

## LINEAR DISCRIMINANT ANALYSIS WITH SPARSE AND DENSE SIGNALS

Ning Wang, Shaokang Ren and Qing Mai\*

*Beijing Normal University, Microsoft Corporation  
and Florida State University*

*Abstract:* A common theme among high-dimensional linear discriminant analysis (LDA) methods is the sparsity assumption. However, in practice, this assumption may be violated, making sparse methods inaccurate. Motivated by this challenge, we propose a novel high-dimensional LDA method that relaxes the sparsity assumption. We assume that there exist a few sparse signals with large effects, and a large number of dense signals with small effects. In the parameter estimation, we combine the group Lasso penalty and the  $\ell_2$  penalty to identify these signals automatically. Our estimation involves a convex optimization problem that can be solved straightforwardly. Theoretical and numerical results support the application of our proposal.

*Key words and phrases:* Group Lasso,  $\ell_2$  penalty, linear discriminant analysis, regularization.

### 1. Introduction

Numerous works have proposed methods for applying the classical linear discriminant analysis (LDA) to high-dimensional data, including Cai and Liu (2011), Clemmensen et al. (2011), Witten and Tibshirani (2011), Fan, Feng and Tong (2012), Mai, Zou and Yuan (2012), Xu et al. (2015), Mai, Yang and Zou (2019), and Yang, Lin and Li (2022). These methods preserve the elegance and simplicity of the classical LDA. They have explicit probabilistic models that yield highly interpretable final classifiers and enable researchers to understand the results, using innovations in formulation, computation, and theory to address the high dimensionality. These methods are shown to have impressive performance in a wide range of applications.

However, most high-dimensional LDA methods rely on sparsity, often assuming that some parameters in the high-dimensional LDA model are sparse, such as the covariance matrix, precision matrix, mean differences, or discriminant coefficients. Without additional parsimony assumptions, accurate model estimation is virtually impossible in high dimensions (Bickel and Levina, 2004; Fan and Fan, 2008), and thus sparsity is a powerful assumption. The sparsity also facilitates interpretation, because only a small subset of predictors are relevant

---

\*Corresponding author. E-mail: [qmai@fsu.edu](mailto:qmai@fsu.edu)

for the prediction. However, it remains an open question if we can relax the sparsity assumption. For example, Witten and Tibshirani (2011) explicitly enforce sparsity in their  $\ell_1$  Fisher’s discriminant analysis ( $\ell_1$ -FDA) method, but in the three real data sets they consider,  $\ell_1$ -FDA produced nonsparse classifiers with thousands of nonzero coefficients and high classification accuracy. The authors argued that this was because sparsity is often only an approximation, in practice. Thus, it is of interest to determine whether we can accommodate such situations using a new high-dimensional LDA model and method.

Motivated by this challenge, we propose a novel high-dimensional LDA method that gives a “sparse+dense” (SD) classifier. We assume that there exists a small subset of predictors with large coefficients, while the rest have small, but possibly nonzero coefficients. Thus, we relax the sparsity assumption by allowing all the coefficients to be nonzero, but to some extent preserve the interpretability that only a few variables have large effects on the final prediction. Under this assumption, we devise an estimator that automatically identifies and estimates the sparse and dense signals using convex optimization. Numerical and theoretical evidence is provided to support our proposal.

Our proposal is inspired by the so-called “lava” estimator in the regression problem described in Chernozhukov, Hansen and Liao (2017). The lava estimator estimates the coefficient in a linear regression problem with a sparse+dense structure. Although we borrow some of their techniques in our study, we investigate the different problem of classification, where sparse+dense estimators have not been developed, to the best of our knowledge. We also address several challenges in LDA problems. First, in a regression, we can treat the predictors as fixed, or at least condition on the predictors, to make an inference about the response, but in an LDA model, we directly model the distribution of the predictors, and have to deal with the randomness in them. Second, in a regression, it is relatively easier to pick the parameter of interest, and then estimate it using a variant of the least squares formula. In an LDA model, we need to carefully determine the parametrization and formula, for efficiency. Third, in a linear regression model, we need only estimate one parameter of the regression coefficient, whereas in multiclass problems, we need to estimate several different directions to separate the classes.

The rest of the article is organized as follows. We explain the proposed model and method in Section 2. The theoretical properties of our proposal are given in Section 3. In Section 4, we present the numerical studies. We further examine our method on several real data sets in Section 5. We provide proofs of the lemmas and theorems in the Supplementary Material.

## 2. Methodology

### 2.1. Background

Consider a pair of random variables  $(Y, \mathbf{X})$ , where the predictor  $\mathbf{X} = (X_1, \dots, X_p)^T \in \mathbb{R}^p$  and the class label  $Y \in \{1, \dots, K\}$ , with  $K$  being a positive integer. LDA assumes that (e.g., see Hastie, Tibshirani and Friedman, 2009)

$$\mathbf{X} \mid Y = k \sim N(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}), \quad \Pr(Y = k) = \pi_k, \quad (2.1)$$

where  $\boldsymbol{\mu}_k \in \mathbb{R}^p$  is the within-class mean,  $\boldsymbol{\Sigma}$  is a  $p \times p$  covariance matrix, and  $\pi_k$  is the prior probability of class  $k$ .

Our goal is to predict the label of any new sample  $\mathbf{X}^*$ . It is known that, under the LDA model, we can minimize the classification error by using the so-called Bayes' rule (Friedman, Hastie and Tibshirani, 2001; Mai, Yang and Zou, 2019)

$$\hat{Y} = \operatorname{argmax}_k \left[ \left\{ \mathbf{X} - \frac{1}{2}(\boldsymbol{\mu}_1 + \boldsymbol{\mu}_k) \right\}^T \boldsymbol{\theta}_k^* + \log \left( \frac{\pi_k}{\pi_1} \right) \right],$$

where the linear discriminant directions are given by

$$\boldsymbol{\theta}_k^* = \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_k - \boldsymbol{\mu}_1), \quad k = 2, \dots, K.$$

Hence, the linear discriminant directions  $\boldsymbol{\theta}_k^*$  are critical to the classification. They project the  $p$ -dimensional predictor  $\mathbf{X}$  onto a  $K - 1$ -dimensional subspace that retains all the information for optimal classification. Consequently, many existing sparse LDA methods assume that  $\boldsymbol{\theta}_k^*$  is sparse, in the sense that the majority of its elements are zero (Cai and Liu, 2011; Fan, Feng and Tong, 2012; Mai, Zou and Yuan, 2012; Mai, Yang and Zou, 2019). In particular, in a multiclass problem where  $K > 2$ , we have multiple directions  $\boldsymbol{\theta}_k^*$  to estimate, and a variable  $X_j$  is unimportant for classification if and only if

$$\theta_{kj}^* = 0, \quad \text{for } k = 2, \dots, K. \quad (2.2)$$

Therefore, the sparsity assumption indicates that (2.2) holds for most  $j$ .

### 2.2. The “sparse+dense” assumption

Our interest is to relax the sparsity assumption in the LDA model. To this end, we decompose the discriminant direction as

$$\boldsymbol{\theta}_k^* = \boldsymbol{\beta}_k^* + \boldsymbol{\delta}_k^*, \quad (2.3)$$

for any  $k$ , where  $\boldsymbol{\delta}_k^* = (\delta_{k1}^*, \dots, \delta_{kp}^*)^T \in \mathbb{R}^p$  is sparse, with only a few nonzero and relatively large elements, while  $\boldsymbol{\beta}_k^* = (\beta_{k1}^*, \dots, \beta_{kp}^*)^T \in \mathbb{R}^p$  have small elements. Specifically, motivated by the sparsity assumption in (2.2), for most

$j \in \{1, \dots, p\}$ , we have

$$\delta_{kj}^* = 0, \quad \text{for } k = 2, \dots, K.$$

For ease of presentation, we also refer to  $\boldsymbol{\delta}_k^*$  as “sparse signals,” and to  $\boldsymbol{\beta}_k^*$  as “dense signals.”

