{R}^p \) are close to each other, we use the operator norm of the difference between the orthogonal projection matrices onto the two subspaces.

**Theorem 4.4.** Suppose that Conditions 1-2 hold. We choose the tuning parameter in the optimization problem (3.3) as \( \kappa_n = \tilde{C}\lambda_1(\Xi)\Lambda_p s_n \), where \( \tilde{C} \) is a constant large enough and independent of \( n \) and \( p \). For any \( 1 \leq i \leq K - 1 \), let \( Q_i \) and \( \hat{Q}_i \) be the orthogonal projection matrices onto the following subspaces of \( \mathbb{R}^p \), respectively,

\[
W_i = \text{span}\{\xi_1, \xi_2, \ldots, \xi_i\}, \quad \hat{W}_i = \text{span}\{\hat{\xi}_1, \hat{\xi}_2, \ldots, \hat{\xi}_i\},
\]

where \( \xi_i = B\alpha_i = \lambda_i(\Xi)\Sigma\alpha_i \). If \( \Lambda_p^2 s_n \to 0 \) as \( n, p \to \infty \), then for each \( 1 \leq i \leq K - 1 \), there exist constants \( D_{i,1}, D_{i,2} \) and \( D_{i,3} \) independent of \( n \) and \( p \) such that in \( \Omega_n \),

\[
\|\hat{\alpha}_i\|_1 \leq D_{i,1}\Lambda_p, \quad \|\hat{\alpha}_i - \alpha_i\|_2 \leq D_{i,2}\Lambda_p^2 s_n, \quad \|Q_i - \hat{Q}_i\|^2 \leq D_{i,3}\Lambda_p^2 s_n.
\]

Hence, for each \( 1 \leq i \leq K - 1 \), \( \hat{\alpha}_i \) is a consistent estimate of \( \alpha_i \), and the projection matrix \( \hat{Q}_i \) is a consistent estimate of \( Q_i \).

Based on Theorem 4.4, we will prove the asymptotic optimality of our classification rule and provide the corresponding convergence rate. When \( K > 2 \), the classification boundary of a linear classification rule is typically complicated and no explicit formula for the error generally exist. In the following, we first prove a theorem which provides the conditions for asymptotic optimality and the corresponding convergence rates for a large family of linear classification rules. Then by applying the general result to our method, we obtain the asymptotic optimality results.

We consider a family of linear classification rules motivated by the following observation. The optimal classification rule \( T_{OPT} \) can be rewritten in the following way. Let

\[
a_{ji} = \Sigma^{-1/2}(\mu_j - \mu_i), \quad b_{ji} = \frac{1}{2}(\mu_j + \mu_i),
\]

where \( 1 \leq i, j \leq K \). Then \( T_{OPT} \) assigns a new observation \( x \) to the \( i \)th class if \( a_{ji}^T \Sigma^{-1/2}(x - b_{ji}) < 0 \) for all \( j \neq i \). Based on this observation, we consider a family of classification rules having the form,

\[
T: \text{to assign a new } x \text{ to the } i \text{th class if } \tilde{a}_{ji}^T \Sigma^{-1/2}(x - \tilde{b}_{ji}) < 0, \text{ for all } j \neq i,
\]

(4.18)
where $\hat{a}_{ji}$ and $\hat{b}_{ji}$ are $p$-dimensional vectors which may depend on the sample $X$, and satisfy
\[
\hat{a}_{ji} = -\hat{a}_{ij}, \quad \hat{b}_{ji} = \hat{b}_{ij}, \quad (4.19)
\]
for all $1 \leq i \neq j \leq K$. Typically, $\hat{a}_{ji}$ and $\hat{b}_{ji}$ are estimates of $a_{ji}$ and $b_{ji}$, respectively. In addition to the optimal rule, many linear classification rules in practice belong to this family. For example, the classic Fisher’s rule (2.9) is of the form (4.18) with $\hat{a}_{ji} = \Sigma^{-1/2} \hat{D}(\bar{x}_j - \bar{x}_i)$ and $\hat{b}_{ji} = \frac{1}{2}(\bar{x}_j + \bar{x}_i)$. The rule of our sparse Fisher’s discriminant analysis method is also a special case of (4.18) with
\[
\hat{a}_{ji} = \Sigma^{-1/2} \hat{D}(\bar{x}_j - \bar{x}_i), \quad \hat{b}_{ji} = \frac{1}{2}(\bar{x}_j + \bar{x}_i), \quad (4.20)
\]
where $\hat{D}$ is defined in (3.10). Now we study the asymptotic optimality of a classification rule $T$ in this family. It is relatively easy to calculate the convergence rates of $\hat{a}_{ji}$ and $\hat{b}_{ji}$ in a given $T$. We will establish the asymptotic optimality of $T$ and the convergence rate for $R_T(X)/R_{OPT} - 1$ based on the convergence rates of $\hat{a}_{ji}$ and $\hat{b}_{ji}$, where $R_T(X)$ is the conditional misclassification rate of $T$ given the training sample $X$.

