Classification of high-dimensional data with spiked covariance matrix structure

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Summary. We study the classification problem for high-dimensional data with \( n \) observations on \( p \) features where the \( p \times p \) covariance matrix \( \Sigma \) exhibits a spiked eigenvalues structure and the vector \( \zeta \), given by the difference between the whitened mean vectors, is sparse with sparsity at most \( s \). We propose an adaptive classifier (adaptive with respect to the sparsity \( s \)) that first performs dimension reduction on the feature vectors prior to classification in the dimensionally reduced space, i.e., the classifier whitened the data, then screen the features by keeping only those corresponding to the \( s \) largest coordinates of \( \zeta \) and finally apply Fisher linear discriminant on the selected features. Leveraging recent results on entrywise matrix perturbation bounds for covariance matrices, we show that the resulting classifier is Bayes optimal whenever \( n \rightarrow \infty \) and \( s \sqrt{n^{-1} \ln p} \rightarrow 0 \). Experimental results on real and synthetic data sets indicate that the proposed classifier is competitive with existing state-of-the-art methods while also selecting a smaller number of features.

Keywords: High-dimensional classification, spiked covariance, Fisher linear discriminant, eigenvector perturbation, whitening matrix

1. Introduction

Classification is one of the most important and widely studied inference task in statistics and machine learning. Among standard classifiers, the Fisher linear discriminant analysis (LDA) rule is especially popular for its ease of implementation and interpretation. More specifically, suppose we are given a \( p \)-variate random vector \( Z \) drawn from a mixture of two multivariate normal distributions \( \pi_1 N_p(\mu_1, \Sigma) + (1 - \pi_1) N_p(\mu_2, \Sigma) \) and our goal is to classify \( Z \) into one of the two classes. The Fisher LDA rule is then given by

\[
\Upsilon_F(Z) = \begin{cases} 
1 & \text{if } (\Sigma^{-1}(\mu_2 - \mu_1))^T (Z - \frac{\mu_2 + \mu_1}{2}) \leq \ln \frac{\pi_1}{1 - \pi_1}, \\
2 & \text{if } (\Sigma^{-1}(\mu_2 - \mu_1))^T (Z - \frac{\mu_2 + \mu_1}{2}) > \ln \frac{\pi_1}{1 - \pi_1}, 
\end{cases}
\]  

(1.1)

provided that \( \Sigma \) is positive definite. The Fisher rule \( \Upsilon_F \) is the Bayes decision rule, i.e., it achieves the smallest mis-classification error with respect to 0-1 loss for classifying \( Z \). The Fisher rule is, however, not applicable in practice as it involves the unknown parameters \( \Sigma^{-1}, \mu_1 \) and \( \mu_2 \); we thus usually compute the sample covariance matrix \( \hat{\Sigma} \) and the sample means \( \hat{X}_1 \) and \( \hat{X}_2 \) from a given training data set with \( n \) observations and then plugged these quantities into Eq. (1.1); the resulting classifier is termed the plug-in LDA rule \( \hat{\Upsilon}_F \).
Traditionally, the classification accuracy of $\hat{\Upsilon}_F$ is justified in the large sample regime where $n \rightarrow \infty$ with $p \ll n$. This theoretical justification is, however, no longer appropriate in the high-dimensional settings where $n \sim p$ or even $n \ll p$, e.g., the sample covariance matrix $\hat{\Sigma}$ is singular in these settings. Remarkably, Bickel and Levina (2004) proved that the error rate for $\hat{\Upsilon}_F$ where we replace $\Sigma^{-1}$ with the Moore–Penrose pseudo-inverse of $\hat{\Sigma}$ could be as bad as random guessing and that, furthermore, the naive Bayes (NB) rule which ignores the correlation structure in $\Sigma$ usually outperforms $\hat{\Upsilon}_F$.

Continuing this line of inquiry, other independence rules (IR) have been proposed in Tibshirani et al. (2002) and Fan and Fan (2008). These classifiers suffer from two major drawbacks, namely (1) the accumulation of error in estimating $\mu_1$ and $\mu_2$ and (2) misspecification of the covariance matrix $\Sigma$. In particular Fan and Fan (2008) demonstrated that the noise accumulation in estimating $\mu_1$ and $\mu_2$ alone is sufficient to degrade the performance of IR classifiers. Shao et al. (2011) extended this result and show that the noise accumulation can also lead to the plug-in LDA classifier being, asymptotically, no better than random guessing even when $\Sigma$ is known. These results indicate the need for assuming sparsity conditions on the features and the important role of features selection for mitigating the estimation errors associated with growing dimensionality. Fan et al. (2012) also showed that ignoring the correlations structure in $\Sigma$ prevents IR classifiers from achieving Bayes optimality.

To address the above limitations of IR classifiers, Shao et al. (2011) proposed thresholding of both $\Sigma$ and $\mu_2 - \mu_1$; this is similar to the motivation for regularized covariance estimators in Bickel and Levina (2009). In contrast, Cai and Liu (2011); Fan et al. (2012); Mai et al. (2012); Witten and Tibshirani (2011) and Cai and Zhang (2019) imposed sparsity conditions on the discriminant direction $\beta = \Sigma^{-1}(\mu_2 - \mu_1)$ and use penalized estimation approaches to recover $\beta$. Cai and Liu (2011) mentioned two major advantages of this framework. Firstly, the assumption of sparsity on $\beta$ is less restrictive than assuming sparsity for both $\Sigma$ (or $\Sigma^{-1}$) and $\mu_2 - \mu_1$ separately. Secondly, $\Upsilon_F$ only uses $\Sigma^{-1}$ and $\mu_2 - \mu_1$ through their product $\Sigma^{-1}(\mu_2 - \mu_1)$ and thus consistent estimation of $\beta$ is sufficient. This framework leads to procedures and results that resemble those for high-dimensional linear regression even though the classification problem is generally not formulated in terms of a linear model plus noises. For example, Cai and Liu (2011) and Cai and Zhang (2019) considered a linear programming approach similar to the Dantzig selector (Candes and Tao, 2005) while Mai et al. (2012) studied a sparse discriminant analysis rule that used the Lasso (Tibshirani, 1996). Nevertheless, it had been observed, empirically, that these approaches can lead to classification rules that select a larger number of features than necessary, and one possible explanation is due to the correlations among the coordinates of the sparse estimate $\hat{\beta}$ as induced by the correlation structure in $\Sigma$.

In this paper we take a different approach for addressing the curse of dimensionality when $n \approx p$ or $n \ll p$ by first performing dimension reduction on the feature vectors prior to classification in the dimensionally reduced space. Since dimension reduction is an important and ubiquitous pre-processing step in high-dimensional data analysis, there is a sizable number of work devoted to these type of classifiers. In particular as LDA is a linear classifier, it is usually combined with other linear algebraic dimension reduction
techniques, with the most prominent being principal component analysis (PCA). For example Section 9.1 of Jolliffe (2002) provides a detailed review of combining LDA with different variants of PCA in the low-dimensional setting while Niu et al. (2015) proposed the use of reduced rank LDA together with class-conditional PCA in the high-dimensional settings. In terms of applications, Belhumeur et al. (1997); Zhao et al. (1998) and Prasad et al. (2010) discussed the use of LDA and PCA in the context of face and images recognition, respectively.

While classifiers based on combining PCA with LDA arise quite naturally, their theoretical properties in the high-dimensional setting remain an open problem. In particular the analysis of these classifiers require possibly different techniques and assumptions compared to those based on direct estimation of the discriminant direction $\beta$. More specifically consistency results for $\beta$ are usually based on ideas from high-dimensional regression and thus adhered to assumptions on bounded and concentrated eigenvalues of $\Sigma$, see e.g., Bickel and Levina (2004); Cai and Zhang (2019); Fan and Fan (2008); Shao et al. (2011). However Wang and Fan (2017) noted that the bounded eigenvalues assumptions disregard the strong signals (eigenvalues) in the data and might be problematic in fields such as genomics, economics and finance. These assumptions are nevertheless imposed mainly due to the limitation of quantifying the estimation error for $\Sigma$ in terms of the spectral norm difference for $\hat{\Sigma} - \Sigma$. In contrast the idealized setting for dimension reduction via PCA is when $\Sigma$ contains a small subset of signal eigenvalues that accounts for most of the variability in $\Sigma$. This idealized setting for PCA is also distinct from the idealized setting for graphical models wherein $\Sigma^{-1}$ is typically assumed to be sparse.

In summary, our contributions in this paper are as follows. We propose a classifier that first perform dimension reduction on the features vectors prior to performing classification in the dimensionally reduced space; see Section 2. We then study the theoretical properties of the proposed classifier under a widely-adopted model for covariance matrix estimation in high-dimensional data, namely the spiked eigenvalues structure where $\Sigma$ contains a few large and/or diverging eigenvalues that are well-separated from the remaining “small” eigenvalues. In particular we show in Section 3 that the proposed classifier achieves the Bayes optimal mis-classification error rate of the Fisher LDA rule $\Upsilon_F$ when $n \to \infty$ and $n^{-1} \ln p \to 0$. This is, to the best of our knowledge, the first Bayes optimal consistency result for classification after performing dimension reduction via PCA. We then demonstrate empirically, for both simulated and real data, that the resulting classifier selects fewer features while also having error rates that are competitive with existing classifiers based on estimating the discriminant direction $\beta$. The theoretical and numerical results provide a clear example of the synergy linking dimension reduction with classification. The proposed classifier can also be extended to (1) classify data from $K \geq 3$ classes or (2) classify data where the feature vectors are elliptical distributed but not necessarily multivariate normal.
2. Methodology

2.1. Notation and settings

For a vector \( x \in \mathbb{R}^p \), the conventional \( \ell_0 \) quasi-norm and the \( \ell_1, \ell_2 \) and \( \ell_\infty \) norms are denoted by \( \| x \|_0, \| x \|_1, \| x \|_2 \) and \( \| x \|_\infty \), respectively. For \( p \in \mathbb{N} \), we denote by \([ p] \) the set \( \{ 1, \ldots, p \} \). Given \( x \in \mathbb{R}^p \) and a non-empty set \( A \subset [ p] \), we denote by \( x_A = ( x_j, j \in A) \) the column vector obtained by keeping only the elements in \( x \) whose indices belong to \( A \).

The symbol ‘\( \circ \)’ represents the Hadamard product. For \( i \in [ p] \), \( e_{(p)}^i \) is the \( i \)th standard basis vector of \( \mathbb{R}^p \) and \( 1_p \) is a vector in \( \mathbb{R}^p \) whose elements are all 1; we also write \( e_i \) and \( 1 \) when the choice of \( p \) is clear from context and \( I_p \) stands for the identity matrix in \( \mathbb{R}^{p \times p} \). For \( x, y \in \mathbb{R}^p \), the standard Euclidean inner product between \( x \) and \( y \) is denoted as \( \langle x, y \rangle \). For a matrix \( M \in \mathbb{R}^{p \times q} \), the Frobenius norm and spectral norm of \( M \) are written as \( \| M \|_F \) and \( \| M \|_2 \), respectively. The two-to-infinity norm of \( M \) is defined as

\[
\| M \|_{2 \to \infty} := \sup_{\| x \|_2 = 1} \| Mx \|_\infty .
\]  

Let \( M_i \) denote the \( i \)th row of \( M \). Proposition 1 in the appendix implies that \( \| M \|_{2 \to \infty} = \max_i \| M_i \|_2 \) where \( \| M_i \|_2 \) denote the \( \ell_2 \) norm of \( M_i \). We note the relationship \( \| M \|_{2 \to \infty} \leq \| M \|_2 \leq \| M \|_F \). Let \( \text{tr} (M) \) denote the trace of a square matrix \( M \). The effective rank of a square matrix \( M \) is defined as \( r(M) := \text{tr}(M)/\| M \|_2 \); the effective rank of a matrix is a useful surrogate measure for its complexity, see e.g., Vershynin (2012). Let \( \mathcal{O}(\cdot), \mathcal{O}^*(\cdot) \) and \( \Theta(\cdot) \) represent the standard big-O, little-o and big-theta relationships. Finally, \( 1(A) \) and \( |A| \) denote the indicator function of a set \( A \) and its cardinality, respectively.

In the subsequent discussion we shall generally assume, unless specified otherwise, that we have access to training sets \( \{ X_{11}, \ldots, X_{n_1} \} \) and \( \{ X_{21}, \ldots, X_{n_2} \} \) whose elements are independently and identically distributed random vector from the \( p \)-variate distributions \( \mathcal{N}_p(\mu_1, \Sigma) \) (class 1) and \( \mathcal{N}_p(\mu_2, \Sigma) \) (class 2). The sample means for each class and the pooled sample covariance matrix are denoted as

\[
\bar{X}_i = \frac{1}{n_i} \sum_{j=1}^{n_i} X_{ij}, \quad i = 1, 2, \tag{2.2}
\]

\[
\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^{2} \sum_{j=1}^{n_i} (X_{ij} - \bar{X}_i)(X_{ij} - \bar{X}_i)^\top, \quad n := n_1 + n_2. \tag{2.3}
\]

On numerous occasions we also need a variant of the sample covariance matrix where we replace the sample means with the true means. We denote this matrix as

\[
\hat{\Sigma}_0 = \frac{1}{n} \sum_{i=1}^{2} \sum_{j=1}^{n_i} (X_{ij} - \mu_i)(X_{ij} - \mu_i)^\top. \tag{2.4}
\]

2.2. Linear discriminant analysis and whitening matrix

Let \( \Sigma \) be a \( p \times p \) positive definite matrix. The whitening matrix or sphering \( \mathcal{W} \) matrix is a linear transformation satisfying \( \mathcal{W} \mathcal{W}^\top = \Sigma^{-1} \) and is generally used to decorrelate
random variables and scale their variances to 1. The whitening transformation is unique only up to orthogonal transformation, i.e., if \( W \) is a whitening transformation then \( WT \) is also a whitening transformation for any \( p \times p \) orthogonal matrix \( T \); see Kessy et al. (2015) for a comparison between several common choices of whitening transformation. In this paper we take the whitening transformation to be \( W = \Sigma^{-1/2} \). Note that \( \Sigma^{-1/2} \) is the whitening transformation that minimizes the expected mean square error between the original data and the whitened data (Eldar and Oppenheim, 2003). Given \( W \), we define the \textit{whitened} direction as \( \zeta = W(\mu_2 - \mu_1) \) and the whitened set \( S_\zeta = \{ j : \zeta_j \neq 0 \} \). We referred to the elements of \( S_\zeta \) as the whitened coordinates or variables. The Fisher linear discriminant rule is then equivalent to

\[
Y_F(Z) = \begin{cases} 
1 & \text{if } \zeta^\top(W(Z - \frac{\mu_1 + \mu_2}{2})) = \zeta_{S_\zeta}^\top(W(Z - \frac{\mu_1 + \mu_2}{2})), S_\zeta \leq \ln \frac{\pi_1}{1 - \pi_1}, \\
2 & \text{otherwise},
\end{cases}
\tag{2.5}
\]

where \( Z \sim \pi_1 N_p(\mu_1, \Sigma) + (1 - \pi_1) N_p(\mu_2, \Sigma) \). Recall that, for a vector \( \zeta \) and a set of indices \( \mathcal{A} \), the vector \( \xi_{\mathcal{A}} \) is obtained from \( \xi \) by keeping only the elements indexed by \( \mathcal{A} \). Since \( \beta = \Sigma^{-1}(\mu_2 - \mu_1) \) is the Bayes direction, a significant portion of previous research is devoted to recovering \( \beta \) and the discriminative set \( S_\beta = \{ j : \beta_j \neq 0 \} \). We refer to the elements of \( S_\beta \) as the discriminative coordinates or variables. We emphasize that in general the discriminative set and whitened set are not the same, except for when \( \Sigma \) has certain special structures, e.g., \( \Sigma \) being diagonal.