Note that the entries in  $\boldsymbol{\theta}_k^*$  are coefficients in the final classifier, and quantify the effect of each predictor. Hence, our SD assumption implies that a few predictors dominate the classification, while most predictors have small effects. Our SD assumption includes the sparsity assumption as a special case, because when  $\boldsymbol{\beta}_k^* = 0$ , the discriminant direction is exactly sparse. However, in general, our SD assumption is weaker than the sparsity assumption. By incorporating the dense signals, we are essentially assuming that the directions are approximately sparse, in which the sparse signals are most relevant for the classification. However, the dense signals contribute to the classification as well, although with less noticeable effects. As a result, our SD assumption allows us to perform variable selection similarly to popular sparse methods. Even though  $\boldsymbol{\theta}_k^*$  does not have to be sparse, we can still exploit the sparsity pattern in  $\boldsymbol{\delta}_k^*$  to identify the most important variables.

In addition, the dense signals are assumed to have small magnitudes. Similar to sparsity, this is also a type of parsimony assumption that limits the parameter space. Such an assumption is important because, in high dimensions, it is challenging to estimate the classifier accurately without appropriate parsimony assumptions. As discussed later, this assumption enables helpful regularization techniques in the estimation. Note that, although the dense signals have small entries individually, jointly, they can significantly improve the classification results.

Our SD assumption in (2.3) is imposed on the discriminant direction  $\boldsymbol{\theta}_k^*$ , because  $\boldsymbol{\theta}_k^*$  is often viewed as the most “direct” parameter for classification. In the literature on sparse LDA methods, researchers sometimes instead assume that the covariance matrix, precision matrix, and the mean differences are sparse (e.g., Shao et al., 2011; Xu et al., 2015). In our context, we choose not to make the SD assumption on these parameters, for two reasons. First, the assumption on the discriminant direction is easy to interpret. Second, the discriminant direction has  $O(p)$  parameters, whereas the covariance and precision matrices have  $O(p^2)$  parameters, and are much more difficult to estimate than the discriminant directions.

Note that our definitions of sparse and dense signals may have identifiability issues. However, as discussed in Section 2.3, we are estimating unique target parameters when we employ regularization.

### 2.3. Estimation

To estimate our model, we first rewrite  $\boldsymbol{\theta}_k^*$  as the solution to the following optimization problem, as suggested by Mai, Yang and Zou (2019):

$$(\boldsymbol{\theta}_2^*, \dots, \boldsymbol{\theta}_K^*) = \underset{\boldsymbol{\theta}_k \in \mathbb{R}^p}{\operatorname{argmin}} \sum_{k=2}^K \left\{ \frac{1}{2} \boldsymbol{\theta}_k^T \boldsymbol{\Sigma} \boldsymbol{\theta}_k - (\boldsymbol{\mu}_k - \boldsymbol{\mu}_1)^T \boldsymbol{\theta}_k \right\}. \quad (2.4)$$

Equation (2.4) cannot be used in the estimation, because it involves the unknown parameters  $\boldsymbol{\Sigma}$  and  $\boldsymbol{\mu}_k$ . More importantly, it does not enforce our SD assumption. We solve these two problems as follows.

To start with, suppose that we observe the data set  $\{Y_i, \mathbf{X}_i\}_{i=1}^n$ , and let  $\mathcal{C}_k$  be the set of indices of the  $n_k$  samples in class  $k$ . We find

$$\hat{\boldsymbol{\mu}}_k = \frac{1}{n_k} \sum_{i \in \mathcal{C}_k} \mathbf{X}_i \quad (2.5)$$

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{n - K} \sum_{k=1}^K \sum_{i \in \mathcal{C}_k} (\mathbf{X}_i - \hat{\boldsymbol{\mu}}_k)(\mathbf{X}_i - \hat{\boldsymbol{\mu}}_k)^T \quad (2.6)$$

as estimates for  $\boldsymbol{\mu}_k$  and  $\boldsymbol{\Sigma}$ , respectively. These are also the standard estimates for a low-dimensional LDA (Hastie, Tibshirani and Friedman, 2009), and popular estimates in many sparse LDA methods (e.g., Cai and Liu, 2011; Fan, Feng and Tong, 2012).

Now, we turn to the more interesting problem of imposing the SD assumption. We use the parametrization in (2.3) and regularize  $\boldsymbol{\beta}_k^*$  and  $\boldsymbol{\delta}_k^*$ . For the sparse signals  $\boldsymbol{\delta}_k^*$ , we use the group lasso penalty (Yuan and Lin, 2006) to honor the sparsity assumption in (2.2). For the dense signals, we use the ridge penalty (Hoerl and Kennard, 1970; Hastie, Tibshirani and Friedman, 2009; Weisberg, 2005). In other words, we consider the penalized problem

$$\begin{aligned} (\hat{\boldsymbol{\beta}}_k, \hat{\boldsymbol{\delta}}_k, k = 2, \dots, K) = & \\ \underset{\boldsymbol{\beta}_k \in \mathbb{R}^p, \boldsymbol{\delta}_k \in \mathbb{R}^p}{\operatorname{argmin}} & \sum_{k=2}^K \left\{ \frac{1}{2} (\boldsymbol{\beta}_k + \boldsymbol{\delta}_k)^T \hat{\boldsymbol{\Sigma}} (\boldsymbol{\beta}_k + \boldsymbol{\delta}_k) - (\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_1)^T (\boldsymbol{\beta}_k + \boldsymbol{\delta}_k) \right\} \\ & + \lambda_1 \sum_{j=1}^p \sqrt{\sum_{k=2}^K \delta_{kj}^2} + \lambda_2 \sum_{j=1}^p \sum_{k=2}^K \beta_{kj}^2, \end{aligned} \quad (2.7)$$

where  $\lambda_1, \lambda_2 > 0$  are tuning parameters. After we obtain  $\hat{\boldsymbol{\beta}}_k$  and  $\hat{\boldsymbol{\delta}}_k$ , we estimate the discriminant direction  $\boldsymbol{\theta}_k^*$  by  $\hat{\boldsymbol{\theta}}_k = \hat{\boldsymbol{\beta}}_k + \hat{\boldsymbol{\delta}}_k$ .

We name this method SD-LDA, where SD refers to the “sparse” and “dense” signals that we target. SD-LDA provides a nonsparse but interpretable classifier, because only a few variables have large effects. When the sparsity assumption does hold, SD-LDA is as powerful as existing sparse methods. However, in the

SD problems of our primary interest, SD-LDA continues to be suitable.