**Theorem 4.5.** Suppose that Conditions 1 and 2 hold and the general classification rule $T$ in (4.18) satisfies: $\hat{a}_{ji} = -\hat{a}_{ij}$ and $\hat{b}_{ji} = \hat{b}_{ij}$. Let $\{\delta_n : n \geq 1\}$ be a sequence of nonrandom positive numbers with $\delta_n \to 0$ and $\lambda_1(\Xi)\delta_n \to 0$ as $n \to \infty$. For any $1 \leq j \neq i \leq K$, let
\[
a_{ji} = t_{ji}\hat{a}_{ji} + (a_{ji})_\perp \quad (4.21)
\]
be an orthogonal decomposition of $a_{ji}$, where $t_{ji}\hat{a}_{ji}$ is the orthogonal projection of $a_{ji}$ along the direction of $\hat{a}_{ji}$, $t_{ji}$ is a real number, and $(a_{ji})_\perp$ is orthogonal to $t_{ji}\hat{a}_{ji}$. Let
\[
\hat{d}_{ji} = a_{ji}^T \Sigma^{-1/2}(\hat{b}_{ji} - \mu_i), \quad d_{ji} = a_{ji}^T \Sigma^{-1/2}(b_{ji} - \mu_i) = \frac{1}{2}\|a_{ji}\|_2^2. \quad (4.22)
\]
If the following conditions are satisfied,
\[
\|a_{ji}\|_2^2 - \|\hat{a}_{ji}\|_2^2 = \|a_{ji}\|_2^2 O_p(\delta_n), \quad t_{ji} = 1 + O_p(\delta_n), \quad (4.23)
\]
\[
d_{ji} - \hat{d}_{ji} = \|\hat{a}_{ji}\|_2^2 O_p(\delta_n),
\]
then the classification rule $T$ is asymptotically optimal and we have
\[
\frac{R_T(X)}{R_{OPT}} - 1 = O_p \left( \sqrt{\lambda_1(\Xi)\delta_n \log \left\{ \frac{\lambda_1(\Xi)\delta_n}{\delta_n} \right\}^{-1}} \right). \quad (4.24)
\]
To apply Theorem 4.5 to a specific linear classification rule with the form (4.18), we need to determine the sequence $\delta_n$ and verify the conditions (4.23). For our classification rule (3.9), which is a special case of (4.18) with $\hat{a}_{ji}$ and $\hat{b}_{ji}$ as given in (4.20), it turns out that we can choose $\delta_n = \Lambda^2_p s_n$ which is the convergence rate in Theorem 4.4.

**Theorem 4.6.** Suppose that Conditions 1 and 2 hold, and $\lambda_1(\Xi)\Lambda^2_p s_n \to 0$ as $n, p \to \infty$. Then our classification rule (3.9) is asymptotically optimal. Moreover, we have

$$\frac{R_T(X)}{R_{OPT}} - 1 = O_p \left( \sqrt{\lambda_1(\Xi)\Lambda^2_p s_n \log \left[ \{\lambda_1(\Xi)\Lambda^2_p s_n\}^{-1}\right]} \right).$$ (4.25)

Comparing Theorem 4.6 with Theorem 4.3, we find that the convergence rate in (4.25) is slower than that for $K = 2$. This may be due to the complicated classification boundary when $K > 2$. It is a future direction to investigate whether the convergence rates in Theorems 4.5 and 4.6 can be improved.