If \( p \ll n \) then the empirical whitening matrix \( \hat{W} = \hat{\Sigma}^{-1/2} \) is well-defined and the empirical whitened variables \( \hat{\zeta} = \hat{W}(\hat{X}_2 - \hat{X}_1) \) are approximately decorrelated in the plug-in LDA rule, i.e., by the law of large numbers, \( \hat{W}\Sigma\hat{W} \to I_p \) and hence \( \text{Var}[\hat{\zeta}] \approx cI \) for some constant \( c \). In contrast, the coordinates of the estimated discriminant direction \( \hat{\beta} \) are not decorrelated since \( \text{Var}[\hat{\beta}] \approx c\Sigma^{-1} \). It is thus easier to quantify the impact of any arbitrary \textit{whitened} feature toward the classification accuracy than to quantify the impact for an arbitrary \textit{raw} feature. We illustrate this point by considering the following simulation example.

**Example 1.** We generate \( n_1 = n_2 = 500 \) samples from the bivariate normal distribution with \( \mu_1 = (0, 0)^\top \), \( \mu_2 = (1, 0)^\top \) and common covariance matrix:

\[
\Sigma = \begin{pmatrix} 
1 & 0.9 \\
0.9 & 1 
\end{pmatrix}.
\]

Figure 1 shows that the synthetic data fall within the ellipses centered at the sample mean of each class while the sphering step scales the data and rotates the ellipses (decorrelation). Example 1 is the conventional low-dimensional setting where \( p = 2 \) and \( n = 1000 \); the sample covariance matrix \( \hat{\Sigma} \) is non-singular and the Bayes direction is estimated by \( \hat{\Sigma}^{-1}(\bar{X}_2 - \bar{X}_1) \) and similarly for the estimated whitened direction \( \hat{\zeta} = \Sigma^{-1/2}(\bar{X}_2 - \bar{X}_1) \). The following procedure compares the impact on classification accuracy when we select the raw features by hard thresholding the estimated discriminant direction versus when we select the whitened features by hard thresholding the estimated whitened direction.

**Step 1:** Hard threshold \( \hat{\beta} \) and \( \hat{\zeta} \) to keep only the largest, in magnitude, coordinate.
Assume without loss of generality that it is the first coordinate for both $\hat{\beta}$ and $\hat{\zeta}$. Now let $\hat{\nu} = \frac{1}{\|\beta\|_2}(\hat{\beta}_1, 0)^T$ and $\hat{\nu}_\zeta = \frac{1}{\|\zeta\|_2}(\hat{\zeta}_1, 0)^T$.

**Step 2**: Project the data and whitened data onto $\hat{\nu}$ and $\hat{\nu}_\zeta$, respectively, then classify using the plugin-LDA rules

\[
\text{Raw data } \hat{\Upsilon}_\nu(Z) = \begin{cases} 
1, & \hat{\nu}^T(Z - \bar{X}_1 + \bar{X}_2) \leq 0 \\
2, & \hat{\nu}^T(Z - \bar{X}_1 + \bar{X}_2) > 0
\end{cases}
\]

\[
\text{Whitened data } \hat{\Upsilon}_{\nu_\zeta}(Z) = \begin{cases} 
1, & \hat{\nu}_\zeta^T\hat{W}(Z - \bar{X}_1 + \bar{X}_2) \leq 0 \\
2, & \hat{\nu}_\zeta^T\hat{W}(Z - \bar{X}_1 + \bar{X}_2) > 0
\end{cases}
\]

Figure 2 compares the in-sample classification accuracy, based on one realization of $n_1 = n_2 = 500$ samples, for the plug-in LDA classifier with different projection directions $\hat{\nu}$ and $\hat{\nu}_\zeta$. Figure 2 suggests that the accuracy of $\hat{\nu}_\zeta$ is substantially higher than that of $\hat{\nu}$. To confirm this, we replicate the above experiment 1000 times and compute the average error rate. The results are given in Table 1 for the plug-in LDA using the projection directions $\hat{\nu}$, $\hat{\nu}_\zeta$ and $\hat{\beta}$. Note that the plug-in LDA rule using $\hat{\beta}$ and $\hat{\zeta}$ are identical for the case $p < n$. The false positives rate (FPR) and the false negative rate (FNR) in Table 1 are computed by labeling data from class 1 and class 2 as true negatives and true positives, respectively. Table 1 indicates that projection onto $\hat{\beta}$ (equivalently projection of whitened data onto $\hat{\zeta}$) yields the best performance among all three directions. This is expected since we lose information when we obtain $\hat{\nu}$ and $\hat{\nu}_\zeta$ by thresholding $\hat{\beta}$ and $\hat{\zeta}$.
Fig. 2. (a) The synthetic data projected onto the first element of the estimated Bayes direction $\hat{\nu}$ (b) The synthetic data projected onto the first element of the estimated whitened direction $\hat{\nu}_\zeta$

Table 1. Average error rate, FPR and FNR of the plug-in LDA using the projection directions $\hat{\nu}$, $\hat{\nu}_\zeta$ and $\hat{\beta}$. The provided numbers are in percentages and are based on 1000 replications of Example 1.

|                | $\hat{\nu}$ | $\hat{\nu}_\zeta$ | $\hat{\beta}$ |
|----------------|--------------|---------------------|----------------|
| Error rate     | 30.88        | 16.55               | 12.56          |
| False positive rate | 30.90        | 16.57               | 12.54          |
| False negative rate | 30.86        | 16.52               | 12.58          |
Nevertheless, the loss in accuracy when using \( \hat{\nu}_\zeta \) is much smaller compared to using \( \hat{\nu} \), and this is due mainly to the (approximate) orthogonality of the whitened features. Note that classification using \( \hat{\nu} \) (correspondingly \( \hat{\nu}_\zeta \)) can also be viewed as first projecting the data (correspondingly whitened data) into 1 dimension followed by learning a plug-in LDA rule in \( \mathbb{R} \).

### 2.3. Combining LDA and PCA

We see from the example in Section 2.2 that thresholding of the whitened direction can lead to better classification accuracy compared to thresholding of the discriminant direction. Furthermore both approaches can be viewed under the framework of first performing dimension reduction and then doing classification in the lower-dimensional spaces with the main difference being that that thresholding of the discriminant direction corresponds to dropping a subset of the raw features while thresholding of the whitened direction corresponds to dropping a subset of the whitened features. Taking this perspective, we are thus interested in estimation of the whitening matrix \( W \).

When \( n \approx p \) then the sample covariance matrix \( \hat{\Sigma} \) is generally ill-conditioned and if \( n < p \) then \( \hat{\Sigma} \) is singular. The estimation of either the precision matrix \( \Sigma^{-1} \) or the whitening matrix \( W \) is thus challenging in these regimes, especially since \( \Sigma^{-1} \) and \( W \) both contains \( O(p^2) \) entries. An universal approach to address this difficulty is to reduce the number of parameters needed for estimating \( \Sigma \), for example by either assuming that \( \Sigma \) has a parametric form (so that \( \Sigma \) can be estimated parametrically), or by introducing regularization terms and induce certain structures in the estimate \( \hat{\Sigma} \).

The use of regularized estimators for covariance matrices are popular in high-dimensional classification, see e.g., Bickel and Levina (2009); Shao et al. (2011), and theoretical analysis for these estimators are usually based on assumptions about the sparsity of either \( \Sigma \) or \( \Sigma^{-1} \) and then bounding the estimation error in terms of the spectral norm differences \( \| \Sigma^{-1} - \hat{\Sigma}^{-1} \| \) or \( \| \Sigma - \hat{\Sigma} \| \). There are, however, several drawbacks to this approach. Firstly, quantifying the estimation error in terms of the spectral norm can be quite loose and the resulting bounds might not capture the difference in geometry between the eigenspaces of \( \Sigma \) and that of the perturbed matrix \( \hat{\Sigma} \). In particular Johnstone (2001) observed that for high-dimensional data, the first few largest eigenvalues of the sample covariance matrix \( \hat{\Sigma} \) are always larger than those for \( \Sigma \). Secondly, while the assumption of sparsity in either \( \Sigma \) or \( \Sigma^{-1} \) is not always appropriate, Cai and Liu (2011) noted that it is generally not feasible to consistently estimate \( \Sigma \) or \( \Sigma^{-1} \) under the spectral norm without sparsity conditions on \( \Sigma \).

In this paper, we assume a different structure for \( \Sigma \) wherein \( \Sigma \) contains a few leading eigenvalues (the spike) that are well-separated from the remaining eigenvalues (the bulk). More specifically, we assume that \( \Sigma \) satisfies the following condition.

**Condition 1** (Spiked covariance matrix). Let \( u_1 \ldots u_d \) be orthonormal vectors in \( \mathbb{R}^p \) and assume that the covariance matrix \( \Sigma \) for the \( p \)-variate normal distributions \( \mathcal{N}_p(\mu_1, \Sigma) \) and
\( N_p(\mu_2, \Sigma) \) is of the form

\[
\Sigma = \sum_{k=1}^{d} \lambda_k u_k u_k^T + \sigma^2 I_p = \mathcal{U} \Lambda \mathcal{U}^T + \sigma^2 I_p.
\]  

(2.6)

Here \( \Lambda = \text{diag}(\lambda_k) \) is a \( d \times d \) diagonal matrix, and \( \mathcal{U} = (u_k), \ k \in [d] \) is a \( p \times d \) orthonormal matrix. We assume implicitly that \( \lambda_1 \geq \cdots \geq \lambda_d > 0, \sigma > 0 \) and \( d \ll p \).

Covariance matrices with spiked structures have been studied extensively in the high-dimensional statistics literature, see e.g., Johnstone (2001) and Chapter 11 of Yao et al. (2015), and there is a significant number of results for consistent estimation of \( \mathcal{U} \) under the assumption that the support of \( \mathcal{U} \) is sparse, e.g., either that the number of non-zero rows of \( \mathcal{U} \) is small compared to \( p \) or that the \( \ell_q \) quasi-norm, for some \( q \in [0, 1] \), of the columns of \( \mathcal{U} \) are bounded. The case when \( q = 0 \) and \( q > 0 \) correspond to “hard” and “soft” sparsity constraints, respectively; see for example Berthet and Rigollet (2012); Birnbaum et al. (2012); Cai et al. (2013); Vu and Lei (2012) and the references therein.

In contrasts to the above cited results, in this paper we do not impose sparsity conditions on \( \mathcal{U} \) but instead assume that \( \mathcal{U} \) have bounded coherence, namely that the maximum \( \ell_2 \) norm of the rows of \( \mathcal{U} \) are of order \( O(p^{-1/2}) \); see Assumption 4 for a precise statement.

The resulting matrix \( \Sigma \) will no longer be sparse. The main rationale for assuming bounded coherence is that the spiked eigenvalues \( \Lambda \) can now even grow linearly with \( p \). There is thus a large gap between the spiked eigenvalues and the bulk eigenvalues, and this justifies the use of PCA as a pre-processing step.

If \( \Sigma \) satisfies Condition 1 then the whitening matrix is given by

\[
\mathcal{W} = \mathcal{U} \mathcal{D} \mathcal{U}^T + \frac{1}{\sigma} (I_p - \mathcal{U} \mathcal{U}^T)
\]

where \( \mathcal{D} = \text{diag}(\eta_k) \) is a \( d \times d \) diagonal matrix with diagonal entries \( \eta_k = (\lambda_k + \sigma^2)^{-1/2} \).

The above form for \( \mathcal{W} \) suggests the following estimation procedure for \( \mathcal{W} \).

(a) Extract the \( d \) largest eigenvalues and corresponding eigenvectors of the pooled sample covariance matrix \( \hat{\Sigma} \). Let \( \hat{\Lambda} \) denote the diagonal matrix of these \( d \) largest eigenvalues and \( \hat{\mathcal{U}} \) denote the \( p \times d \) orthonormal matrix whose columns are the corresponding eigenvectors.

(b) Estimate the non-spiked eigenvalues by

\[
\hat{\sigma}^2 = \frac{\text{tr}(\hat{\Sigma}) - \text{tr}(\hat{\Lambda})}{p - d}.
\]  

(2.7)

(c) Let \( \hat{\mathcal{D}} = (\hat{\Lambda} + \hat{\sigma}^2 I_d)^{-1/2} \) and estimate \( \mathcal{W} \) by \( \hat{\mathcal{W}} = \hat{\mathcal{U}} \hat{\mathcal{D}} \hat{\mathcal{U}}^T + \hat{\sigma}^{-1} (I_p - \hat{\mathcal{U}} \hat{\mathcal{U}}^T) \).