It is easy to see that  $(\hat{\beta}_k, \hat{\delta}_k, k = 2, \dots, K)$  produced by (2.7) approximate

$$\begin{aligned} (\beta_k^\dagger, \delta_k^\dagger, k = 2, \dots, K) = \\ \underset{\beta_k \in \mathbb{R}^p, \delta_k \in \mathbb{R}^p}{\operatorname{argmin}} \sum_{k=2}^K \left\{ \frac{1}{2} (\beta_k + \delta_k)^T \Sigma (\beta_k + \delta_k) - (\mu_k - \mu_1)^T (\beta_k + \delta_k) \right\} \\ + \lambda_1 \sum_{j=1}^p \sqrt{\sum_{k=2}^K \delta_{kj}^2} + \lambda_2 \sum_{j=1}^p \sum_{k=2}^K \beta_{kj}^2. \end{aligned} \quad (2.8)$$

Note that, compared with (2.7), in (2.8), we use the true parameters  $\Sigma$  and  $\mu_k$ . Hence, for any fixed pair of tuning parameters  $(\lambda_1, \lambda_2)$ ,  $(\beta_k^\dagger, \delta_k^\dagger, k = 2, \dots, K)$  are parameters. With the corresponding penalties,  $\beta_k^\dagger$  is dense, while  $\delta_k^\dagger$  is sparse. Moreover, unlike  $\delta_k^*$  and  $\beta_k^*$ , defined intuitively in Section 2.2,  $(\beta_k^\dagger, \delta_k^\dagger, k = 2, \dots, K)$  do not have identifiability issues, because (2.8) is strictly convex and has a unique minimizer. Admittedly, similar to many penalized problems,  $(\beta_k^\dagger, \delta_k^\dagger, k = 2, \dots, K)$  are generally biased in the sense that, in general,  $\theta_k^* \neq \beta_k^\dagger + \delta_k^\dagger$ . However, if the tuning parameters  $(\lambda_1, \lambda_2)$  are chosen properly, the discrepancy is small, and (2.7) consistently estimates the discriminant directions. See Section 3 for rigorous theoretical justifications.

To better understand SD-LDA, we present the following toy example.

**Example 1.** Consider a binary classification problem, where  $\Sigma = \sigma^2 \mathbf{I}_p$  is known. Then, we have the following solution to SD-LDA:

$$\hat{\delta}_{2j} = \operatorname{sign}(\hat{\mu}_{2j} - \hat{\mu}_{1j}) \left\{ \left| \frac{\hat{\mu}_{2j} - \hat{\mu}_{1j}}{\sigma^2} \right| - \lambda_1 \left( \frac{1}{2\lambda_2} + \frac{1}{\sigma^2} \right) \right\}_+ \quad (2.9)$$

and

$$\hat{\beta}_{2j} = \frac{\hat{\mu}_{2j} - \hat{\mu}_{1j} - \sigma^2 \hat{\delta}_{2j}}{2\lambda_2 + \sigma^2}, \quad (2.10)$$

for any  $j$ , where the soft-thresholding operator  $(x)_+ = \max\{x, 0\}$ , for any  $x \in \mathbb{R}$ .

Example 1 illustrates how (2.7) obtains the “sparse signals” and “dense signals” in  $\hat{\delta}_2$  and  $\hat{\beta}_2$ . According to (2.9), each  $\hat{\delta}_{2j}$  produces a shrunken standardized mean difference. Therefore,  $\hat{\delta}_{2j}$  is only nonzero when  $(\hat{\mu}_{2j} - \hat{\mu}_{1j})/\sigma^2$  is large enough with respect to the choices of  $\lambda_1$  and  $\lambda_2$ . Benefiting from this feature,  $\hat{\delta}_2$  is able to identify the signals with large magnitude exclusively. On the other hand,  $\hat{\beta}_{2j}$  is essentially a rescaled standardized mean difference, reduced by  $\lambda_2$ . When  $\lambda_2$  is large, (2.10) gives a small  $\hat{\beta}_{2j}$ , ensuring that  $\hat{\beta}_2$  contains the “dense signals.” Therefore, the two types of penalties in (2.7) help identify the “sparse signals” and “dense signals” effectively. The ability to capture the two types of signals is made possible by the  $\ell_1$  and  $\ell_2$  regularization.

Example 1 assumes that  $\Sigma$  is diagonal and known to obtain explicit formulae for the estimates. However, in practice, SD-LDA does not need any knowledge of  $\Sigma$ . It simply plugs in our sample estimate in (2.6). In what follows, we discuss another special case where  $\Sigma$  does not have any special structure and is unknown. Suppose that  $\lambda_1 = \infty$ , and thus the sparse signal is estimated as zero. Then, the dense signals are estimated by

$$\hat{\beta}_k = (\hat{\Sigma} + 2\lambda_2 \mathbf{I})^{-1}(\hat{\mu}_k - \hat{\mu}_1). \quad (2.11)$$

It is easy to see that the sample covariance is stabilized by adding  $2\lambda_2 \mathbf{I}$ , and resembles the Ledoit–Wolf estimator (Ledoit and Wolf, 2004). The estimator in (2.11) also has a similar form to the regularized discriminant analysis (RDA; Friedman, 1989). However, in the Ledoit–Wolf estimator and RDA, the added identity matrix is intended only to make the sample covariance well-conditioned, and usually  $\lambda_2$  is chosen to be small. In our work,  $\lambda_2$  is usually reasonably large, to encourage the signals to have small magnitudes. When  $\lambda_2$  is large,  $\hat{\beta}_k$  in (2.11) is close to the shrunken mean difference. The nearest centroids classifier (Tibshirani et al., 2002, 2003) also uses the shrunken mean difference to construct a classifier. However, it uses the soft-thresholding operator to obtain a sparse classifier, whereas (2.11) obtains a dense coefficient using the  $\ell_2$  penalty.

Our proposal is inspired by the lava estimator in Chernozhukov, Hansen and Liao (2017) for regression. Similarly to their estimator, we separate the coefficients into sparse signals and dense signals, and use a sparsity-inducing penalty and a ridge penalty, accordingly. Our estimator for the classification problem has many unique challenges. For example, in a regression problem, there is one coefficient vector to be estimated, whereas in classification problems, we need to estimate several discriminant directions when  $K > 2$  so that we can separate the classes.

Moreover, compared with the lava estimator for a regression, the formulation for classification requires additional considerations. In regression problems, the least squares formula is the foundation of most methods, as is the case for the lava estimator. However, in a discriminant analysis, although there are various approaches to finding the directions in high dimensions, no formula dominates the others like the least squares problem does in a regression. Consequently, we examined numerous different high-dimensional LDA formulae to find the one most suitable to be generalized to our context. Our SD-LDA is related to the multiclass sparse discriminant analysis (MSDA) method (Mai, Yang and Zou, 2019) in that when we are confident in the sparsity assumption, we can set the dense signals to zero, and (2.7) reduces to the MSDA. In this sense, (2.7) is a generalization of the MSDA to SD problems. We choose to generalize the MSDA rather than other candidates for computational reasons. Note that SD-LDA is convex. This is partially because its predecessor, MSDA, is convex.

However, many other high-dimensional LDA methods are nonconvex, and their generalizations to the SD problem will continue to be nonconvex and potentially challenging in terms of computation. For example, Clemmensen et al. (2011) and Fan, Feng and Tong (2012) both consider nonconvex optimization problems with equality constraints. In principle, we could also modify these methods by reparametrizing the parameters of interest into sparse and dense signals, and adding appropriate penalty functions. However, the resulting methods would be nonconvex.

Note that our method is significantly different from the elastic net (Zou and Hastie, 2005), even though we also combine a nonsmooth penalty function (group lasso) with the ridge penalty. Elastic net imposes both penalties on the same parameter to stabilize the estimator when the predictors are highly correlated. In our method, the penalties are enforced on the sparse and dense signals separately to exploit their own structure. In principle we could use other group selection penalty functions to pursue sparsity, such as a group smoothly clipped absolute deviation (SCAD) and a group minimax concave penalty (MCP) (Fan and Li, 2001; Zhang, 2010; Huang, Breheny and Ma, 2012). However, these penalty functions are nonconvex, which is likely to lead to instability in computation. The corresponding theoretical study is also expected to be more challenging, because there could be local minima.