## 5 Simulation studies

In the previous section, we have shown that the revised sparse Fisher’s discriminant analysis method with soft thresholding (SFDA-threshold) has good theoretical properties. In this and the following section, we will show that SFDA-threshold also has good predictive performance as the original method (SFDA) in Qi *et al.* (2015) by comparing them with regularized discriminant analysis (RDA) (Guo *et al.* (2007), R package “rda”) and penalized discriminant analysis (PDA) (Witten and Tibshirani (2011), R package “penalizedLDA”) through simulation studies and applications to real data sets.

Three simulation models are considered. In each simulation, 50 independent data sets are simulated each of which has 1500 observations and three classes. In each dataset, for each observation, we randomly select a class label and then generate the value of $x$ based on the distribution of that class. Then the 1500 observations in each dataset are randomly split into the training set with 150 observations and the test set with 1350 observations. There are 500 features ($p = 500$) in these datasets. For our methods, SFDA-threshold and SFDA, we use the usual cross-validation procedure to select tuning parameters $\tau$ from $\{0.5, 1, 5, 10\}$, and $\lambda$ from $\{0.01, 0.05, 0.1, 0.2, 0.3, 0.4\}$. For SFDA-threshold, we choose $\kappa$ in (3.3) from the
three values which are equal to $\|\hat{B}\hat{\alpha}\|_1$ multiplied by 0, 0.001 and 0.01, respectively. For RDA and PDA, the default cross-validation procedure in the corresponding packages are used. The details of the three simulation studies are provided below.

(a). Simulation 1: There is no overlap between the features for different classes. There are correlations among some feature variables. Specifically, let $x_{ij}$ be the $i^{th}$ observation on the $j^{th}$ variable, $1 \leq j \leq 500$ and $1 \leq i \leq 1500$. If the $i^{th}$ observation is in class $k (= 1, 2, 3)$, then $x_{ij} = \mu_{kj} + Z_i + \epsilon_{ij}$ if $1 \leq j \leq 30$, and $x_{ij} = \mu_{kj} + \epsilon_{ij}$ if $j \geq 31$, where $Z_i \sim \text{Normal}(0, 1)$ and $\epsilon_{ij} \sim \text{Normal}(0, \sigma^2)$ are independent. Here $\mu_{1j} \sim \text{Normal}(1, 0.8^2)$ if $1 \leq j \leq 20$, $\mu_{2j} \sim \text{Normal}(4, 0.8^2)$ if $21 \leq j \leq 30$, $\mu_{3j} \sim \text{Normal}(1, 0.8^2)$ if $31 \leq j \leq 50$ and $\mu_{kj} = 0$ otherwise. We consider the cases that $\sigma^2 = 1, 1.5^2$ and 4, respectively.

(b). Simulation 2: There are overlaps between the features for different classes and the variables are correlated. The $i^{th}$ observation, $\mathbf{x}_i = (x_{i1}, x_{i2}, \ldots, x_{i500}) \sim \text{Normal}(\mu_k, \Sigma)$, where $\mu_k = (\mu_{k,1}, \mu_{k,2}, \ldots, \mu_{k,500})$, if it is in class $k$, $1 \leq k \leq 3$. The covariance matrix $\Sigma$ is block diagonal, with five blocks each of dimension $100 \times 100$. The five blocks are the same and have $(j, j')$ element $0.6|j - j'| \times \sigma^2$. Also, $\mu_{1j} \sim \text{Normal}(1, 1)$, $\mu_{2j} \sim \text{Normal}(2, 1)$ and $\mu_{3j} \sim \text{Normal}(3, 1)$ if $1 \leq j \leq 10$ or $101 \leq j \leq 110$ and $\mu_{kj} = 0$ otherwise. We consider $\sigma^2 = 1, 2$ and 3.