Although the sample covariance matrix \( \hat{\Sigma} \) is generally a poor estimate of \( \Sigma \) when \( n \ll p \), the eigenvectors \( \hat{\mathcal{U}} \) corresponding to the largest eigenvalues of \( \hat{\Sigma} \) are nevertheless accurate estimates of \( \mathcal{U} \). In particular, Fan et al. (2018) and Cape et al. (2019) provide uniform error bound for \( \min_T \| \hat{\mathcal{U}}^T \mathcal{U} \|_{2 \rightarrow \infty} \) where the minimum is taken over all \( d \times d \) orthogonal
transformations $T$; see also Theorem 1 of the current paper. We can thus transform $\hat{U}$ by an orthogonal transformation $T$ so that the resulting (transformed) rows of $\hat{U}$ are uniformly close to the corresponding rows of $\mathcal{U}$.

Given the above estimate for $\mathcal{W}$, we now introduce our PCLDA classifier.

**Algorithm 1:** PCLDA rule

**Input:** $\bar{X}_1, \bar{X}_2$, $\hat{\Sigma}$ and the test sample $Z$

**Output:** $\hat{\Upsilon}_{\text{PCLDA}}(Z)$

**Step 1:** Perform PCA on the feature vectors for the training data. Extract the $d$ largest principal components to obtain $\hat{W}$.

**Step 2:** Take $\tilde{X}_i = \hat{W} \bar{X}_i$, $i = 1, 2$ and $\tilde{X}_a = 0.5(\tilde{X}_1 + \tilde{X}_2)$. Let $\hat{\zeta} = \tilde{X}_2 - \tilde{X}_1$ and form the indices set $\hat{S}$ by selecting the $s$ largest coordinates of $\hat{\zeta}$ in absolute values.

**Step 3:** Given the test sample $Z$, take $\tilde{Z} = \hat{W}Z$ and plug the sub-vector of $\hat{\zeta}$, $\tilde{Z}$ and $\tilde{X}_a$ corresponding to the indices in $\hat{S}$ into the Fisher discriminant rule, i.e.,

$$
\hat{\Upsilon}_{\text{PCLDA}}(Z) = \begin{cases} 
1 & \text{if } \hat{\zeta}^T [\tilde{Z} - \tilde{X}_a]_{S} \leq \ln \frac{n_1}{n_2}, \\
2 & \text{otherwise}
\end{cases} \quad (2.8)
$$

The above description of PCLDA contains two tuning parameters, namely $d$, the number of principal components in the PCA step and $s$, the number of coordinates of estimated whitened direction $\hat{\zeta}$ that we preserve. The choices for $d$ and $s$ correspond to the number of spiked eigenvalues in $\Sigma$ and the sparsity level of the whitened direction $\zeta$. We show in Section 3 that, under certain mild conditions, one can consistently estimate $d$ and $s$ and hence the PCLDA classifier is adaptive with respect to $d$ and $s$.

We now discuss the relationship between PCLDA and two other relevant classifiers, namely the features annealed independence rule (FAIR) of Fan and Fan (2008) and the LDA with CAT scores (CAT-LDA) of Zuber and Strimmer (2009). FAIR is the independence rule applied to the features prescreened by the two-sample t test while CAT-LDA scores decorrelate $t$ statistics by whitening the sample correlation matrix $\text{diag}(\Sigma)^{-1/2} \Sigma \text{diag}(\Sigma)^{-1/2}$; CAT-LDA is motivated by the observation that accounting for correlations is essential when analyzing proteomic and metabolic data. If there are no correlation or if the correlations are negligible, i.e., when $\Sigma$ is diagonal or approximately diagonal, then PCLDA is essentially equivalent to both FAIR and CAT-LDA. However, when the correlations are not negligible, the performance of IR classifiers such as FAIR degrades significantly due to mis-specification of the covariance structure (Fan et al., 2012). The decorrelation idea shared by PCLDA and CAT-LDA are quite similar as they both apply a whitening transformation before doing LDA; the choice of whitening matrices are, however, different between the two approaches. In particular CAT-LDA uses the asymmetric whitening transformation $\text{Corr}(\Sigma)^{-1/2} \text{diag}(\Sigma)^{-1/2}$ where $\text{Corr}(\Sigma)$
is the matrix of correlations. The choice of whitening transformation is not important if $\Sigma$ is known or if we are in the low-dimensional setting where $p \ll n$ for which consistent estimation of $\Sigma$ is straightforward. It is only when $p \gg n$ when the different regularization strategies used in CAT-LDA and PCLDA lead to possibly different behaviors for the resulting classifiers; see for example the numerical comparisons given in Section 4 of the current paper. Finally we view the theoretical results in Section 3 as not only providing justification for PCLDA but also serve as examples of theoretical analysis that can be extended to other classifiers in which dimension reduction is done prior to performing LDA. Indeed, to the best of our knowledge, there are no theoretical guarantees for the error rate of the CAT-LDA classifier in the high-dimensional setting.

We end this section by noting that our paper is also not the first work to study high-dimensional classification under spiked covariance matrices of the form in Condition 1. In particular Hao et al. (2015) examined the effects of spiked eigenvalues when trying to find an orthogonal transformation $T$ of the discriminant direction $\beta$ so that $T\beta$ is sparse. More specifically they show that if $\Sigma$ is known then $T$ can be computed using the eigen-decomposition of the matrix $\Sigma_{\text{rot}}$ where

$$\Sigma_{\text{rot}} = \Sigma + \gamma \Delta \mu \Delta \mu^T,$$

for a given $\gamma > 0$. (2.9)

Recall that $\Delta \mu = \mu_2 - \mu_1$ is the vector of mean differences between the two classes. Let $\mathcal{U}_{\text{rot},m}$ be the $p \times m$ matrix whose columns consist of the orthonormal eigenvectors of $\Sigma_{\text{rot}}$ corresponding to the $m$ largest eigenvalues. When $m = p$ then the matrix $\mathcal{U}_{\text{rot},p}$ diagonalizes $\Sigma_{\text{rot}}$ and Hao et al. (2015) showed that $\mathcal{U}_{\text{rot},p}$ also sparsifies $\beta$ in that

$$\|\mathcal{U}_{\text{rot},p}^T \beta\|_0 \leq d + 1,$$

whenever $\Sigma$ satisfies the spiked covariance assumption in Condition 1. Eq. (2.10) suggests that we should rotate the data before performing classification.

When $\Sigma$ is unknown Hao et al. (2015) propose the following procedure for estimating $\mathcal{U}_{\text{rot},m}$ for some choice of $m \leq \min\{n, p\}$; here $\gamma > 0$ is a user-specified parameter.

**Step 1:** Perform PCA on $\hat{\Sigma}_{\text{rot}} = \hat{\Sigma} + \gamma (\bar{X}_2 - \bar{X}_1)(\bar{X}_2 - \bar{X}_1)^\top$ to extract the $m$ largest principal components. Let $\hat{\mathcal{U}}_{\text{rot},m}$ be the resulting $p \times m$ matrix.

**Step 2:** Rotate the training sets to $\{\hat{\mathcal{U}}_{\text{rot},m}^\top X_{i1}, \ldots, \hat{\mathcal{U}}_{\text{rot},m}^\top X_{in_i}\}$ where $\hat{\mathcal{U}}_{\text{rot},m}^\top X_{ij} \in \mathbb{R}^m$ for $i \in \{1, 2\}$ and $j \in \{1, 2, \ldots, n_i\}$.

**Step 3:** Apply some discriminant direction based LDA method such as Cai and Liu (2011); Fan et al. (2012); Mai et al. (2015) on the rotated dataset $\{\hat{\mathcal{U}}_{\text{rot},m}^\top X_{ij}\}$.

We will use this pre-processing step in some of our numerical experiments in Section 4.

Finally we emphasize that the theoretical results of Hao et al. (2015) are presented only in the context where $\Sigma$ is known as the main objective of Hao et al. (2015) is in delineating different approaches for sparsifying $\beta$ and they thus explicitly chose not to address the important issue of how the estimation error for $\mathcal{U}_{\text{rot},m}$ impacts the classification accuracy.
3. Theoretical properties

In this section we derive theoretical properties of the PCLDA rule for the case where the features vector \( X \) is sampled from a mixture of two multivariate Gaussians. Extensions of these results to the case where \( X \) is a mixture of \( K \geq 2 \) elliptical but not necessarily multivariate normal distributions are discussed in Section 5.1 and Section 5.2.

If \( X \sim \pi_1 \mathcal{N}(\mu_1, \Sigma) + (1 - \pi_1) \mathcal{N}(\mu_2, \Sigma) \) then the Fisher’s rule \( \Upsilon_F \) has error rate
\[
R_F = \pi_1 \Phi \left( -\frac{1}{2} \|\zeta\|^2 + \|\zeta\|^{-1} \ln \frac{1 - \pi_1}{\pi_1} \right) + (1 - \pi_1) \Phi \left( -\frac{1}{2} \|\zeta\|^2 - \|\zeta\|^{-1} \ln \frac{1 - \pi_1}{\pi_1} \right).
\]

Here \( \Phi \) is the cumulative distribution function for \( \mathcal{N}(0, 1) \) and \( \zeta = \Sigma^{-1/2}(\mu_2 - \mu_1) \) is the whitened direction, see e.g., Ripley (1996, Section 2.1). We note that \( R_F \) is the smallest mis-classification error achievable by any classifier \( \hat{\Upsilon} \) and, furthermore, is monotone decreasing as \( \|\zeta\| \) increases. More specifically, if \( \|\zeta\|_2 \to 0 \) then \( R_F \to \min \{\pi_1, 1 - \pi_1\} \) and \( \Upsilon_F \) is no better than assigning every data point to the most prevalent class while if \( \|\zeta\|_2 \to \infty \), then \( R_F \to 0 \) and \( \Upsilon_F \) achieves perfect accuracy. The cases where \( R_F \to 0 \) or \( R_F \to \min \{\pi_1, 1 - \pi_1\} \) as \( p \to \infty \) are not interesting and hence, in this paper, we will only focus on the case where \( 0 < \|\zeta\| < \infty \). We therefore make the following assumption.

**Condition 2.** Let \( |S_\zeta| = s_0 > 0 \). Recall that \( S_\zeta \) is the set of indices \( i \) for which \( \zeta_i \neq 0 \). Let \( C_0 > 0 \), \( M > 0 \) and \( C_\zeta > 0 \) be constants not depending on \( p \) such that \( s_0 \leq M \) and
\[
\min_{j \in S_\zeta} |\zeta_j| > C_0, \quad \max \left\{ \|\Sigma^{-1/2} \mu_1\|_2, \|\Sigma^{-1/2} \mu_2\|_2 \right\} < C_\zeta.
\]

Condition 2 implies \( 0 < s_0 C_0 < \|\zeta\|_2 < 2C_\zeta < \infty \).

Our theoretical results are large-sample results in which the sample sizes \( n_1 \) and \( n_2 \) for the training data increase as the dimension \( p \) increases. The next assumption specifies the asymptotic relationships among these quantities and the eigenvalues of \( \Sigma \).

**Condition 3.** Let \( \sigma > 0 \) be fixed and that, for sufficiently large \( p \), \( n_1, n_2 \) and \( p \) satisfy
\[
\frac{n_1}{n_2} = \Theta(1), \quad \ln p = o(n).
\]

Furthermore, for sufficiently large \( p \), the spiked eigenvalues \( \lambda_1, \ldots, \lambda_d \) satisfy
\[
\lambda_k = O(p), \quad \text{for all } k \in [d].
\]

If \( \Sigma \) satisfies Condition 3 then \( \text{tr}(\Sigma) = O(p) \) and \( r(\Sigma) = \|\Sigma\|/\text{tr}(\Sigma) = O(1) \). Recall that \( r(\Sigma) \) is the effective rank of \( \Sigma \). Condition 3 also implies that the spiked eigenvalues of \( \Sigma \) are unbounded as \( p \) increases and this assumption distinguishes our theoretical results from existing results in the literature wherein it is generally assumed that the eigenvalues of \( \Sigma \) are bounded; see Bickel and Levina (2004); Cai and Zhang (2019); Fan and Fan (2008); Shao et al. (2011) for a few examples of results under the bounded eigenvalues assumption. However, while the bounded eigenvalues value assumption is prevalent, it can also be problematic for high-dimensional data; see Fan et al. (2013); Wang and Fan...
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(2017) for some insightful discussions of this issue. Our work is thus one of a few to consider divergent eigenvalues in the context of high-dimensional classification. If \( \Sigma \) has a spiked eigenvalues structure as in Condition 1 then \( W \) is given by

\[
W = \Sigma^{-1/2} = U(\Lambda + \sigma^2 I)^{-1/2}U^T + \sigma^{-1}(I - UU^T)
\]  

(3.2)

and an appropriate estimate for \( W \) is

\[
\hat{W} = \hat{U}(\hat{\Lambda} + \hat{\sigma}^2 I)^{-1/2}\hat{U}^T + \hat{\sigma}^{-1}(I - \hat{U}\hat{U}^T)
\]  

(3.3)

where \( \hat{\Lambda} \) is the diagonal matrix containing the \( d \) largest eigenvalues of the pooled covariance matrix, \( \hat{U} \) is the \( p \times d \) orthonormal matrix whose columns are the corresponding eigenvectors, and \( \hat{\sigma}^2 \) is the estimate of \( \sigma^2 \) as given in Eq. (2.7). We now make the following assumption on \( U \).