## 2.4. Algorithm

In this section, we derive an algorithm to solve (2.7). SD-LDA is jointly convex over  $(\boldsymbol{\beta}_k, \boldsymbol{\delta}_k)$ , but it is most straightforward to derive updates for one of  $\boldsymbol{\beta}_k$  and  $\boldsymbol{\delta}_k$  while fixing the other, and iterate between them. To this end, we derive the following lemma.

**Lemma 1.** *Denote  $\hat{\mathbf{Q}} = 2\lambda_2 \mathbf{I}_p + \hat{\Sigma}$ ,  $\bar{\Sigma} = 2\lambda_2 \hat{\Sigma} \hat{\mathbf{Q}}^{-1}$ ,  $\hat{\boldsymbol{\mu}}_{dk} = \hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_1$ , and  $\bar{\boldsymbol{\mu}}_{dk} = \hat{\boldsymbol{\mu}}_{dk}^T (2\lambda_2 \hat{\mathbf{Q}}^{-1})$ . Then, we have*

1. *for a fixed  $\boldsymbol{\delta}_k$ , the optimizer of  $\boldsymbol{\beta}_k$  to (2.7) is*

$$\hat{\boldsymbol{\beta}}_k(\boldsymbol{\delta}_k) = (2\lambda_2 \mathbf{I}_p + \hat{\Sigma})^{-1}(\hat{\boldsymbol{\mu}}_k - \hat{\boldsymbol{\mu}}_1 - \hat{\Sigma} \boldsymbol{\delta}_k); \quad (2.12)$$

2. *the optimizer of  $\boldsymbol{\delta}_k$  to (2.7) is*

$$(\hat{\boldsymbol{\delta}}_2, \dots, \hat{\boldsymbol{\delta}}_K) = \underset{\boldsymbol{\delta}_k \in \mathbb{R}^p}{\operatorname{argmin}} \sum_{k=2}^K \left\{ \frac{1}{2} [\boldsymbol{\delta}_k^T \bar{\Sigma} \boldsymbol{\delta}_k] - \bar{\boldsymbol{\mu}}_{dk}^T \boldsymbol{\delta}_k \right\} + \lambda_1 \sum_{j=1}^p \sqrt{\sum_{k=2}^K \delta_{kj}^2}. \quad (2.13)$$

According to Lemma 1, we first solve (2.13), and then plug its results into (2.12) to find the SD-LDA estimate. Note that the  $\ell_2$  regularization enables us to invert the covariance matrix in (2.12), so that (2.12) is feasible, even in high dimensions. For the solution of (2.13), although it does not have an explicit

form, we can find it by modifying the groupwise coordinate descent algorithm of Mai, Yang and Zou (2019). We replace their  $\widehat{\Sigma}$  with  $\bar{\Sigma}$ , and  $\hat{\mu}_k - \hat{\mu}_1$  with  $\bar{\mu}_{dk}$ , respectively, to solve (2.13).

### 3. Theory

In this section, we present the theoretical properties of SD-LDA. The entire theoretical study is based on the LDA model setup given by (2.1). For ease of presentation, for two quantities  $A$  and  $\xi$ , we write  $A \lesssim \xi$  if  $A \leq C\xi$ , for some  $C > 0$ .

We also make the following assumptions:

- (A1)  $\|\Sigma\|_2 \leq u$  and  $\|\Sigma^{-1}\|_2 \leq U$ , for some constants  $U$  and  $u$ ,
- (A2)  $\max_k \|\mu_k - \mu_1\|_2 \leq w_1$ , for some constant  $w_1$ ,
- (A3)  $0 < c_2 < \pi_k < c_1 < 1$ , for some constants  $c_1$  and  $c_2$ .

Assumptions (A1) and (A2) are technical conditions that facilitate our proof. Assumption (A1) implies that the eigenvalues of  $\Sigma$  are finite and bounded away from zero, and Assumption (A2) requires a bound on the  $\ell_2$ -norm of the mean difference. Assumption (A3) guarantees that our data set is not extremely unbalanced. This yields the following theorem.

**Theorem 1.** *Let  $\hat{\theta}_k = \hat{\delta}_k + \hat{\beta}_k$ , with  $\hat{\beta}_k$  and  $\hat{\delta}_k$  defined as in (2.12) and (2.13), respectively, and Assumptions (A1), (A2), and (A3) hold. Then, with probability at least  $1 - O(p^{-1})$ , we have*

$$\|\hat{\theta}_k - \theta_k^*\|_2 \lesssim \sqrt{\frac{p \log p}{n}}, \quad (3.1)$$

for  $\lambda_2 = O(\sqrt{\log p/n})$  and  $\lambda_1 = O(\sqrt{\log p/n})$ .

Theorem 1 shows that the estimators for the linear discriminant directions consistently converge to the truth when  $p \log p/n \rightarrow 0$ . This implies that SD-LDA approaches the Bayes rule under the same dimensionality. Hence, in theory, SD-LDA works similarly to the true Bayes rule as the sample size increases.

Although SD-LDA allows  $p$  to diverge, we acknowledge that it has a stronger requirement on the dimensionality than those of sparse methods. Sparse methods often allow  $p$  to diverge at an exponential rate (Cai and Liu, 2011; Fan, Feng and Tong, 2012; Mai, Zou and Yuan, 2012). Theorem 1 has a stronger requirement, because we no longer make the sparsity assumption, and the problem is more difficult. However, the difficulty could be technical, because SD-LDA works out well on high-dimensional problems with  $p > n$  in our numerical studies. In addition, in the special case of exact sparsity where we know  $\beta_k^* = 0$ , SD-LDA reduces to the sparse classifier MSDA (Mai, Yang and Zou, 2019), which has

an optimal convergence rate of  $\sqrt{s \log p/n}$  (Min, Mai and Junge, 2023), with  $s$  being the number of important variables. Moreover, even though SD-LDA is inspired by the lava estimator in regression, our proof differs significantly from theirs, because most of their proof conditions on  $\mathbf{X}$ , but we have to directly handle the randomness in  $\mathbf{X}$  as a consequence of the LDA model assumption. Furthermore, in multiclass problems, we have multiple directions to estimate, which adds to the technical difficulty of the proof. In addition, compared with the sparse classifier MSDA, SD-LDA involves much more complicated functionals, such as  $\widehat{\Sigma}(\widehat{\Sigma} + 2\lambda_2 \mathbf{I})^{-1}$ . We need to establish bounds for these terms, which are not available in the literature. Because we focus on method development, we leave a more careful theoretical investigation of the SD-LDA as a future topic of research.