(c). Simulation 3: Observations from different classes have different distributions about the class means. If the $i^{th}$ observation is in class $k$, $\mathbf{x}_i \sim \text{Normal}(\mu_k, \Sigma_k)$. We take $\mu_{1j} = 3$ if $1 \leq j \leq 10$, $\mu_{2j} = 2$ if $1 \leq j \leq 20$, $\mu_{3j} = 1$ if $1 \leq j \leq 30$, and $\mu_{kj} = 0$ otherwise. The covariance matrix $\Sigma_1$ is diagonal with the diagonal elements generated from the uniform distribution in $(0.5, 2) \times \sigma^2$. $\Sigma_2$ is block diagonal, with five blocks each of dimension $100 \times 100$. The blocks have $(j, j')$ element $0.9|j - j'| \times \sigma^2$. And $\Sigma_3$ is block diagonal, with five blocks each of dimension $100 \times 100$. The blocks have $(j, j')$ element $0.6 \times \sigma^2$ if $j \neq j'$ and $\sigma^2$ otherwise. We consider $\sigma^2 = 1, 2$ and 3.

The mean misclassification rates (percentages) of 50 data sets for each simulation are shown in Table 1, with standard deviations in parentheses. The PDA has the highest misclassification rates.
fication rate in all simulations. SFDA-threshold performs similarly with SFDA and both methods have good prediction accuracies in all the simulations.

Table 1: The averages and standard deviations (in parentheses) of the misclassification rates (%) for the simulations in Section 5.

| Simulation | $\sigma^2$ | SFDA-threshold | SFDA     | RDA      | PDA      |
|------------|------------|----------------|----------|----------|----------|
| Simulation 1 | 1          | 0.21(0.26)     | 0.24(0.26) | 0.32(0.39) | 2.37(1.46) |
|            | 1.5$^2$    | 1.52(0.77)     | 1.54(0.71) | 1.75(0.96) | 5.40(2.07) |
|            | 4          | 8.78(4.06)     | 8.60(3.71) | 10.20(4.41)| 12.73(4.32)|
| Simulation 2 | 1          | 0.48(0.43)     | 0.48(0.47) | 0.79(0.73) | 0.86(0.57) |
|            | 2          | 3.15(2.40)     | 3.29(2.38) | 3.61(2.15) | 4.84(2.45) |
|            | 3          | 5.05(2.57)     | 5.10(2.43) | 6.05(2.99) | 8.55(3.52) |
| Simulation 3 | 1          | 4.86(1.12)     | 4.85(1.12) | 7.71(2.03) | 9.51(4.20) |
|            | 2          | 13.02(2.73)    | 12.84(2.79)| 18.74(2.84)| 20.42(5.72)|
|            | 3          | 21.49(3.45)    | 21.48(3.35)| 26.56(3.58)| 29.74(7.61)|

6 Application to multivariate functional data

With the advance of techniques, multiple curves can be extracted and recorded simultaneously for one subject in a single experiment. In this section, we consider two real datasets where observations are classified into multiple categories and for each subject, multiple curves were measured. We first apply the wavelet transformation to those curves, and then apply our method to the obtained wavelet coefficients. The setting for the tuning parameters is the same as that in the simulation studies.

6.1 Daily and sports activities data

This motion sensor data set, available in UCI Machine Learning Repository (Bache and Lichman, 2013), recorded several daily and sports activities each performed by 8 subjects (Altun et al., 2010; Barshan and Yüksel, 2013; Altun and Barshan, 2010) in 60 time segments. Nine
sensors (x, y, z accelerometers, x, y, z gyroscopes, x, y, z magnetometers) were placed on each of five body parts (torso, right arm, left arm, right leg, left leg) and calibrated to acquire data at 25 Hz sampling frequency. Therefore, for each activity, there are 480 observations. In each observation, 45 curves are recorded and each of them has 125 discrete time points. The purpose of the study is to build a classification rule to identify the corresponding activity based on the observed curves.

We first apply the Fast Fourier Transformation to each of 45 curves to convert it from time domain to the frequency domain and get its spectrum curve. After filtering out the higher frequency, we use the first 64 frequency points for each of 45 frequency curves. Then we apply wavelet transformation with 64 wavelet basis functions to each of 45 spectrum curves and obtain 64 wavelet coefficients. In this way, for each observation, a vector with \(64 \times 45 = 2880\) wavelet coefficients is obtained as the features to make classifications.