**Condition 4. (Bounded Coherence)** There exists a positive constant \( C_U \geq 1 \) independent of \( n \) and \( p \) such that

\[
\|U\|_{2 \to \infty} \leq C_U \sqrt{\frac{d}{p}}.
\]

The bounded coherence assumption appears frequently in matrix estimation and random matrix theory. The motivation behind this assumption is as follows. Since every column in \( U \) has \( \ell_2 \) norm equal to 1, the entries of \( U \) are, on average, of order \( 1/\sqrt{p} \). Condition 4 guarantees that the maximum entry is also of order \( 1/\sqrt{p} \). That is to say, the entries of \( U \) are sufficiently homogeneous, i.e., delocalized. For more discussions about the bounded coherence assumption in the context of matrix completion and covariance matrix estimation, see Candès and Recht (2009); Fan et al. (2018), and for discussion about eigenvectors delocalization in random matrix theory, see Bloemendal et al. (2014); Rudelson and Vershynin (2016). Finally we note that if \( U \) satisfies the bounded coherence assumption then there exists a constant \( C > 0 \) such that

\[
\Sigma_{ii} \leq C \left( \frac{\lambda_1}{p} + \sigma^2 \right), \quad \forall i \in [p].
\]

Hence, if \( \lambda_1 \) satisfies Condition 3 then \( \max_{i \in [p]} \Sigma_{ii} = \mathcal{O}(1) \). In summary, the bounded coherence assumption allows for the spiked eigenvalues \( \lambda_1, \ldots, \lambda_d \) of the covariance matrix \( \Sigma \) to diverge with \( p \) while also guaranteeing that the entries of \( \Sigma \) remains bounded, i.e., each variable in \( X \) has finite variance.

We next state a result on the estimation accuracy of \( \hat{U} \). This result is a slight extension of an earlier result in Cape et al. (2019). More specifically, in Cape et al. (2019) the authors assume that the feature vectors \( X \) has mean 0 and hence the sample covariance matrix is simply \( \frac{1}{n}X^TX \). In this paper we used the pooled sampled covariance matrix which requires first centering the feature vectors by the sample means of each class.

**Theorem 1.** Let \( X \) be a \( n \times p \) matrix where the rows \( X_1, \ldots, X_n \) are i.i.d sample from \( \pi_1 \mathcal{N}(\mu_1, \Sigma) + (1 - \pi_1) \mathcal{N}(\mu_2, \Sigma) \) where \( \Sigma \) satisfies Condition 3 and Condition 4. Let \( \hat{U} \) be the matrix of eigenvectors corresponding to the \( d \) largest eigenvalues of the pooled
sampled covariance matrix $\hat{\Sigma}$. Then there exists a $d \times d$ orthogonal matrix $\Xi U$ and a constant $C > 0$ such that with probability at least $1 - O(p^{-1})$,

$$\|\hat{U} - U\Xi U\|_{2 \to \infty} \leq C \sqrt{\frac{d^3 \max\{r(\Sigma), \ln p\}}{np}}. \tag{3.4}$$

We now consider the classification accuracy of the PCLDA rule. Recall that the main idea behind the PCLDA rule is that we first construct an estimate $\hat{\zeta}$ for the whitened direction $\zeta$ and then project our whitened data onto the $d$ largest coordinates, in magnitude, of $\hat{\zeta}$. Now recall Eq. (3.1); in particular the Bayes error rate $R_F$ is a monotone decreasing function of $\|\zeta\|$ and hence, to achieve $R_F$ it is only necessary to recover the indices in $S_\zeta = \{i : \zeta_i \neq 0\}$. Therefore the error rate for PCLDA rule will converge to the Bayes error rate $R_F$ provided that we can (1) bound the estimation error $\hat{\zeta} - \zeta$ and then (2) show that there exists a thresholding procedure for $\hat{\zeta}$ that perfectly recovers $S_\zeta$.

We first provide a bound, in $\ell_\infty$ norm, for $\hat{\zeta} - \zeta$.

**Theorem 2.** Under Condition 1-4, there exists a constant $C > 0$ such that with probability at least $1 - O(p^{-1})$,

$$\|\hat{\zeta} - \zeta\|_\infty \leq C \sqrt{\frac{\ln p}{n}}. \tag{3.5}$$

We next consider the recovery of $S_\zeta$. From Condition 2, we have $\zeta_i \neq 0$ if and only if $\zeta_i > C_0$ for some constant $C_0$ not depending on $p$. Therefore, by Theorem 2, if $\hat{\zeta}_i = O((n^{-1} \ln p)^{1/2})$ then with high probability $\zeta_i = 0$. We therefore consider the estimate $\tilde{\zeta}$ obtained by hard thresholding $\hat{\zeta}$ as follows

$$\tilde{\zeta}_j = \hat{\zeta}_j 1(|\hat{\zeta}_j| > t_n), \quad j \in [p] \tag{3.6}$$

where $t_n = C (\ln p/n)^\alpha$ for some constant $C > 0$ and $0 < \alpha < \frac{1}{2}$. Given $\tilde{\zeta}$, define the corresponding active set $\tilde{S} = \{j : \tilde{\zeta}_j \neq 0\}$. The mis-classification rate for the PCLDA rule, conditional on the training data $\{X_{11}, \ldots, X_{1n_1}\}$ and $\{X_{21}, \ldots, X_{2n_2}\}$, is then

$$\hat{R}_{PCLDA} = \Pr(\text{label}(Z) \neq \hat{\Upsilon}_{PCLDA}(Z) | \{X_{11}, \ldots, X_{1n_1}\}, \{X_{21}, \ldots, X_{2n_2}\}) \tag{3.7}$$

The following result shows that $\tilde{S}$ recovers $S_\zeta$ exactly and hence $\hat{R}_{PCLDA} \to R_F$, i.e., the PCLDA rule is asymptotically Bayes-optimal.

**Theorem 3.** Suppose that $Z \sim \pi_1 \mathcal{N}_p(\mu_1, \Sigma) + (1 - \pi_1) \mathcal{N}_p(\mu_2, \Sigma)$ where $\pi_1 \in (0, 1)$. Suppose Condition 1 through Condition 4 are satisfied. We then have

$$\Pr(\hat{S} \neq S_\zeta) = O(p^{-2}). \tag{3.8}$$

Furthermore, suppose that $\ln p = \mathcal{O}(n)$. We then have

$$|\hat{R}_{PCLDA} - R_F| \to 0 \tag{3.9}$$

almost surely as $n, p \to \infty$. 
Remark 1. Theorem 2 and Theorem 3 appear, at first blush, quite similar to the results in Mai et al. (2012) for lassoed LDA using the discriminant direction $\beta = \Sigma^{-1}(\mu_1 - \mu_2)$. However the underlying assumptions behind these results are very different. In particular the lassoed LDA relies on the irrepresentable condition analogous to that in Zhao and Yu (2006) to achieve variable selection consistency. The discriminative variables therefore cannot be highly correlated with the irrelevant variables. In contrast, the results for PCLDA do not assume an irrepresentable condition and furthermore Condition 1 only assume boundedness of the non-spiked eigenvalues but allows for diverging spiked eigenvalues.

4. Numerical results

In this section we present simulation results and real data analysis to demonstrate the performance of the PCLDA rule. For comparisons we also considered the nearest shrunk centroids method (NSC) of Tibshirani et al. (2002), the sparse linear discriminant analysis (SLDA) of Shao et al. (2011), the direct sparse discriminant analysis (DSDA) of Mai et al. (2012), the adaptive linear discriminant analysis (AdaLDA) of Cai and Zhang (2019) and the LDA rule with CAT scores (CAT-LDA) of Zuber and Strimmer (2009); note that CAT-LDA uses a different sphering transformation compared to the proposed PCLDA rule. There are three other commonly used classifiers that are not included in our comparisons, namely the naive Bayes rule, the linear programming discriminant (LPD) (Cai and Liu, 2011) and the regularized optimal affine discriminant (ROAD) (Fan et al., 2012). We omit these classifiers because (1) the naive Bayes rule is a special case of the NSC rule without soft thresholding the mean vectors (2) Mai and Zou (2013) showed that the ROAD classifier is equivalent to the DSDA classifier and (3) Cai and Zhang (2019) showed that the AdaLDA rule is a refinement of the LPD rule, i.e., compared to the LPD rule, the AdaLDA rule allows for “heteroscedastic constraints” and requires no tuning parameters.

Implementations of the DSDA and CAT-LDA rules are based on the TULIP and sda library in R while the implementation of the AdaLDA rule is based on Matlab codes from ADAM. We also consider the rotation pre-processing step of Hao et al. (2015), which yields the transformed data $\{U_{\text{rot},1}^\top x_{11}, \ldots, U_{\text{rot},1}^\top x_{1n_1}\}$ and $\{U_{\text{rot},2}^\top x_{21}, \ldots, U_{\text{rot},2}^\top x_{2n_2}\}$ based on Matlab codes from HDRotation with $\gamma = 0.25$ in Eq. (2.9) (corresponding to $\rho$ in their code). These transformed data are then used as input to the DSDA and AdaLDA rules; we denote the resulting classifiers as DSDA(rot) and AdaLDA(rot).

4.1. Simulated examples

We evaluate the performance of the PCLDA rule using three different simulation settings. For each simulation setting we set the number of features to $p = 800$ and we generate $n_1 = n_2 = 100$ data points from each class for the training data and also generate $n_1 = n_2 = 100$ data points from each class for the testing data. The classification accuracy of the classifiers in each simulation setting are computed based on 200 Monte Carlo replications. For the mean vectors of the two classes, we set $\mu_1 = 0_{p100}^\top$ and $\mu_2 = (1_{10}^\top, 0_{790}^\top)^\top$, i.e., the vector $\mu_2$ contains 10 non-zero entries with values all equal
to 1.

We consider the following models for the covariance matrix $\Sigma$. These models were considered previously in Cai and Liu (2011); Cai and Zhang (2019); Fan et al. (2012); Mai et al. (2012), among others.

(a) **Model 1 (equal correlation)**: Here $\Sigma = (\sigma_{ij})_{p \times p} = \rho \mathbf{1} \mathbf{1}^T + (1 - \rho) \mathbf{I}$, i.e., $\sigma_{ij} = \rho$ for $i \neq j$ and $\sigma_{ij} = 1$ for $i = j$. With this covariance structure $\Sigma$, the discriminant direction $\beta = \Sigma^{-1}(\mu_1 - \mu_0)$ and the whitened direction $\zeta = \Sigma^{-1/2}(\mu_1 - \mu_0)$ are non-sparse, i.e., all the entries of $\beta$ and $\zeta$ are non-zero.

(b) **Model 2 (block diagonal with equal correlation)** Here $\Sigma = (\sigma_{ij})_{p \times p}$ is assumed to be a block diagonal matrix with two blocks of size $20 \times 20$ and $(p - 20) \times (p - 20)$. Both diagonal blocks are also of the form $\rho \mathbf{1} \mathbf{1}^T + (1 - \rho) \mathbf{I}$ where the correlation $\rho$ is the same for both blocks. The discriminant direction $\beta$ and whitened direction $\zeta$ are sparse in this model, with $\beta$ and $\zeta$ both having 20 non-zero entries.

(c) **Model 3 (random correlation)** Here $\Sigma = \mathcal{L} \mathcal{L}^T + c_{\mathcal{L}} \mathbf{I}_p$ where $\mathcal{L} \in \mathbb{R}^{p \times 10}$ with $\mathcal{L}_{ij}$ generated from $\mathcal{N}(0, 1)$ and $c_{\mathcal{L}} = \min_{i \in \{\mathcal{L} \mathcal{L}^T\}}$. We emphasize that in this setting we generate a new $\mathcal{L}$ for every Monte Carlo replicate. For further comparison, we also consider $\mathcal{L}_{ij}$ generated from the uniform distribution on $[-1, 1]$ and the Student’s $t$-distribution with 5 degrees of freedom. The discriminant direction $\beta$ and $\zeta$ are generally non-sparse in this model, i.e., all of their entries are non-zero.

The tuning parameters for the algorithms listed above are chosen using five-fold CV. In particular, the SLDA rule of Shao et al. (2011) typically requires two tuning parameters, namely one parameter for the number of non-zero entries in $\mu_1 - \mu_2$ and the other parameter for the number of non-zero entries in $\Sigma$. For simplicity we shall assume that the sparsity of $\mu_1 - \mu_2$ is known when implementing SLDA and thus the only tuning parameter required is for estimating $\Sigma$: following Cai and Zhang (2019), this tuning parameter is selected among the possible values of $\{\sqrt{n^{-1}} \ln p, 1.5 \sqrt{n^{-1}} \ln p, \ldots, 5 \sqrt{n^{-1}} \ln p\}$ using five-fold cross validation (CV). The proposed PCLDA rule in this paper also requires two tuning parameters, namely (1) the number of spikes $d$ in the estimation of $\Sigma$ and (2) the sparsity level $s$ in $\zeta$. These tuning parameters are selected as follows. The number of spikes $d$ is chosen so as to account for at least 90% of the total variability as given by $\text{tr}(\hat{\Sigma})$, i.e., we chose $d$ so that $(\sum_{i=1}^{d} \lambda_i)/\text{tr}(\hat{\Sigma}) \geq 0.9$; here $\lambda_1 \geq \lambda_2 \geq \ldots$ are the eigenvalues of the pooled sampled covariance matrix $\hat{\Sigma}$. The sparsity level $s$ is chosen among the candidate set $s \in \{1, 2, \ldots, 30\}$ using five-fold CV. Similarly, the number of features in CAT-LDA is selected among the top $\{1, 2, \ldots, 30\}$ features ranked by CAT scores using five-fold CV.