#### 4. Simulation

Here, we present a simulation study to examine the performance of our proposed method. We consider two scenarios separately: settings where the sparsity assumption holds, and the settings where the sparsity assumption does not hold, but the SD assumption holds. The sparse models are given by S1 and S2 and the SD models are given by Models D1–D6. Throughout the simulation, we set the sample size  $n_k = 50$  for each class and  $p = 250K$ . Simulations of imbalanced classes can be found in Section S1 in the Supplementary Material. For each class, we set  $\mathbf{X} | Y = k \sim N(\boldsymbol{\mu}_k, \sigma^2 \boldsymbol{\Sigma})$ , where  $\sigma^2$  is a constant that varies from model to model. For each model, we have different  $\boldsymbol{\delta}_k^*$  and  $\boldsymbol{\beta}_k^*$ , with  $\boldsymbol{\mu}_1 = \mathbf{0}$  and  $\boldsymbol{\mu}_k = \sigma^2 \boldsymbol{\Sigma}(\boldsymbol{\beta}_k^* + \boldsymbol{\delta}_k^*)$ , for  $k = 2, \dots, K$ . In the sparse models,  $\boldsymbol{\beta}_k^* = \mathbf{0}$  for all  $k$ . For the five SD models, We choose  $q$  from  $\{0.1, 0.15, 0.2\}$  for each model, where  $q$  represents the signal strength of “dense signals.” The models are given as follows:

- S1.  $K = 2$ ,  $\sigma = 0.5$ .  $\boldsymbol{\Sigma}$  is block-diagonal, with each block  $\boldsymbol{\Sigma}_s$  being a  $4 \times 4$  auto-regressive matrix with parameter 0.5,  $\boldsymbol{\delta}_2^* = (\mathbf{2}_5, \mathbf{0}_{495})$ .
- S2.  $K = 3$ ,  $\sigma = 0.5$ .  $\boldsymbol{\Sigma}$  is block-diagonal, with each block  $\boldsymbol{\Sigma}_s$  being a  $4 \times 4$  auto-regressive matrix with parameter 0.5,  $\boldsymbol{\delta}_2^* = (\mathbf{2}_5, \mathbf{0}_{745})$ ,  $\boldsymbol{\delta}_3^* = (\mathbf{0}_5, -\mathbf{2}_5, \mathbf{0}_{740})$ .
- D1.  $K = 2$ ,  $\sigma = 0.5$ .  $\boldsymbol{\Sigma} = \mathbf{I}_p$ ,  $\boldsymbol{\delta}_2^* = (2.5, \mathbf{0}_{499})$ , and  $\boldsymbol{\beta}_2^* = (0, \mathbf{q}_{499})$ ,  $q \in \{0.1, 0.2\}$ .
- D2.  $K = 2$ ,  $\sigma = 0.5$ .  $\boldsymbol{\Sigma}$  is block-diagonal, with each block  $\boldsymbol{\Sigma}_s$  being a  $4 \times 4$  compound symmetry matrix with parameter 0.5,  $\boldsymbol{\delta}_2^* = (2.5, \mathbf{0}_{499})$  and  $\boldsymbol{\beta}_2^* = (0, \mathbf{q}_{499})$ ,  $q \in \{0.1, 0.2\}$ .
- D3.  $K = 2$ ,  $\sigma = 0.5$ .  $\boldsymbol{\Sigma}$  is block-diagonal, with each block  $\boldsymbol{\Sigma}_s$  being a  $4 \times 4$  auto-regressive matrix with parameter 0.5,  $\boldsymbol{\delta}_2^* = (2.5, \mathbf{0}_{499})$  and  $\boldsymbol{\beta}_2^* = (0, \mathbf{q}_{499})$ ,  $q \in \{0.1, 0.2\}$ .

D4.  $K = 3$ ,  $\sigma = 0.6$ .  $\Sigma = \mathbf{I}_p$ ,  $\boldsymbol{\delta}_2^* = (2.5, \mathbf{0}_{749})$ ,  $\boldsymbol{\delta}_3^* = (-2.5, \mathbf{0}_{749})$ ,  $\boldsymbol{\beta}_2^* = (0, \mathbf{q}_{749})$ , and  $\boldsymbol{\beta}_3^* = (0, -\mathbf{q}_{749})$ ,  $q \in \{0.15, 0.2\}$ .

D5.  $K = 3$ ,  $\sigma = 0.5$ .  $\Sigma$  is block-diagonal, with each block  $\Sigma_s$  being a  $4 \times 4$  auto-regressive matrix with parameter 0.5,  $\boldsymbol{\delta}_2^* = (2.5, \mathbf{0}_{749})$ ,  $\boldsymbol{\delta}_3^* = (-2.5, \mathbf{0}_{749})$ ,  $\boldsymbol{\beta}_2^* = (0, \mathbf{q}_{749})$ , and  $\boldsymbol{\beta}_3^* = (0, -\mathbf{q}_{749})$ ,  $q \in \{0.1, 0.15\}$ .

D6.  $K = 5$ ,  $\sigma = 0.5$ . The covariance matrix  $\Sigma$  has an auto-regressive structure, namely,  $\sigma_{ij} = 0.8^{|i-j|}$ . The number of nonzero elements of parameter  $\boldsymbol{\beta}$ 's is five instead of one. Specifically, we let  $(\boldsymbol{\delta}_2^*, \dots, \boldsymbol{\delta}_5^*) = (\mathbf{1.5}_5, -\mathbf{1.5}_5, \mathbf{1}_5, -\mathbf{1}_5)$  and  $(\boldsymbol{\beta}_2^*, \dots, \boldsymbol{\beta}_5^*) = (2\mathbf{q}_{495}, -2\mathbf{q}_{495}, \mathbf{q}_{495}, -\mathbf{q}_{495})$ ,  $q \in \{0.075, 0.1\}$ .

In addition to SD-LDA, we include the following competitors in our simulation: the MSDA (Mai, Yang and Zou, 2019), a logistic regression with a lasso penalty (Hastie, Tibshirani and Friedman, 2009) or elastic-net penalty (Zou and Hastie, 2005) (denoted as lasso and elastic-net, respectively), a support vector machine (SVM) (Joachims, 1998), and sparse optimal scoring (Clemmensen et al., 2011, denoted as SOS). MSDA is implemented using the R package `msda`, lasso and elastic-net are implemented using the R package `glmnet`, and the SVM is implemented using the R package `e1071`. SOS is implemented using the R package `sparseLDA` for multiclass models and the R package `TULIP` in binary models (Pan, Mai and Zhang, 2020).

The tuning parameters in all methods are chosen using five-fold cross-validation, and a grid search is implemented if there are multiple tuning parameters. We run the simulation 100 times for each model, and the means and standard errors of the prediction error (PE in %) are reported in Table 1. The means of the numbers of correctly and incorrectly selected variables are given in Table 2. Recall that the sparse signals dominate in terms of their effects, and thus we focus on their selection. For all the competitors, a variable is selected if and only if it has a nonzero coefficient, while for SD-LDA, a variable is selected if it has a nonzero coefficient in  $\hat{\boldsymbol{\delta}}_k$ .

As shown in Table 1, even when the true models are sparse, SD-LDA still gives a comparable, or even significantly better result than those of the sparse competitors. This may be because the SD-LDA can approximate a sparse classifier by using a large  $\lambda_2$ , but it explores more classifiers using cross-validation over  $\lambda_2$ , yielding better empirical results. For the SD models, SD-LDA has a clear advantage over the sparse methods, indicating that the latter are vulnerable when dense signals exist, and the SD-LDA is preferable under such circumstances.

In Table 2, we see that the SD-LDA continues to give excellent variable selection results across all models. In the SD models, the variable selection becomes worse as  $q$  increases. This is expected, because as  $q$  increases, the boundary between sparse and dense signals becomes blurred. However, the sparse competitors struggle much more than the SD-LDA does. Because they

Table 1. The prediction accuracy results. The means and standard errors (in the parentheses) of the prediction error of 100 replicates are reported as percentages.