We consider nine activities which can be divided into three groups. Group 1 includes three activities: walking in a parking lot, ascending and descending stairs; Group 2 has three activities: running on a treadmill with a speed of 8 km/h, exercising on a stepper and exercising on a cross trainer; Group 3 includes rowing, jumping and playing basketball. We will consider seven classification problems. In each of the first three problems, we consider the classification of the three activities in each of the three groups. In each of the next three problems, we combine any two of the three groups and consider the classification of the six activities in the combined groups. The last problem is the classification of all nine activities. In each problem, for each class, we randomly select 30 observations as the training sample and all the other 450 observations as the test sample. The procedure is repeated 50 times for each of the seven problems and the averages and standard deviations of misclassification rates are reported in Table 2. SFDA-threshold performs similarly with SFDA and both methods have higher prediction accuracies than RDA and PDA in all cases.

6.2 Australian sign language data

The data is available in UCI Machine Learning Repository and the details of the experiments can be founded in Kadous (2002). This data set consists of samples of Auslan (Australian
Table 2: The averages and standard deviations (in parentheses) of the misclassification rates (%) for the daily and sports activities data.

| Classes included | SFDA-threshold | SFDA     | RDA    | PDA    |
|------------------|----------------|----------|--------|--------|
| Group 1          | 0.23(0.23)     | 0.23(0.23)| 1.94(1.91)| 1.96(2.10) |
| Group 2          | 0.14(0.43)     | 0.14(0.44)| 0.58(0.66)| 0.21(0.58) |
| Group 3          | 0.12(0.07)     | 0.12(0.08)| 0.58(1.08)| 0.23(0.36) |
| Group 1+2        | 0.45(0.44)     | 0.46(0.43)| 1.13(0.79)| 2.39(1.52) |
| Group 1+3        | 1.50(0.84)     | 1.54(0.96)| 1.92(0.99)| 4.79(2.33) |
| Group 2+3        | 0.53(0.26)     | 0.54(0.24)| 1.06(0.72)| 0.80(0.37) |
| Group 1+2+3      | 1.63(0.60)     | 1.53(0.63)| 1.78(0.65)| 4.20(2.01) |

Sign Language) signs. Twenty seven examples of each sign were captured from a native signer using high-quality position trackers and instrumented gloves. This was a two-hand system. For each hand, 11 time series curves were recorded simultaneously, including the measurements of x, y, z positions, the direction of palm and five finger bends. The frequency curve of each of the 22 curves were extracted by the Fast Fourier Transformation and then were transformed by 16 wavelet basis functions. Hence, for each sign, we obtained 352 features. We choose nine signs and divide them into three groups: Group 1 contains the three signs with meanings “innocent”, “responsible” and “not-my-problem”, respectively; Group 2 contains “read”, “write” and “draw”; Group 3 contains “hear”, “answer” and “think”. As in the previous example, we consider seven classification problems. For each class, we randomly choose 20 observations as the training sample and the other 7 as the test sample. The procedure is repeated 50 times and the averages and standard deviations of misclassification rates are reported in Table 3. As in previous studies, SFDA-threshold performs similarly with SFDA and both methods have higher prediction accuracies than RDA and PDA in all cases.

Acknowledgments

Xin Qi is supported by NSF DMS 1208786.
Table 3: The averages and standard deviations (in parentheses) of the misclassification rates (%) for the Australian sign language data.

| Classes included | SFDA-threshold | SFDA | RDA     | PDA     |
|------------------|----------------|------|---------|---------|
| Group 1          | 0(0)           | 0(0) | 1.24(2.32) | 0.19(0.94) |
| Group 2          | 0(0)           | 0(0) | 1.43(2.76) | 4.57(5.61) |
| Group 3          | 1.24(2.11)     | 1.14(2.05) | 3.05(3.94) | 3.9(6.5) |
| Group 1+2        | 0.19(0.65)     | 0.62(1.26) | 0.76(1.31) | 3.81(2.93) |
| Group 1+3        | 0.81(1.71)     | 0.62(1.16) | 1.29(1.94) | 2.24(2.38) |
| Group 2+3        | 0.93(1.45)     | 1.06(1.68) | 1.72(2.13) | 5.16(4.34) |
| Group 1+2+3      | 0.73(1.02)     | 0.57(0.95) | 1.14(1.11) | 6.0(2.78) |

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