For data generated according to Model 1, Table 2 and Table 3 show that the PCLDA rule achieves the highest accuracy while using only a small number of features compared to the other classifiers. Note that although CAT-LDA also apply a whitening transformation before performing LDA, the accuracy of CAT-LDA is much worse compared to that for PCLDA. The DSDA and DSDA(rot) classifiers have slightly better accuracies compared to those for the AdaLDA and AdaLDA(rot) classifiers; recall that the DSDA(rot) and AdaLDA(rot) classifiers first applied the rotation pre-processing step of...
Table 2. Misclassification rate (%) with standard deviations (%) in parentheses for equal correlation setting (model 1).

| $\rho$ | 0.50 | 0.60 | 0.70 | 0.80 | 0.90 |
|--------|------|------|------|------|------|
| Oracle | 1.37 (0.87) | 0.61 (0.53) | 0.19 (0.30) | 0.19 (0.30) | 0.00 (0.00) |
| PCLDA  | 1.74 (1.00) | 1.00 (0.82) | 0.55 (0.67) | 0.55 (0.67) | 0.22 (0.39) |
| CAT-LDA| 7.18 (2.22) | 4.70 (1.77) | 2.60 (1.34) | 1.10 (0.88) | 0.38 (0.56) |
| DSDA   | 3.27 (1.47) | 1.96 (1.08) | 0.74 (0.62) | 0.76 (0.65) | 0.00 (0.04) |
| DSDA(rot)| 6.31 (1.83) | 3.26 (1.27) | 1.16 (0.83) | 0.30 (0.41) | 0.01 (0.06) |
| AdaLDA | 4.15 (1.61) | 2.62 (1.24) | 1.22 (0.91) | 0.31 (0.42) | 0.00 (0.04) |
| AdaLDA(rot) | 7.04 (2.07) | 3.70 (1.26) | 1.19 (0.79) | 0.13 (0.26) | 0.00 (0.00) |
| SLDA   | 17.97 (3.53) | 14.46 (2.99) | 11.14 (2.43) | 11.14 (2.43) | 1.64 (0.92) |
| NSC    | 20.38 (8.53) | 22.60 (8.38) | 24.64 (8.36) | 24.64 (8.36) | 29.26 (8.04) |

Table 3. Average number of nonzero coefficients with standard deviations in parentheses for equal correlation setting (model 1).

| $\rho$ | 0.50 | 0.60 | 0.70 | 0.80 | 0.90 |
|--------|------|------|------|------|------|
| PCLDA  | 12.04 (4.53) | 11.31 (4.10) | 9.52 (4.01) | 9.52 (4.01) | 3.68 (0.98) |
| CAT-LDA| 24.85 (3.74) | 24.70 (3.58) | 24.60 (3.97) | 22.29 (3.93) | 15.45 (2.39) |
| DSDA   | 96.20 (31.06) | 106.42 (32.57) | 117.15 (30.52) | 117.05 (29.97) | 96.48 (8.66) |
| DSDA(rot)| 33.78 (32.71) | 36.88 (38.13) | 57.23 (61.02) | 147.57 (66.97) | 176.29 (5.08) |
| AdaLDA | 46.54 (5.95) | 45.84 (5.25) | 46.72 (6.41) | 47.86 (5.88) | 48.65 (5.02) |
| AdaLDA(rot) | 5.68 (1.82) | 5.57 (1.84) | 5.86 (1.82) | 7.83 (2.54) | 19.85 (9.96) |
| SLDA   | 728.84 (226.63) | 788.16 (95.69) | 799.96 (0.21) | 799.96 (0.21) | 799.96 (0.21) |

Hao et al. (2015) before running DSDA and AdaLDA on the transformed data. The NSC classifier has the largest mis-classification error; this is a consequence of the NSC rule ignoring the correlation structure in $\Sigma$. Finally, the oracle classifier correspond to the LDA rule where $\pi_1, \mu_0, \mu_1$ and $\Sigma$ are all known, i.e., the error rate for the oracle classifier is the Bayes error rate from Eq. (3.1).

Remark 1. Recall that for Model 1, all entries of the discriminant direction $\beta$ and the whitened direction $\zeta$ are non-zero. These entries however can be classified into those representing strong signals vs weak signals based on their magnitudes; see Table 4. The strong signals appear in the first 10 entries of $\beta$ (similarly $\zeta$) and the remaining $p - 10$ entries of $\beta$ (similarly $\zeta$) correspond to the weak signals. For example, if $\rho = 0.5$ then the first 10 entries of $\beta$ are all equal to 1.98 and the remaining $p = 10$ entries are all equal to $-0.02$. From Table 3 we see that the PCLDA rule kept all of the coordinates corresponding to the strong signals and only added a few coordinates corresponding to the weak signals; this explains the small number of features used in the PCLDA rule.

Table 4. Strong and faint signals for equal correlation setting (model 1). See the discussion in Remark 1.

| $\rho$ | 0.50 | 0.60 | 0.70 | 0.80 | 0.90 |
|-------|------|------|------|------|------|
| strong signal $\beta$ | 1.98 | 2.47 | 3.29 | 4.94 | 9.88 |
| strong signal $\zeta$ | 1.40 | 1.56 | 1.80 | 2.21 | 3.12 |
| faint signal $\beta$ | -0.02 | -0.03 | -0.04 | -0.06 | -0.12 |
| faint signal $\zeta$ | -0.02 | -0.02 | -0.02 | -0.03 | -0.04 |
In contrast, the DSDA and SLDA rules include a large number of (noisy) features with weak signals.

For Model 2, Table 5 shows that SLDA performs slightly better than the PCLDA rule and DSDA rule. However, from Table 6, we see that the SLDA rule also selects a much larger number of features compared to both the PCLDA and DSDA rules. Recall that, for model 2, both \( \beta \) and \( \zeta \) contains exactly 20 non-zero entries and hence the SLDA rule is selecting a large number of extraneous, non-informative features; a similar, albeit much less severe, phenomenon is observed for the DSDA rule. Table 5 and Table 6 shows that the PCLDA, CAT-LDA, and AdaLDA rules have comparable accuracy with a similar number of selected features. The NSC rule once again has the largest mis-classification error due to it ignoring the correlation structure in \( \Sigma \). Finally we see that the rotation pre-processing step described in Hao et al. (2015) lead to a substantial loss in accuracy for the DSDA and AdaLDA rules; to understand why this happens, we need to extend the theoretical analysis in Hao et al. (2015) (which assume that \( \Sigma \) and \( \mathbf{U}_{\text{rot}, p} \) are known) to the current setting where \( \Sigma \) and \( \mathbf{U}_{\text{rot}, p} \) have to be estimated. We leave this investigation for future work.

Finally for Model 3, Table 7 and Table 8 show that the PCLDA rule has both the highest accuracy as well as the smallest number of selected features among all the considered classifiers; the DSDA classifier has a slightly worse accuracy and also selected a much larger number of features, when compared to PCLDA. The SLDA classifier now has the worst accuracy and also selects almost all \( p = 800 \) features, and this is a consequence of \( \Sigma \) being a dense matrix with high probability. The mis-classification error for the AdaLDA and AdaLDA(rot) rules are also quite large, and we surmise that this is due to the numerical instability when solving the linear programming problem in AdaLDA. Indeed, the condition numbers for \( \Sigma \) are, in general, quite large; Table 13 presents the summary statistics for these conditions numbers using the same 200 Monte Carlo replicates as that for generating Table 7. Following the suggestion in Cai and Zhang (2019), we replace the sample covariance matrix \( \hat{\Sigma} \) used in the optimization problem for AdaLDA and AdaLDA(rot) (see Eq. (8) and Eq. (9) in Cai and Zhang (2019)) with the matrix \( \Sigma = \hat{\Sigma} + \sqrt{n^{-1} \ln p} I_p \); the resulting classifiers are denoted as AdaLDA(reg) and AdaLDA(rot + reg), respectively. Table 7 however shows that using \( \hat{\Sigma} \) lead only to a negligible gain in accuracy. Finally we observe that the rotation pre-processing step once again leads to a substantial loss in accuracy for the DSDA and AdaLDA classifiers.

### 4.2. Real data analysis

We now assess the performance of our proposed procedure PCLDA on two popular gene expression data sets for leukaemia and lung cancer. The leukaemia dataset (Golub et al., 1999) includes \( p = 7128 \) gene measurements on 72 patients with either acute lymphoblastic leukemia (ALL) or acute myeloid leukemia (AML) and we wish to classify patients into either ALL or AML based on their gene expressions. The training set consists of the gene expressions for \( n_1 = 27 \) patients with ALL and \( n_2 = 11 \) patients with AML while the test set contains the gene expression data for 20 patients with ALL and 14 patients with AML. The lung cancer data was originally analyzed in Gordon et al. (2002) and we use a version of the data wherein the predictor variables with low
Table 5. Misclassification rate (%) with standard deviations (%) in parentheses for block diagonal setting (model 2)

| $\rho$ | 0.50  | 0.60  | 0.70  | 0.80  | 0.90  |
|--------|-------|-------|-------|-------|-------|
| Oracle | 5.30 (1.71) | 5.21 (1.52) | 5.34 (1.64) | 5.48 (1.62) | 5.40 (1.74) |
| PCLDA  | 9.08 (2.71) | 8.61 (2.59) | 8.30 (2.55) | 8.26 (2.45) | 8.12 (2.58) |
| CAT-LDA | 10.08 (3.00) | 9.36 (2.57) | 9.31 (2.50) | 9.25 (2.59) | 9.21 (2.89) |
| DSDA  | 9.63 (2.61) | 9.62 (2.64) | 9.50 (2.66) | 9.58 (2.67) | 9.47 (2.42) |
| DSDA(rot) | 20.64 (4.16) | 20.52 (3.99) | 20.75 (4.18) | 21.02 (4.44) | 20.90 (4.40) |
| AdaLDA | 12.70 (2.99) | 13.06 (3.39) | 13.88 (3.45) | 13.75 (3.48) | 14.68 (3.86) |
| AdaLDA(rot) | 23.91 (3.70) | 23.81 (3.72) | 24.33 (4.10) | 23.89 (3.92) | 24.12 (3.94) |
| SLDA  | 6.99 (2.89) | 6.66 (1.92) | 6.71 (2.17) | 6.62 (1.97) | 6.56 (1.90) |
| NSC  | 25.14 (3.11) | 26.47 (3.31) | 28.61 (3.35) | 29.59 (3.24) | 30.52 (3.82) |

Table 6. Average number of nonzero coefficients with standard deviations in parentheses for block diagonal setting (model 2)

| $\rho$ | 0.50  | 0.60  | 0.70  | 0.80  | 0.90  |
|--------|-------|-------|-------|-------|-------|
| PCLDA  | 20.19 (4.87) | 20.48 (5.06) | 20.48 (4.88) | 20.96 (4.96) | 20.58 (4.44) |
| CAT-LDA | 20.02 (4.95) | 19.86 (4.31) | 20.05 (4.62) | 20.32 (4.21) | 20.33 (4.54) |
| DSDA  | 50.28 (26.61) | 50.74 (28.92) | 47.48 (25.77) | 43.66 (22.42) | 45.15 (23.78) |
| DSDA(rot) | 51.02 (39.23) | 46.13 (29.09) | 51.93 (36.08) | 45.56 (31.15) | 49.62 (33.50) |
| AdaLDA | 19.45 (2.37) | 18.53 (2.23) | 17.93 (2.27) | 17.40 (2.20) | 16.85 (2.07) |
| AdaLDA(rot) | 14.40 (3.14) | 14.81 (3.53) | 15.16 (3.40) | 15.69 (3.99) | 14.97 (3.84) |
| SLDA  | 405.98 (390.84) | 320.17 (380.33) | 210.99 (336.12) | 242.19 (352.81) | 172.00 (309.62) |

Table 7. Misclassification rate (%) with standard deviations (%) in parentheses for random correlation setting (model 3)

| Method | $\mathcal{U}(-1, 1)$ | $\mathcal{N}(0, 1)$ | $t_5$ |
|--------|-----------------|----------------|-------|
| PCLDA  | 5.07 (2.40) | 12.39 (4.17) | 13.72 (5.00) |
| CAT-LDA | 11.93 (4.04) | 23.67 (6.13) | 25.68 (6.82) |
| DSDA  | 7.32 (3.05) | 16.92 (5.21) | 17.90 (5.49) |
| DSDA(rot) | 18.51 (6.37) | 31.81 (7.11) | 33.65 (7.28) |
| AdaLDA | 17.94 (6.03) | 44.55 (7.12) | 47.89 (5.10) |
| AdaLDA(rot) | 23.00 (7.49) | 39.29 (6.11) | 42.52 (6.28) |
| AdaLDA(reg) | 29.48 (7.58) | 47.49 (4.52) | 48.96 (4.04) |
| AdaLDA(reg+rot) | 21.23 (7.43) | 38.93 (6.60) | 42.52 (6.28) |
| SLDA  | 50.10 (4.40) | 49.98 (4.25) | 50.09 (3.70) |
| NSC  | 30.30 (6.28) | 44.55 (5.16) | 46.70 (4.49) |


Table 8. Model size with standard deviations in parentheses for random correlation setting (model 3)

| Method      | $U(-1,1)$ | $N(0,1)$ | $t_5$         |
|-------------|-----------|-----------|---------------|
| PCLDA       | 11.93 (4.10) | 11.48 (3.88) | 11.37 (3.92) |
| CAT-LDA     | 21.19 (6.51) | 20.64 (6.88) | 20.75 (6.90) |
| DSDA        | 66.00 (31.92) | 65.63 (34.45) | 64.91 (30.51) |
| DSDA(rot)   | 51.08 (34.82) | 71.94 (41.64) | 77.56 (49.29) |
| AdaLDA      | 15.99 (2.32)  | 10.46 (1.97)  | 8.51 (2.22)   |
| AdaLDA(rot) | 14.62 (4.61)  | 19.08 (3.93)  | 16.26 (3.43)  |
| AdaLDA(reg) | 11.38 (1.77)  | 8.50 (2.00)   | 7.12 (1.96)   |
| AdaLDA(reg+rot) | 9.86 (4.71) | 15.99 (3.63) | 16.26 (3.43) |
| SLDA        | 799.51 (1.31) | 800.00 (0.07) | 800.00 (0.00) |
| NSC         | 12.21 (8.47)  | 55.38 (131.65)| 102.89 (192.83)|

Table 9. Misclassification rate and model size of various methods for the leukaemia data

| Method      | Training Error | Test Error | Model Size |
|-------------|----------------|------------|------------|
| PCLDA       | 0/38           | 1/34       | 12         |
| DSDA        | 0/38           | 1/34       | 36         |
| AdaLDA (reg)| 0/38           | 1/34       | 18         |
| NSC         | 1/38           | 3/34       | 24         |

variances are removed; see Pun and Hadimaja (2021). The resulting dataset contains tumor tissues with $p = 1577$ features collected from patients with adenocarcinoma (AD) or malignant pleural mesothelioma (MPM). According to Gordon et al. (2002), MPM is highly lethal but distinguishing between MPM and AD is quite challenging in both clinical and pathological settings. The training set consists of $n_1 = 120$ gene expressions for patients with AD and $n_2 = 25$ gene expressions for patients with MPM, and the test set consists of gene expressions for 30 patients with AD and 6 patients with MPM. Table 9 and Table 10 presents the classification accuracy and number of selected features for various classifiers when applied to the leukemia and lung cancer data, respectively. The hyperparameters for these classifiers are selected using leave-one-out CV. Table 9 and 10 indicate that the proposed PCLDA rule has classification accuracy that are competitive with existing state-of-the-art classifiers while also selecting fewer features.