Models	$q$	BE	SD-LDA	MSDA	Lasso	elastic-net	SVM	SOS
S1	0	6.4	6.51(0.23)	7.83(0.28)	8.58(0.3)	7.20(0.27)	22.93(0.44)	8.69(0.3)
S2	0	8.3	8.54(0.24)	9.29(0.26)	11.45(0.3)	10.51(0.26)	29.15(0.36)	17.23(0.31)
D1	0.1	20.1	25.27(0.45)	27.26(0.47)	28.40(0.5)	26.28(0.46)	40.79(0.55)	28.20(0.5)
	0.2	10.0	21.08(0.45)	27.18(0.52)	28.35(0.53)	25.40(0.47)	28.18(0.48)	27.57(0.45)
D2	0.1	13.5	18.90(0.38)	26.59(0.47)	26.99(0.48)	24.18(0.42)	25.13(0.45)	25.91(0.49)
	0.2	2.8	5.63(0.22)	21.65(0.48)	19.46(0.44)	10.94(0.33)	5.92(0.23)	17.08(0.49)
D3	0.1	15.2	20.42(0.42)	26.24(0.46)	26.76(0.45)	24.34(0.41)	29.30(0.44)	27.14(0.45)
	0.2	4.1	7.99(0.28)	22.67(0.41)	21.18(0.42)	13.99(0.35)	9.33(0.28)	21.79(0.47)
D4	0.15	9.9	28.57(0.37)	31.23(0.41)	33.90(0.4)	32.47(0.32)	34.43(0.4)	35.61(0.41)
	0.2	8.3	20.76(0.38)	31.59(0.41)	33.75(0.37)	31.15(0.31)	23.38(0.32)	35.00(0.39)
D5	0.1	20.4	28.63(0.39)	35.36(0.42)	38.00(0.38)	35.11(0.38)	31.09(0.38)	39.06(0.41)
	0.15	5.9	17.54(0.4)	35.04(0.42)	35.41(0.39)	29.26(0.33)	14.66(0.3)	37.45(0.37)
D6	0.075	6.3	9.11(0.18)	28.12(0.26)	33.41(0.36)	28.10(0.29)	11.51(0.20)	27.34(0.31)
	0.1	2.4	3.10(0.10)	26.14(0.31)	28.52(0.33)	18.47(0.28)	4.00(0.14)	24.15(0.32)

Table 2. The means and standard errors of correctly selected variables (denoted as C) and incorrectly selected variables (denoted as IC). The true numbers of important/dense signals are 5 for Model S1, 10 for Model S2, and 1 for all SD models.

Models	$q$	SD-LDA		MSDA		Lasso		elastic net		SOS	
		C	IC	C	IC	C	IC	C	IC	C	IC
S1	0	4.5(0.7)	4.6(5)	4.5(0.8)	5.60(6.8)	4.7(0.5)	19.50(8.6)	4.90(0.2)	43.6(30.3)	4.8(0)	19.4(2.3)
S2	0	9.2(1)	5.1(6.7)	9.1(1.1)	4.60(6.9)	1.8(1.1)	33.20(7.4)	5.50(2.6)	67.0(36.2)	10.0(0)	4.4(0.1)
D1	0.1	1.0(0)	4.2(4.4)	1.0(0)	4.50(6.3)	1.0(0)	9.20(9)	1.00(0)	15.0(20.6)	1.0(0)	13.6(2.2)
	0.2	1.0(0.1)	4.7(5.2)	1.0(0)	6.70(7.5)	1.0(0)	18.20(13.4)	1.00(0)	56.0(52.1)	1.0(0)	30.8(3.5)
D2	0.1	1.0(0)	1.8(3.1)	1.0(0)	10.50(10.9)	1.0(0)	22.90(13.1)	1.00(0)	65.8(51)	1.0(0)	23.5(3)
	0.2	0.9(0.3)	1.5(2.8)	1.0(0)	24.00(12.1)	1.0(0)	46.20(7.5)	1.00(0)	189.1(29.7)	1.0(0)	68.8(3.1)
D3	0.1	1.0(0)	2.7(3.7)	1.0(0)	7.70(9)	1.0(0)	18.7(12.9)	1.00(0)	51.1(43.5)	1.0(0)	17.3(2.6)
	0.2	0.9(0.2)	1.1(2)	1.0(0)	21.90(11.1)	1.0(0)	42.1(10.1)	1.00(0)	175.1(44.2)	1.0(0)	58.2(3.3)
D4	0.15	1.0(0.1)	0.6(3.4)	1.0(0)	1.20(3.4)	0(0)	19.9(11.6)	0(0.1)	57.0(69.5)	1.0(0)	22.8(0)
	0.2	0.9(0.3)	0(0)	1.0(0)	5.40(13)	0(0)	23.1(12.8)	0(0.1)	109.7(87.4)	1.0(0)	26.7(0.1)
D5	0.1	1.0(0.1)	1.2(4.4)	1.0(0)	5.30(14.3)	0(0)	19.6(10.8)	0(0.1)	102.2(79.4)	1.0(0)	28.7(0.1)
	0.15	0.9(0.3)	1.6(6.2)	1.0(0)	30.40(26.5)	0(0)	22.9(10.1)	0.10(0.3)	168.2(66.5)	1.0(0)	18.9(0)
D6	0.075	2.6(0.2)	17.5(3.1)	3.3(0.1)	0.11(0)	0(0)	26.89(0.7)	0.31(0.1)	137.7(3.6)	2.3(0.1)	139.9(3.9)
	0.1	2.4(0.1)	11.3(2.7)	3.8(0.1)	0.81(0.2)	0(0)	26.70(0.6)	0.36(0.1)	153.0(1.3)	2.3(0.1)	139.0(3.7)

are incapable of modeling dense signals, they drastically overselect the variables in the hope of achieving higher accuracy.

Finally, we report the computation cost for SD-LDA and its competitors in Table 3. For brevity, we report only the results for Models D1 and D6 with  $q = 0.1$  at the optimal tuning parameters. The computation time is averaged over 100 replicates. Most methods take much less than 1 second to finish one replicate. SD-LDA is slower than most of the competitors, which is the price we pay to model the dense signals and achieve better prediction accuracy. Among the discriminant analysis methods (SD-LDA, MSDA, and SOS), SD-LDA is slower

Table 3. Average computation time based on 100 replicates.

Time ( $s \times 10^{-2}$ )	SD-LDA	MSDA	Lasso	elastic-net	SVM	SOS
D1	11.3	2.3	0.18	0.18	2.5	1.2
D6	17.9	5.2	8.40	9.00	10.4	104.7

than MSDA because it needs to calculate  $(\hat{\Sigma} + 2\lambda_2 \mathbf{I})^{-1}$  when estimating the dense signals. SD-LDA is slower than SOS in the relatively simple Model (D1). However, in the more difficult Model (D6), SD-LDA is much faster than SOS, even though SOS estimates only the sparse signals.

## 5. Real Data Set Analysis

We demonstrate the performance of SD-LDA on five real-world data sets: The IBD data set from Burczynski et al. (2006), the small-blue-round-cell tumour data set (SBRCT) from Khan et al. (2001), the prostate cancer data set from Singh et al. (2002), the gene time data set, and the cancer genome atlas data set. The screened IBD data set is imported from the R package `msda` directly. It contains 127 samples in three classes and 127 gene expressions. The SBRCT data set has 84 samples in four classes, and the prostate cancer data set has 102 samples in two classes. Because the dimensions of the SBRCT and the prostate cancer data sets are extremely high, we first apply t-test screening, as in Fan and Fan (2008), before performing our proposal. The reduced data sets are generated by the t-test screening with  $p$ -values of screening set to 0.001 and 0.05, respectively. The numbers of their gene expressions are reduced to 594 and 477, respectively.

The gene time course data (GTC) describes the clinical response to treatment for multiple sclerosis (MS) patients based on gene expression time course data. This data set was originally described in Baranzini et al. (2004). Fifty-three patients were given recombinant human interferon beta (rIFN $\beta$ ), which is often used to control the symptoms of MS. Gene expression was measured for 76 genes of interest before treatment (baseline) and at six follow-up time points over the next two years (3 months, 6 months, 9 months, 12 months, 18 months, 24 months). Afterward, patients were classified into good responders or poor responders to rIFN $\beta$ , based on clinical characteristics. There are 20 good responders and 33 bad responders in all the 53 patients. The dimension for this data set is  $76 \times 7 = 532$ .