Table 10. Misclassification rate and model size of various methods for the lung cancer data

| Method      | Training Error | Test Error | Model Size |
|-------------|----------------|------------|------------|
| PCLDA       | 0/145          | 0/36       | 20         |
| DSDA        | 1/145          | 0/36       | 25         |
| AdaLDA (reg)| 0/145          | 0/36       | 388        |
| NSC         | 1/145          | 0/36       | 1206       |
5. Extensions

5.1. Extending PCLDA to non-normal distribution

A random vector $X \in \mathbb{R}^p$ is said to have an elliptical distribution with mean $\mu$ and covariance matrix $\Sigma$ if the probability density function for $X$ is of the form

$$f(x) = C_f |\Sigma|^{-1/2} h((x - \mu)\Sigma^{-1}(x - \mu)), \quad \text{for all } x \in \mathbb{R}^p. \quad (5.1)$$

Here $C_f$ is a normalization constant, $|\Sigma|$ is the determinant of $\Sigma$ and $h$ is a monotone function on $[0, \infty)$. The class of elliptical distributions is analytically tractable and many results that hold for multivariate normal distributions can be extended to general elliptical distributions. In particular Fang and Anderson (1992) showed that Fisher's LDA rule in Eq. (1.1) is also Bayes optimal whenever the feature vectors $X$ are sampled from a mixture of two elliptical distributions with known covariance matrix $\Sigma$ and known class conditional means $\mu_1$ and $\mu_2$. Shao et al. (2011) and Cai and Liu (2011) leveraged this fact to show that, under certain conditions on the sparsity of either $\mu_1 - \mu_2$ and $\Sigma$ or the sparsity of $\Sigma^{-1}(\mu_1 - \mu_2)$, the SLDA and AdaLDA classifier also achieves the Bayes error rate for elliptical distributions with unknown $\Sigma, \mu_1$ and $\mu_2$. Analogously, the theoretical properties for the PCLDA rule in section 3 can also be extended to elliptical distributions, provided that these distributions have sub-Gaussian tails as define below.

**Definition 1.** Let $\Psi : [0, \infty) \rightarrow [0, \infty)$ be a non-decreasing and non-zero convex function with $\Psi(0) = 0$. Let $Z$ be a mean 0 random variable. The Birnbaum-Orlicz $\Psi$-norm of $Z$ is then defined as

$$\|Z\|_\Psi = \inf \left\{ s \geq 0 : \mathbb{E}\Psi \left( \frac{Z}{s} \right) \leq 2 \right\}. \quad (5.2)$$

Similarly, let $Z$ be a mean 0 random vector taking values in $\mathbb{R}^p$. The Birnbaum-Orlicz $\Psi$-norm for $Z$ is then defined as

$$\|Z\|_\Psi = \sup_{w \in \mathbb{R}^p, \|w\|_2 = 1} \left\| w^T Z \right\|_{\Psi}. \quad (5.3)$$

Let $\Psi_1(x) = \exp(|x|)$ and $\Psi_2(x) = \exp(x^2)$. A mean 0 random vector $Z$ is said to be sub-exponential if $\|Z\|_{\Psi_1} < \infty$ and is said to be sub-Gaussian if $\|Z\|_{\Psi_2} < \infty$. If $Z \in \mathbb{R}^p$ is a mean 0 sub-Gaussian random vector then $w^T Z$ is a sub-Gaussian random variable for all $w \in \mathbb{R}^p$. Furthermore, if $Z$ is a sub-Gaussian random variable then there exists a universal constant $K$ such that for all $t > 0$, we have

$$\mathbb{P}(Z > t) \leq 2 \exp(-t^2/(K\|Z\|_{\Psi_2}^2)).$$

In other words the tails of $Z$ decay at a rate similar to that for a Gaussian distribution with variance $\|Z\|_{\Psi_2}^2$. For more on sub-Gaussian random vectors, see Section 2.5 and Section 3.4 of Vershynin (2018).

**Remark 2.** If $Z \in \mathbb{R}^p$ is a mean 0 sub-Gaussian random vector with covariance matrix $\Sigma$ then $\|w^T V\|_{\Psi_2}^2 \geq w^T \Sigma w$ for all $w \in \mathbb{R}^p$. In this paper we shall assume that a converse inequality also holds, namely that there exist a constant $c_1 > 0$ such that,

$$w^T \Sigma w \geq c_1 \|w^T Z\|_{\Psi_2}^2, \quad \text{for all } w \in \mathbb{R}^p. \quad (5.4)$$
We note that the constant $c_1$ in Eq. (5.4) can depend on $Z$ but does not depend on the choice of $w \in \mathbb{R}^p$. If $Z$ is multivariate normal then Eq. (5.4) always hold. If $Z$ is a mean 0 sub-Gaussian random vector but not a multivariate normal then Eq. (5.4) allows us to bound the Orlicz norm of $w^T Z$ for any $w \in \mathbb{R}^p$ in terms of its variance. This then allow us to obtain better estimate for $\hat{\Sigma} - \Sigma$ in spectral norm, especially in the setting where the spiked eigenvalues could diverge with $p$. See for example Theorem 4.7.1 in Vershynin (2018) and Theorem 9 in Koltchinskii and Lounici (2017).

We can now reformulate the classification problem in the earlier part of this paper to the case of elliptical distributions as follows. Let $\{\epsilon_{11}, \ldots, \epsilon_{1n_1}\}$ and $\{\epsilon_{21}, \ldots, \epsilon_{2n_2}\}$ be independently and identically distributed mean 0 random vectors with pdf of the form given in Eq. (5.1) and suppose that the training sample is given by

$$
X_{1j} = \mu_1 + \epsilon_{1j1}, \quad j_1 \in [n_1], 
$$

$$
X_{2j} = \mu_2 + \epsilon_{2j2}, \quad j_2 \in [n_2].
$$

Given these training samples $\{X_{ij}\}$, let $X$ be the $(n_1 + n_2) \times p$ matrix whose rows are the $\{X_{ij}\}$. Then Theorem 1, in particular Eq. (3.4), also holds for these $X$ as long as the $\{\epsilon_{ij}\}$ satisfy Eq. (5.4). Eq. (3.4) then implies that Theorem 2, in particular Eq. (3.5), also holds when the $X$ are sub-Gaussian random vectors. The resulting bound for $\|\hat{\zeta} - \zeta\|_\infty$ allows us to recover $S_\zeta$ by thresholding $\hat{\zeta}$, and hence $\hat{R}_{PCLDA} \to R_F$. In summary, the PCLDA rule is asymptotically Bayes optimal whenever the feature vectors $\{X_{ij}\}$ are sampled from a mixture of elliptical distributions with sub-Gaussian tails.

### 5.2. Extending PCLDA to multi-class classification

The PCLDA rule can also be extended to the setting for $K \geq 3$ classes. Let us assume that we are given training data from $K$ classes where, for each class, the training samples are independently and identically distributed according to a $p$-dimensional multivariate normal distribution, i.e.,

$$
X_{i1}, \ldots, X_{im_i} \sim \mathcal{N}_p(\mu_i, \Sigma), \quad i \in [K].
$$

Here $n_i$ denote the number of training data points from class $i \in [K]$. The testing data point $Z$ is drawn from a mixture of $K$ multivariate normal distributions namely, $Z \sim \sum_{i=1}^{K} \pi_i \mathcal{N}_p(\mu_i, \Sigma)$ with $\pi_i \geq 0$ and $\sum_{i=1}^{K} \pi_i = 1$. Note that, for ease of exposition, the $\{X_{ij}\}$ are assumed to be multivariate normals but the following results also hold when $\{X_{ij}\}$ are elliptically distributed as in Section 5.1.

Now define, for $2 \leq i \leq K$, the whitened direction $\zeta^{(i)}$ and the corresponding whitened indices $S_i$, via

$$
\zeta^{(i)} = W(\mu_i - \mu_1), \quad S_i = \{j : \zeta_j^{(i)} \neq 0\}.
$$

Define the global whitened set as the union $S_\zeta = \bigcup_{i=2}^{K} S_i$. The set $S_\zeta$ is the target that we wish to recover from feature selection.

The $K$-class PCLDA rule $\hat{\Upsilon}_{PCLDA}$ can now be described as follows.
Algorithm 2: $K$-class PCLDA rule

Input: $\bar{X}_i$, $i \in [K]$, $\Sigma$ and the test sample $Z$

Output: $\hat{\Upsilon}_{\text{PCLDA}}(Z)$

Step 1: Perform PCA on the feature vectors for the training data. Extract the $d$ largest principal components to obtain $\hat{W}$.

Step 2: For $2 \leq i \leq K$, let $\hat{X}_i = \hat{W} \bar{X}_i$ and $\hat{\zeta}^{(i)} = \hat{X}_i - \hat{X}_1$. Also let $\hat{S}_i$ be the set of indices corresponding to the $s_i$ largest elements of $\hat{\zeta}^{(i)}$ in absolute values. The value of $s_i$ is, in general, a user-specified or tuning parameter. Nevertheless, under certain conditions, we can also estimate $s_i$; see Eq. (5.10) below.

Step 3: Given the test data point $Z$, let $\hat{Z} = \hat{W}Z$ and denote by $\hat{\zeta}^{(i)}_{\hat{S}_i}$ the vector obtained from $\hat{\zeta}^{(i)}$ by keeping only those coordinates belonging to $\hat{S}_i$.

Step 4: Set $\hat{D}_1 = 0$ and calculate, for $2 \leq i \leq K$, the discriminant score for class $i$ relative to class 1 as

$$\hat{D}_i = \left[ \hat{Z} - \left( \frac{\hat{X}_i + \hat{X}_1}{2} \right) \right]^T \hat{S}_i \hat{\zeta}^{(i)}_{\hat{S}_i} + \ln \frac{n_i}{n_1}. \quad (5.7)$$

Step 5: Assign the label of $Z$ to the class that maximizes the discriminant score, i.e.,

$$\hat{\Upsilon}_{\text{PCLDA}}(Z) = \arg \max_{i \in [K]} \hat{D}_i. \quad (5.8)$$
We now assume that the whitened directions \(\{\zeta^{(i)}\}\), the whitened indices \(\{S_i\}\), and the covariance matrix \(\Sigma\) satisfy the following two conditions; these conditions are natural generalizations of Condition 2 and Condition 3 to the multi-class setting.

**Condition 5.** Let \(|S_i| = s_{i0} > 0 \) for each \(i = 2, \ldots, K\). Recall that \(S_i\) is the set of indices \(j\) for which \(\zeta_{ij} \neq 0\). Let \(C_0 > 0\), \(M > 0\) and \(C_\zeta > 0\) be constants not depending on \(p\) such that \(\min_{i=2, \ldots, K} s_{i0} \leq M\) and
\[
\min_{i=2, \ldots, K} \min_{j \in S_i} |\zeta_{ij}| > C_0, \quad \max_{i \in [K]} \|\Sigma^{-1/2} \mu_i\|_2 < C_\zeta.
\]

**Condition 6.** Let \(\sigma > 0\) be fixed and that, for sufficiently large \(p, n_1, \ldots, n_K\) and \(p\) satisfy
\[
\frac{n_i}{n_j} = \Theta(1), \quad i \neq j, \quad i, j \in [K]; \quad \ln p = o(n).
\]
Furthermore, for sufficiently large \(p\), the spiked eigenvalues \(\lambda_1, \ldots, \lambda_d\) satisfy
\[
\lambda_k = O(p), \quad \text{for all } k \in [d].
\]

Given the above conditions, the following result generalizes Theorem 2 and provides an \(\ell_\infty\) bound for \(\hat{\zeta}_i - \zeta_i\) for \(i \geq 2\).

**Theorem 4.** Under Condition 1, 4, 5 and 6, there exists a constant \(C > 0\) such that with probability at least \(1 - O(p^{-1})\),
\[
\max_{i=2, \ldots, K} \|\hat{\zeta}^{(i)} - \zeta^{(i)}\|_\infty \leq C \sqrt{\frac{\ln p}{n}}. \tag{5.9}
\]

We now consider a hard thresholding estimate \(\tilde{\zeta}^{(i)}\) for recovering \(\zeta^{(i)}\) as follows. For a given \(i \geq 2\), let
\[
\tilde{\zeta}_j^{(i)} = \begin{cases} 
\hat{\zeta}_j^{(i)} & \text{if } |\hat{\zeta}_j^{(i)}| > t_n, \\
0 & \text{otherwise}
\end{cases}, \quad j \in [p] \tag{5.10}
\]
where \(t_n = C \left(\ln n/p\right)^\alpha\) for some constant \(C > 0\) and \(0 < \alpha < \frac{1}{2}\). Here we assume, for simplicity, that \(C\) and \(\alpha\) are the same for all classes. Given \(\tilde{\zeta}^{(i)}\), define the associated active set \(\tilde{S}_i = \{j : \tilde{\zeta}_j^{(i)} \neq 0\}\). The next result extends Theorem 3 and show that the PCLDA rule is also asymptotically Bayes-optimal in the multi-class setting.

**Theorem 5.** Suppose that \(Z \sim \sum_{i=1}^K \pi_i N_p(\mu_i, \Sigma)\) where \(\pi_i \geq 0\) and \(\sum_{i=1}^K \pi_i = 1\). Suppose Condition 1, 4, 5 and 6 are satisfied. We then have
\[
\max_{i=2, \ldots, K} \Pr(\tilde{S}_i \neq S_i) = O(p^{-2}). \tag{5.11}
\]
Furthermore, suppose that \(\ln p = o(n)\). We then have
\[
|\hat{R}_{\text{PCLDA}} - R_F| \rightarrow 0 \tag{5.12}
\]
almost surely as \(n, p \rightarrow \infty\).
6. Discussion

In this paper we addressed the classification problem for high-dimensional data by proposing the PCLDA classifier that first performs dimension reduction on the feature vectors prior to classification in the dimensionally reduced space. We show that, under a spiked eigenvalues structure for $\Sigma$, the PCLDA classifier is asymptotically Bayes optimal whenever $n \to \infty$ and $n^{-1} \ln p \to 0$. While the consistency property of PCLDA is similar to other classifiers based on estimating the discriminant direction $\beta$, the underlying assumptions and motivations for this paper are substantially different. Indeed, the focus on PCA and the whitening matrix leads to the natural assumption that $\Sigma$ has spiked/diverging eigenvalues while earlier results that focus on estimation of $\beta$ had generally assumed that $\Sigma$ is sparse or that the eigenvalues of $\Sigma$ are bounded. Numerical experiments indicate that the classification accuracy of PCLDA is competitive with other existing state-of-the-art classifiers, such as DSDA and AdaLDA, while also selecting a smaller number of features.

We now mention two interesting issues for future research. The first issue is to extend the theoretical results in this paper for LDA $\odot$ PCA to other, possibly non-linear, dimension reduction techniques such as (classical) multidimensional scaling, kernel PCA, and Laplacian eigenmaps (Belkin and Niyogi, 2003), followed by learning a classifier (such as LDA) in the dimensionally reduced space. The second issue concerns the spiked covariance structure in Condition 1. In particular while Condition 1 is widely used in earlier papers, see e.g., Birnbaum et al. (2012); Cai et al. (2013); Hao et al. (2015); Johnstone (2001), its assumption on the non-spiked eigenvalues might be somewhat restrictive. We can relax Condition 1 by assuming that $\Sigma$ arises from an approximate factor model (Fan et al., 2013) or that $\Sigma$ can be decomposed into a low-rank plus sparse matrix structure (Agarwal et al., 2011). We surmise that, due to the focus on the whitening matrix $\Sigma^{-1/2}$, theoretical analysis of PCLDA under these more general covariance structure also leads to interesting technical developments; e.g., while perturbation results for $\hat{\Sigma}^{-1} - \Sigma^{-1}$ given $\hat{\Sigma} - \Sigma$ are well-studied, much less is known about perturbation bounds for $\hat{\Sigma}^{-1/2} - \Sigma^{-1/2}$ given $\hat{\Sigma} - \Sigma$.

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Table 11. Average number of strong discriminative and whitened variable with standard deviations in parentheses for equal correlation setting (model 1)

| $\rho$  | 0.50    | 0.60    | 0.70    | 0.80    | 0.90     |
|---------|---------|---------|---------|---------|---------|
| PCLDA   | 9.59 (0.82) | 9.42 (0.85) | 8.53 (1.41) | 8.53 (1.41) | 3.68 (0.98) |
| DSDA    | 10.00 (0.00) | 9.99 (0.07) | 9.99 (0.07) | 9.99 (0.07) | 10.00 (0.00) |
| AdaLDA  | 9.95 (0.22) | 9.93 (0.26) | 9.95 (0.23) | 10.00 (0.07) | 10.00 (0.07) |
| SLDA    | 9.98 (0.22) | 9.98 (0.28) | 10.00 (0.00) | 10.00 (0.00) | 10.00 (0.00) |

Table 12. Average number of weak discriminative and whitened variable with standard deviations in parentheses for equal correlation setting (model 1)

| $\rho$  | 0.50    | 0.60    | 0.70    | 0.80    | 0.90     |
|---------|---------|---------|---------|---------|---------|
| PCLDA   | 2.44 (4.22) | 1.90 (3.73) | 0.98 (3.35) | 0.98 (3.35) | 0.00 (0.00) |
| DSDA    | 86.20 (31.06) | 96.42 (32.57) | 107.16 (30.53) | 107.06 (29.96) | 86.48 (8.66) |
| AdaLDA  | 36.59 (5.94) | 35.91 (5.22) | 36.78 (6.36) | 37.86 (5.88) | 38.65 (5.02) |
| SLDA    | 718.86 (226.57) | 778.18 (95.53) | 789.96 (0.21) | 789.96 (0.21) | 789.96 (0.21) |

Appendix A: Supplementary Numerical Results

We provide here several tables that supplement the simulation results in Section 4. Table 11 and 12 reports the average number of strong signals and weak signals captured by PCLDA, DSDA, AdaLDA and SLDA under Model 1. Looking at Table 12 we see that PCLDA generally includes only a few features corresponding to the weak signals and thus selects only a small number of features compared to the other classifiers. We also report in Table 13 the summary statistics for the condition numbers of the covariance matrix $\Sigma$ in Model 3; these summary statistics indicate that the classification accuracy of could be adversely impacted since AdaLDA finds an estimate of $\beta$ by solving a linear programming problem and this optimization problem can be numerically unstable when $\Sigma$ have large condition numbers.

Table 13. Summary statistics of condition numbers of generated $\Sigma$ from uniform, normal and student distributions

| Statistics | $\mathcal{U}(-1, 1)$ | $\mathcal{N}(0, 1)$ | $t_5$ |
|------------|-----------------------|---------------------|------|
| Mean       | 415.3                 | 688.0               | 1059.2 |
| SD         | 102.4                 | 195.2               | 400.0 |
| Median     | 391.5                 | 658.5               | 966.3 |
| IQR        | 108.0                 | 205.9               | 314.1 |
| Max        | 849.9                 | 1622.1              | 3708.4 |
| Min        | 266.3                 | 396.9               | 536.0 |
Appendix B: Proofs of Stated Results

This section contains the proofs of Theorem 1 through Theorem 3. We will present the proofs under the more general assumption that the feature vectors \( \{X_{ij}\} \) are sub-Gaussian random vectors; see also the discussion in Section 5.1.

B.1. Preliminary results

We start by listing some elementary but useful facts about the \( 2 \rightarrow \infty \) norm and its relationships with other matrix norms.

Proposition 1. Let \( A \in \mathbb{R}^{p_1 \times p_2} \) and \( B \in \mathbb{R}^{p_2 \times p_3} \) be arbitrary matrices. Let \( x \in \mathbb{R}^{p_2} \) be an arbitrary vector. We then have

\[
\|A\|_{2 \rightarrow \infty} = \max_{i \in [p_1]} \|A^T e_i(p_1)\|_2; \quad (B.1)
\]

\[
\|Ax\|_\infty \leq \|A\|_{2 \rightarrow \infty} \|x\|_2; \quad (B.2)
\]

\[
\|AB\|_{2 \rightarrow \infty} \leq \|A\|_{2 \rightarrow \infty} \|B\|_2. \quad (B.3)
\]

Eq. (B.1) states that the two-to-infinity norm of a matrix \( A \) is equivalent to the maximum \( \ell_2 \) norm of the rows of \( A \). Eq. (B.2) provides a bound for \( \|Ax\|_\infty \) that is tighter than the naive bound \( \|Ax\|_\infty \leq \|A\|_2 \|x\|_2 \); prior works that bound \( \|Ax\|_\infty \leq \|A\|_2 \|x\|_2 \) generally have to assume that the eigenvalues or singular values of \( A \) are bounded.

Let \( \xi_i = \bar{X}_i - \mu_i \) and \( E_i = \xi_i \xi_i^T \), \( i = 1, 2 \). Recall that \( \eta_k = (\lambda_k + \sigma^2)^{-1/2} \), \( k \in [d] \) and \( \sigma^2 = (\text{tr}(\Sigma) - \text{tr}(\Lambda))/(p - d) \), simply the eigenvalues of \( W \). The next lemma provides several concentration inequalities for \( \hat{\Sigma} - \Sigma \), \( \hat{\eta}_k - \eta_k \) and \( \sigma^2 - \hat{\sigma}^2 \).

Lemma 1. Assume that the random variables \( \{X_i\} \) satisfy Eq. (5.4) and the covariance matrix \( \Sigma \) satisfies Condition 3 and Condition 4. Then the following bounds hold simultaneously with probability at least \( 1 - O(p^{-1}) \),

\[
\|\hat{\Sigma} - \Sigma\|_2 = O(p \sqrt{n^{-1} \ln p}), \quad (B.4)
\]

\[
\|\hat{\xi}_i\|_2 = O(p n^{-1} \ln p), \quad (B.5)
\]

\[
\|\hat{\Sigma} - \Sigma\|_2 = O(p \sqrt{n^{-1} \ln p}), \quad (B.6)
\]

\[
|\hat{\eta}_k - \eta_k| = O(\sqrt{p n^{-1} \ln p}), \quad (B.7)
\]

\[
|\sigma^2 - \hat{\sigma}^2| = O(\sqrt{n^{-1} \ln p}). \quad (B.8)
\]

Eq. (B.4) is given in Lounici (2014) and Koltchinskii and Lounici (2017) while Eq. (B.5) follows from an application of Bernstein inequality; see Section 2.8 of Vershynin (2018). Eq. (B.6) follows from Eq. (B.4) and Eq. (B.5) together with the observation that \( \|\xi_i\|_2 = \|E_i\|_2 \) and \( \hat{\Sigma}_0 - \hat{\Sigma} = n_1/n \ E_1 + n_2/n \ E_2 \). Finally, Eq. (B.7) and Eq. (B.8) follow from Eq. (B.6) and Weyl’s inequality.
B.2. Proof of Theorem 1

Recall that \( \mathbf{U} \) and \( \hat{\mathbf{U}} \) denote the \( p \times d \) matrices whose columns are the eigenvectors corresponding to the \( d \) largest eigenvalues of \( \Sigma \) and the pooled sample covariance matrix \( \hat{\Sigma} \), respectively. Now let \( \mathbf{U}_\perp \) and \( \hat{\mathbf{U}}_\perp \) be the \( p \times (p - d) \) matrices whose columns are the remaining eigenvectors of \( \Sigma \) and \( \hat{\Sigma} \), respectively, i.e., \( \mathbf{I}_p - \mathbf{U}\mathbf{U}^T = \mathbf{U}_\perp \mathbf{U}_\perp^T \) and \( \mathbf{I}_p - \hat{\mathbf{U}}\hat{\mathbf{U}}^T = \hat{\mathbf{U}}_\perp \hat{\mathbf{U}}_\perp^T \).

Let \( \Xi \) be the \( d \times d \) orthogonal matrix that minimizes

\[
\min_{\mathbf{W}} \|\mathbf{W} - \mathbf{U}^T \hat{\mathbf{U}}\|_F
\]

among all orthogonal matrices. Let \( \mathbf{E}_n = \hat{\Sigma} - \Sigma \). We bound \( \|\hat{\mathbf{U}} - \mathbf{U}\Xi\|_{2 \to \infty} \) using following expansion.

\[
\begin{align*}
\|\hat{\mathbf{U}} - \mathbf{U}\Xi\|_{2 \to \infty} & \leq C \left( \|\mathbf{U}_\perp \mathbf{E}_n \mathbf{U}_\perp^T\|_{2 \to \infty} / (\lambda_d + \sigma^2) \right. \\
& \quad + C \left. \|\mathbf{U}_\perp \mathbf{E}_n \mathbf{U}_\perp^T\|_{2 \to \infty} \sin \Theta(\hat{\mathbf{U}}, \mathbf{U}) \right)_{2 \to \infty} / (\lambda_d + \sigma^2) \\
& \quad + C \|\mathbf{U}_\perp \mathbf{E}_n \mathbf{U}_\perp^T\|_{2 \to \infty} \sin \Theta(\hat{\mathbf{U}}, \mathbf{U})_{2 \to \infty} / (\lambda_d + \sigma^2) \\
& \quad + \| \sin \Theta(\hat{\mathbf{U}}, \mathbf{U}) \|_2 \|\mathbf{U}\|_{2 \to \infty}. \quad (a-4)
\end{align*}
\]

See also Theorem 3.7 in Cape et al. (2019). Now recall the matrix \( \hat{\Sigma}_0 \) from Eq. (2.4). We then have

\[
\hat{\Sigma} - \Sigma = \hat{\Sigma}_0 - \Sigma - \frac{n_1}{n} \left( \overline{x}_1 - \mu_1 \right) \left( \overline{x}_1 - \mu_1 \right)^T - \frac{n_2}{n} \left( \overline{x}_2 - \mu_2 \right) \left( \overline{x}_2 - \mu_2 \right)^T.
\]

Using the same argument as that for the proof of Theorem 1.1 in Cape et al. (2019), there exists a constant \( C > 0 \) such that, with probability at least \( 1 - \mathcal{O}(p^{-2}) \),

\[
\begin{align*}
\|\mathbf{U}_\perp \mathbf{U}_\perp \mathbf{E}_n \mathbf{U}_\perp^T\|_{2 \to \infty} & \leq C \sqrt{d} \max_{i \in [p]} \Sigma_{ii} \sqrt{\lambda_1 + \sigma^2} \sqrt{\max\{\mathbf{r}(\Sigma), \ln p\} / n} \\
\|\mathbf{U}_\perp \mathbf{U}_\perp^T \mathbf{E}_n \mathbf{U}_\perp^T\|_{2 \to \infty} & \leq C \sqrt{\lambda_1 + \sigma^2} \sqrt{\max\{\mathbf{r}(\Sigma), \ln p\} / n}.
\end{align*}
\]

(B.9) (B.10)

Therefore to complete the proof of Theorem 1, it suffices to show that for \( j \in \{1, 2\} \), the terms \( \|\mathbf{U}_\perp \mathbf{U}_\perp \mathbf{E}_n \mathbf{U}_\perp^T\|_{2 \to \infty} \) and \( \|\mathbf{U}_\perp \mathbf{U}_\perp^T \mathbf{E}_n \mathbf{U}_\perp^T\|_{2 \to \infty} \) is of the same order or smaller order than the terms in Eq. (B.9) and Eq. (B.10), respectively.