The Cancer Genome Atlas (TCGA) Research Network has profiled and analyzed large numbers of human tumors to discover molecular aberrations at the DNA, RNA, protein, and epigenetic levels. These data are part of the pan-cancer data set, and is a random extraction of gene expressions of patients with different types of tumors: BRCA, KIRC, COAD, LUAD, and PRAD. We downloaded the data from <https://archive.ics.uci.edu/dataset/401/gene+expression+cancer+rna+seq>, which was kindly shared by Samuele Fiorini in

Table 4. The means and standard errors (in parentheses) of the prediction error(%) of SD-LDA and other competitors of 100 replicates for each data set.

DataSet	SD-LDA	MSDA	Lasso	elastic-net	SVM	SOS
IBD	3.71(0.28)	8.00(0.37)	6.76(0.36)	5.10(0.34)	8.27(0.38)	6.93(0.33)
SBRCT	0.08(0.08)	14.08(0.9)	1.58(0.2)	0(0)	0.92(0.17)	2.15(0.26)
Prostate	0(0)	29.06(0.74)	19.06(0.58)	2.79(0.28)	0(0)	15.33(0.63)
GTC	17.40(0.74)	33.60(0.97)	31.70(0.85)	21.20(0.87)	31.60(0.51)	45.20(1.31)
TCGA	0.20(0.02)	1.57(0.14)	0.58(0.02)	0.42(0.01)	0.37(0.01)	4.90(0.12)

Table 5. The means and standard errors of the number of selected variables by SD-LDA and other competitors of 100 replicates are reported.

Methods	SD-LDA	MSDA	Lasso	elastic-net	SOS
IBD	9.40(0.82)	29.46(0.7)	10.67(0.18)	69.83(0.5)	52.36(1.89)
SBRCT	7.62(0.47)	17.32(0.54)	10.97(0.23)	140.45(0.67)	59.07(0.99)
Prostate	11.37(0.52)	12.66(0.4)	43.59(0.59)	233.70(0.93)	64.67(1.15)
GTC	2.04(0.18)	6.09(0.34)	12.52(0.66)	110.07(2.84)	25.65(1.15)
TCGA	19.13(0.76)	38.71(0.84)	9.01(0.19)	125.51(0.74)	108.34(2.71)

2016. The original data set is maintained by the cancer genome atlas pan-cancer analysis project (<https://www.synapse.org/>). The data set has 801 samples in five classes and 20,531 gene expressions. As with the previous data sets, we first use t-test screening to select 801 genes.

We perform SD-LDA and the competitors included in Section 4 on the first four data sets. We run 100 replicates, and in each replicate the data sets are split in a 2:1 ratio in a balanced manner to form training and testing sets. The tuning parameters are chosen using five-fold cross-validation and by checking their prediction errors. For the TCGA data, almost all the methods perform perfectly. To make the classification problem more challenging, we run 100 replicates, with the data set split in a 1:9 ratio in a balanced manner to form training and testing sets; that is, we have 80 training samples and 721 test samples.

The average prediction errors are reported in Table 4. SD-LDA is either the best classifier, or statistically no different from the best classifier. These results support the application of SD-LDA in practice. Note that the sparse methods may perform better if we preprocess the data sets a little differently. For example, Mai, Zou and Yuan (2012) reported a prediction error of 5.9% for MSDA (its binary equivalence, to be exact) if the data set is not screened. However, the error is still significantly larger than that of SD-LDA on the screened data in Table 4.

We further check the variable selection results in Table 5. By considering the “dense signals”, SD-LDA actually selects the fewest sparse signals. Therefore, SD-LDA could help researchers focus on a smaller set of key features for a more in-depth study. Because the gene names for the IBD, Prostate, and TCGA data

sets are missing from the original resources, we report only the selected genes for the SBRCT and GTC data sets. For the SBRCT data, SD-LDA selects 10 genes, including WASp, CAV1, CDH2, HBE1, anti-CD99, Psmb10, HLA-DMA, SYNGR1, EHD1, and PSMB8. Some of these genes have been shown to have close relationship with the development of cancer. For example, CAV1 appears to act as a tumor suppressor protein at early stages of cancer progression (Sáinz-Jaspeado et al., 2011); CD99 appears to be a robust marker of cancer stem cells and a promising therapeutic target in these malignancies (Pasello, Manara and Scotlandi, 2018); and HLA-DMA antigen expression by tumor cells influences the tumor antigen (TA)-specific immune responses and, depending on the cancer type, the clinical course of the disease (Seliger, Kloot and Ferrone, 2017). For the GTC data set, SD-LDA selects two genes, Caspase 6 and FLIP. This agrees with the findings in the existing literature. For example Julien et al. (2016) showed that Caspase 6 is related to MS, and (Hauser and Oksenberg, 2006) showed that FLIP is related to MS.

## 6. Discussion

SD-LDA is proposed as a convex high-dimensional classification method that is robust to the changing signal pattern in linear discriminant directions. It is obtained by separating the linear discriminant directions into “sparse signals” and “dense signals” and applying suitable penalties to estimate them. To the best of our knowledge, this is the first SD classifier, to perform well over a wide range of data sets. Similar techniques could be combined with linear classifiers, such as the logistic regression or SVM, to enable them to capture the “sparse signals” and “dense signals.” We can further consider a similar modification for nonlinear models, such as the quadratic discriminant analysis (QDA; Fan et al., 2015; Li and Shao, 2015; Jiang, Wang and Leng, 2018).

Although our work is developed under the LDA model, in which the within-class distribution is normal. It can be extended easily to a semiparametric framework that has been reasonably well studied (Lin and Jeon, 2003; Liu, Lafferty and Wasserman, 2009; Mai and Zou, 2015; Jiang and Leng, 2016). In such a semiparametric framework,  $\mathbf{X}$  does not have to be normal within each class, but there must exist a set of unknown transformations  $g = (g_1, \dots, g_p)$  such that  $(g(\mathbf{X}), Y)$  follows the LDA model. When considering high-dimensional data, existing works frequently adopt the sparsity assumption. However, following our work, we can consider a semiparametric model with sparse+dense signals to achieve greater flexibility. We leave this topic as an interesting future research direction, for which some recent theoretical works on estimating the transformation may be helpful (Mai, He and Zou, 2022). However, such studies are beyond the scope of this research.

## Supplementary Material

The derivation for algorithms and the proof for theorems are available in the Supplementary Material. Section S2 contains the derivation for Lemma 1 and Section S3 contains the proof for Theorem 1.

## Acknowledgments

The authors are grateful to the editor, associate editor and referees for their helpful suggestions. Mai's research was partially supported by National Science Foundation (CCF-1908969).

## References

Baranzini, S. E., Mousavi, P., Rio, J., Caillier, S. J., Stillman, A., Villoslada, P. et al. (2004). Transcription-based prediction of response to IFN $\beta$  using supervised computational methods. *PLoS Biology* **3**, e2.

Bickel, P. J. and Levina, E. (2004). Some theory for Fisher's linear discriminant function, naive Bayes', and some alternatives when there are many more variables than observations. *Bernoulli* **10**, 989–1010.

Burczynski, M. E., Peterson, R. L., Twine, N. C., Zuberek, K. A., Brodeur, B. J., Casciotti, L. et al. (2006). Molecular classification of Crohn's disease and ulcerative colitis patients using transcriptional profiles in peripheral blood mononuclear cells. *The Journal of Molecular Diagnostics* **8**, 51–61.

Cai, T. and Liu, W. (2011). A direct estimation approach to sparse linear discriminant analysis. *Journal of the American Statistical Association* **106**, 1566–1577.

Chernozhukov, V., Hansen, C. and Liao, Y. (2017). A lava attack on the recovery of sums of dense and sparse signals. *The Annals of Statistics* **45**, 39–76.

Clemmensen, L., Hastie, T., Witten, D. and Ersbøll, B. (2011). Sparse discriminant analysis. *Technometrics* **53**, 406–413.

Fan, J. and Fan, Y. (2008). High dimensional classification using features annealed independence rules. *The Annals of Statistics* **36**, 2605–2637.

Fan, J., Feng, Y. and Tong, X. (2012). A road to classification in high dimensional space: The regularized optimal affine discriminant. *Journal of the Royal Statistical Society. Series B (Statistical Methodology)* **74**, 745–771.

Fan, J., Ke, Z. T., Liu, H. and Xia, L. (2015). Quadro: A supervised dimension reduction method via rayleigh quotient optimization. *The Annals of Statistics* **43**, 1498–1534.

Fan, J. and Li, R. (2001). Variable selection via nonconcave penalized likelihood and its oracle properties. *Journal of the American Statistical Association* **96**, 1348–1360.

Friedman, J., Hastie, T. and Tibshirani, R. (2001). *The Elements of Statistical Learning*. Springer, New York.

Friedman, J. H. (1989). Regularized discriminant analysis. *Journal of the American Statistical Association* **84**, 165–175.

Hastie, T., Tibshirani, R. and Friedman, J. (2009). *The Elements of Statistical Learning: Data Mining, Inference, and Prediction*. Springer Science & Business Media.

Hauser, S. L. and Oksenberg, J. R. (2006). The neurobiology of multiple sclerosis: Genes, inflammation, and neurodegeneration. *Neuron* **52**, 61–76.

Hoerl, A. E. and Kennard, R. W. (1970). Ridge regression: Biased estimation for nonorthogonal problems. *Technometrics* **12**, 55–67.

Huang, J., Breheny, P. and Ma, S. (2012). A selective review of group selection in high-dimensional models. *Statistical Science* **27**, 481–499.

Jiang, B. and Leng, C. (2016). High dimensional discrimination analysis via a semiparametric model. *Statistics & Probability Letters* **110**, 103–110.

Jiang, B., Wang, X. and Leng, C. (2018). A direct approach for sparse quadratic discriminant analysis. *The Journal of Machine Learning Research* **19**, 1098–1134.

Joachims, T. (1998). Making large-scale SVM learning practical. Technical report. University of Dortmund, Dortmund.

Julien, O., Zhuang, M., Wiita, A. P., O'Donoghue, A. J., Knudsen, G. M., Craik, C. S. et al. (2016). Quantitative MS-based enzymology of caspases reveals distinct protein substrate specificities, hierarchies, and cellular roles. *Proceedings of the National Academy of Sciences* **113**, E2001–E2010.

Khan, J., Wei, J. S., Ringner, M., Saal, L. H., Ladanyi, M., Westermann, F. et al. (2001). Classification and diagnostic prediction of cancers using gene expression profiling and artificial neural networks. *Nature medicine* **7**, 673–679.

Ledoit, O. and Wolf, M. (2004). A well-conditioned estimator for large-dimensional covariance matrices. *Journal of Multivariate Analysis* **88**, 365–411.

Li, Q. and Shao, J. (2015). Sparse quadratic discriminant analysis for high dimensional data. *Statistica Sinica* **25**, 457–473.

Lin, Y. and Jeon, Y. (2003). Discriminant analysis through a semiparametric model. *Biometrika* **90**, 379–392.

Liu, H., Lafferty, J. and Wasserman, L. (2009). The nonparanormal: Semiparametric estimation of high dimensional undirected graphs. *Journal of Machine Learning Research* **10**, 2295–2328.

Mai, Q., He, D. and Zou, H. (2022). Coordinatewise Gaussianization: Theories and applications. *Journal of the American Statistical Association* **118**, 2329–2343.

Mai, Q., Yang, Y. and Zou, H. (2019). Multiclass sparse discriminant analysis. *Statistica Sinica* **29**, 97–111.

Mai, Q. and Zou, H. (2015). Sparse semiparametric discriminant analysis. *Journal of Multivariate Analysis* **135**, 175–188.

Mai, Q., Zou, H. and Yuan, M. (2012). A direct approach to sparse discriminant analysis in ultra-high dimensions. *Biometrika* **99**, 29–42.

Min, K., Mai, Q. and Junge, L. (2023). Optimality in high-dimensional tensor discriminant analysis. *Pattern Recognition* **143**, 109803.

Pan, Y., Mai, Q. and Zhang, X. (2020). Tulip: A toolbox for linear discriminant analysis with penalties. *The R Journal* **12**, 134–154.

Pasello, M., Manara, M. C. and Scotlandi, K. (2018). CD99 at the crossroads of physiology and pathology. *Journal of Cell Communication and Signaling* **12**, 55–68.

Sáinz-Jaspeado, M., Martin-Liberal, J., Lagares-Tena, L., Mateo-Lozano, S., Del Muro, X. G. and Tirado, O. M. (2011). Caveolin-1 in sarcomas: Friend or foe? *Oncotarget* **2**, 305–312.

Seliger, B., Kloot, M. and Ferrone, S. (2017). HLA class II antigen-processing pathway in tumors: Molecular defects and clinical relevance. *Oncoimmunology* **6**, e1171447.

Shao, J., Wang, Y., Deng, X. and Wang, S. (2011). Sparse linear discriminant analysis by thresholding for high dimensional data. *The Annals of statistics* **39**, 1241–1265.

Singh, D., Febbo, P. G., Ross, K., Jackson, D. G., Manola, J., Ladd, C. et al. (2002). Gene expression correlates of clinical prostate cancer behavior. *Cancer cell* **1**, 203–209.

Tibshirani, R., Hastie, T., Narasimhan, B. and Chu, G. (2002). Diagnosis of multiple cancer types by shrunken centroids of gene expression. *Proceedings of the National Academy of Sciences* **99**, 6567–6572.

Tibshirani, R., Hastie, T., Narasimhan, B. and Chu, G. (2003). Class prediction by nearest shrunken centroids, with applications to DNA microarrays. *Statistical Science* **18**, 104–117.

Weisberg, S. (2005). *Applied Linear Regression*. John Wiley & Sons.

Witten, D. M. and Tibshirani, R. (2011). Penalized classification using Fisher's linear discriminant. *Journal of the Royal Statistical Society. Series B (Statistical Methodology)* **73**, 753–772.

Xu, P., Zhu, J., Zhu, L. and Li, Y. (2015). Covariance-enhanced discriminant analysis. *Biometrika* **102**, 33–45.

Yang, H., Lin, D. and Li, Q. (2022). An efficient greedy search algorithm for high-dimensional linear discriminant analysis. *Statistica Sinica* **33**, 1343–1364.

Yuan, M. and Lin, Y. (2006). Model selection and estimation in regression with grouped variables. *Journal of the Royal Statistical Society. Series B (Statistical Methodology)* **68**, 49–67.

Zhang, C.-H. (2010). Nearly unbiased variable selection under minimax concave penalty. *The Annals of Statistics* **38**, 894–942.

Zou, H. and Hastie, T. (2005). Regularization and variable selection via the elastic net. *Journal of the Royal Statistical Society. Series B (Statistical Methodology)* **67**, 301–320.

(Received July 2022; accepted May 2023)