We now analyze \( \|\mathbf{U}_\perp \mathbf{U}_\perp \mathbf{E}_n \mathbf{U}_\perp^T\|_{2 \to \infty} \) and \( \|\mathbf{U}_\perp \mathbf{U}_\perp^T \mathbf{E}_n \mathbf{U}_\perp^T\|_{2 \to \infty} \) for \( j = 1 \). The case where \( j = 2 \) is identical. From Condition 4 and Proposition 1, we have

\[
\|\mathbf{U}_\perp \mathbf{U}_\perp^T\|_\infty \leq C \sqrt{d}, \quad \text{and} \quad \|\mathbf{U}_\perp \mathbf{U}_\perp^T \mathbf{E}_n \mathbf{U}_\perp^T\|_{2 \to \infty} \leq C \sqrt{d} \|\mathbf{E}_n \mathbf{U}\|_{2 \to \infty}. \quad (B.11)
\]

Furthermore, we also have

\[
\|\mathbf{E}_n \mathbf{U}\|_{2 \to \infty} \leq \sqrt{d} \max_{i \in [p], j \in [d]} \|\mathbf{E}_n \mathbf{U}_i \mathbf{U}_j\| = \sqrt{d} \max_{i \in [p], j \in [d]} \|\mathbf{E}_n \mathbf{U}_i \mathbf{U}_j\|.
\]
Since $X_i$ is sub-Gaussian, by the properties of Orlicz norms we have
\[
\|((\bar{X}_1 - \mu_1)^T u_i) \cdot ((\bar{X}_1 - \mu_1)^T u_j)\|_{\psi_1} \leq \|((\bar{X}_1 - \mu_1)^T e_i^{(p)})\|_{\psi_1} \|((\bar{X}_1 - \mu_1)^T u_j)\|_{\psi_2}
\]
Eq. (5.4) implies that there exists a constant $C > 0$ such that for any $i \in [p]$ and $j \in [d]$,
\[
\|((\bar{X}_1 - \mu_1)^T e_i^{(p)})\|_{\psi_1} \leq C \sqrt{\frac{\sum_{ii}^p}{n_1}} \leq \frac{C}{\sqrt{n_1}} \max_{i \in [p]} \Sigma_{ii},
\]
\[
\|((\bar{X}_1 - \mu_1)^T u_j)\|_{\psi_2} \leq C \sqrt{\text{Var}(u_j^T (\bar{X}_1 - \mu_1))} \leq C \sqrt{u_j^T \Sigma u_j} \leq C \sqrt{\frac{\lambda_1 + \sigma^2}{n_1}}.
\]
Now fix an arbitrary pair $(i, j)$ with $i \in [p]$ and $j \in [d]$. Then from Condition 4 and Bernstein inequality for sub-Gaussian random variables (Vershynin, 2018), there exists a constant $C > 0$ such that with probability at least $1 - O(p^{-3})$,
\[
|\mathbb{E}[\langle e_i^{(p)}, u_j \rangle]| \leq C \frac{\lambda_1 + \sigma^2}{n_1} \sqrt{\frac{d}{p}} \quad \text{(B.12)}
\]
\[
|\langle e_i^{(p)}, u_j \rangle| \leq \mathbb{E}[|\langle e_i^{(p)}, u_j \rangle|] + C \max_{i \in [p]} \{r(\Sigma), \ln p\} \sqrt{\frac{\max_{i \in [p]} \Sigma_{ii}}{n_1}} \sqrt{\frac{\lambda_1 + \sigma^2}{n_1}}. \quad \text{(B.13)}
\]
Now recall Eq. (B.11). Then by Eq. (B.13) together with a union bound over all $i \in [p]$ and $j \in [d]$, we have, with probability at least $1 - O(p^{-2})$,
\[
\|U_1 U_1^T E_1 U^T \|_{2 \to \infty} \leq C \sqrt{d} \|E_1 U\|_{2 \to \infty} \leq C d \max_{i,j} |\langle e_i^{(p)}, u_j \rangle| \leq C \sqrt{d \ln p}. \quad \text{(B.14)}
\]
An almost identical argument also yields
\[
\|U_1 U_1^T E_2 U^T \|_{2 \to \infty} \leq C \sqrt{d \ln p}. \quad \text{(B.15)}
\]
with probability at least $1 - O(p^{-2})$. The above two bounds are all of smaller order than that in Eq. (B.9), as desired. Under Condition 3, there exist $C > 0$ such that $\lambda_1 + \sigma^2 \leq C(\lambda_d + \sigma^2)$ for sufficiently large enough $p$ and $n$ and with probability at least $1 - O(p^{-2})$, we bound the term $(a - 1)$ as
\[
\|U_1 U_1^T E_n (U^T U)\|_{2 \to \infty} / (\lambda_d + \sigma^2)
\]
\[
\leq C \left( \sqrt{\frac{\max \{r(\Sigma), \ln p\}}{n}} + \frac{\max \{r(\Sigma), \ln p\}}{n} \right) \sqrt{\frac{\max_{i \in [p]} \Sigma_{ii}}{\lambda_d + \sigma^2}} \quad \text{(B.15)}
\]
We next consider $\|U_1 U_1^T E_1 U_1 U_1^T \|_{2 \to \infty}$. Then for $j > d$, we have
\[
\|((\bar{X}_1 - \mu_1)^T u_j)\|_{\psi_2} \leq C \sqrt{u_j^T \Sigma u_j} \leq C n^{-1/2} \sigma.
\]
Then following the same argument as that used for showing Eq. (B.14), we have
\[
\| (I - uu^T) E_1 I - uu^T \|_{2 \to \infty} \leq C \sqrt{pd} \sigma \sqrt{\max_{i \in [p]} \Sigma_{ii} \frac{\max \{r(\Sigma), \ln p\}}{n}} \leq C \sigma \sqrt{pd} \frac{\ln p}{n} \quad \text{(B.16)}
\]
with probability at least \(1 - O(p^{-2})\), and similarly for \( (I - uu^T)^2 (I - uu^T)^T \|_{2 \to \infty} \). The above bounds for \( \| (I - uu^T) E_2 (I - uu^T)^T \|_{2 \to \infty} \) imply Eq. (B.10).

We then have, by the Davis-Kahan theorem and Lemma 1, that
\[
\| \sin \Theta(\hat{u}, u) \|_2 \leq \frac{\| E_n \|_2}{\sigma^2} \leq C \sqrt{\max \{r(\Sigma), \ln p\}} \frac{\max \{r(\Sigma), \ln p\}}{n} \quad \text{(B.17)}
\]
for some \(C > 0\) with probability at least \(1 - O(p^{-1})\). We now bound the term in Eq. (a - 2). From Eq.(B.17) and Eq.(B.10), together with a similar argument as that for showing Eq.(B.15), we have
\[
\| (I - uu^T)^2 E_n (I - uu^T)^T \|_{2 \to \infty} \| \sin \Theta(\hat{u}, u) \|_2 (\lambda_d + \sigma^2)^{-1/2} \leq C \sqrt{\max \{r(\Sigma), \ln p\}} \frac{\max \{r(\Sigma), \ln p\}}{n} \quad \text{(B.18)}
\]
with probability at least \(1 - O(p^{-2})\). This then imply, by Eq.(B.17) and the bounded coherence assumption for \( U \), a bound for the term in Eq. (a - 4) of the form
\[
\| \sin \Theta(\hat{u}, u) \|_2 \| u \|_{2 \to \infty} \leq C \frac{\max \{r(\Sigma), \ln p\}}{n} \sqrt{\frac{d}{p}} = O \left( \frac{\ln p}{n} \frac{1}{\sqrt{p}} \right). \quad \text{(B.19)}
\]
with probability at least \(1 - O(p^{-2})\). Note that \( \Sigma U_\perp = \sigma^2 U_\perp \) and \( \| (I - uu^T) \Sigma (I - uu^T)^T \|_{2 \to \infty} = \sigma^2 \). Therefore, with probability at least \(1 - O(p^{-2})\), we can bound the term in Eq. (a - 3) by
\[
\| (I - uu^T)^2 (I - uu^T)^T \|_{2 \to \infty} \leq \| \sin \Theta(\hat{u}, u) \|_2 (\lambda_d + \sigma^2)^{-1/2} \leq C \sqrt{\frac{\max \{r(\Sigma), \ln p\}}{n}} = O \left( \frac{\ln p}{n} \frac{1}{\sqrt{p}} \right). \quad \text{(B.20)}
\]
Upon combining the bounds for the terms (a - 1), (a - 2), (a - 3) and (a - 4) in Eq.(B.15), Eq.(B.18), Eq.(B.19) and Eq.(B.20), we then have, with probability at least \(1 - O(p^{-2})\)
and for some constant $C > 0$, that

$$
\|\hat{u} - u\Xi\|_{2,\infty} \leq C \left( \sqrt{\frac{\max\{r(\Sigma), \ln p\}}{n}} + \frac{\max\{r(\Sigma), \ln p\}}{n} \right) \frac{d\sqrt{\max_{i \in [p]} \Sigma_{ii}}}{\sqrt{\lambda_d + \sigma^2}}
$$

$$
+ C \frac{\sigma}{\sqrt{\lambda_d + \sigma^2}} \frac{\max\{r(\Sigma), \ln p\}}{n} + \leq C \sqrt{\frac{\max_{i \in [p]} \Sigma_{ii}}{\lambda_d + \sigma^2}} \left( \frac{\max\{r(\Sigma), \ln p\}}{n} \right)^{3/2}
$$

We now bound the terms in \((B)\) and \((C)\). Let $\hat{D}$ and $D$ be diagonal matrices where

$$
\hat{D} = (\hat{\Lambda} + \hat{\sigma}^2 I_d)^{-1/2}, \quad D = (\Lambda + \sigma^2 I_d)^{-1/2}.
$$

We start by decomposing $\hat{W} - W$ as

$$
\hat{W} - W = (\hat{U} \hat{D} \hat{U}^T - U D U^T) + (\hat{\sigma}^{-1} - \sigma^{-1})(I_p - \hat{U} U^T) + \hat{\sigma}^{-1}(\hat{U} \hat{U}^T - U U^T).
$$

(B.21)

B.3. **Proof of Theorem 2**

First recall that $\hat{\zeta} = \hat{W}(\bar{X}_2 - \bar{X}_1)$ and $\zeta = W(\mu_2 - \mu_1)$ where the whitening matrix $W$ and its estimate $\hat{W}$ are given by Eq. (3.2) and Eq. (3.3), respectively. We now consider the decomposition

$$
\hat{\zeta} - \zeta = W\left[(\bar{X}_2 - \bar{X}_1) - (\mu_2 - \mu_1)\right]
$$

\(A\)

$$
+ (\hat{W} - W)\left[(\bar{X}_2 - \bar{X}_1) - (\mu_2 - \mu_1)\right]
$$

\(B\)

$$
+ (\hat{W} - W)(\mu_2 - \mu_1)
$$

\(C\)

We will now bound each of the term in the right hand side of the above display. We start with the term in \(A\). Let $\delta = (\bar{X}_2 - \bar{X}_1) - (\mu_2 - \mu_1)$ and let $\xi = W\delta$. We then have $\mathbb{E}[\xi] = 0$ and $\text{Var}[\xi] = c n^{-1} I_p$ for some $c > 0$ and $c = \mathcal{O}(1)$. Since $\delta$ satisfies Eq. (5.4), $\xi$ also satisfies Eq. (5.4). Hence, by Bernstein inequality for sub-Gaussian random vectors, there exists a constant $C > 0$ such that with probability at least $1 - \mathcal{O}(p^{-2})$,

$$
\|W((\bar{X}_2 - \bar{X}_1) - (\mu_2 - \mu_1))\|_\infty = \|\xi\|_\infty \leq C \sqrt{\frac{\ln p}{n}}.
$$

We now bound the terms in \(B\) and \(C\). Let $\hat{D}$ and $D$ be diagonal matrices where

$$
\hat{D} = (\hat{\Lambda} + \hat{\sigma}^2 I_d)^{-1/2}, \quad D = (\Lambda + \sigma^2 I_d)^{-1/2}.
$$

We start by decomposing $\hat{W} - W$ as

$$
\hat{W} - W = (\hat{U} \hat{D} \hat{U}^T - U D U^T) + (\hat{\sigma}^{-1} - \sigma^{-1})(I_p - \hat{U} U^T) + \hat{\sigma}^{-1}(\hat{U} \hat{U}^T - U U^T).
$$

(B.21)
Now consider the term \((\hat{\sigma}^{-1} - \sigma^{-1})(I_p - \mathbf{UU}^T)\delta\) obtained by combining the expressions in (B) and (II). The covariance matrix for \(\hat{\sigma}\) is \(n^{-1}\Sigma\) and hence \((I_p - \mathbf{UU}^T)\delta\) satisfies Eq. (5.4) with covariance matrix \(n^{-1}(I_p - \mathbf{UU}^T)\). Therefore, by Bernstein inequality, there exists a constant \(C > 0\) such that with probability at least \(1 - O(p^{-2})\),

\[
\| (I_p - \mathbf{UU}^T)\delta \|_\infty \leq C\sigma\sqrt{\frac{\ln p}{n}}.
\]

Furthermore, from Lemma 1, we have with probability at least \(1 - O(p^{-2})\) that

\[
|\hat{\sigma}^{-1} - \sigma^{-1}| = \frac{|\hat{\sigma}^2 - \sigma^2|}{\hat{\sigma}\sigma(\hat{\sigma} + \sigma)} \leq C\sqrt{\frac{\ln p}{n}}. \tag{B.22}
\]

Combining the above bounds, we obtain

\[
\| (\hat{\sigma}^{-1} - \sigma^{-1})(I_p - \mathbf{UU}^T)\delta \|_\infty \leq C\frac{\ln p}{n}. \tag{B.23}
\]

with probability at least \(1 - O(p^{-2})\).

We next consider the term \((\hat{\sigma}^{-1} - \sigma^{-1})(I_p - \mathbf{UU}^T)(\mu_2 - \mu_1)\). Recall that if \(\mathcal{U}\) has bounded coherence as in Condition 4 then \(\|I_p - \mathbf{UU}^T\|_\infty \leq (1 + C_\mathcal{U})\sqrt{d}\) where \(C_\mathcal{U}\) is the constant appearing in Condition 4. We therefore have, by Lemma 1, that

\[
\| (\hat{\sigma}^{-1} - \sigma^{-1})(I_p - \mathbf{UU}^T)\delta \|_\infty \leq \| (\hat{\sigma}^{-1} - \sigma^{-1})(I_p - \mathbf{UU}^T)\|_\infty \leq (1 + C_\mathcal{U})\sqrt{d} \times \|\delta\|_\infty \leq C\sqrt{\frac{\ln p}{n}} \times \|\delta\|_\infty,
\]

with probability at least \(1 - O(p^{-2})\).

We now focus our effort on the terms involving \(\hat{\mathcal{U}}\hat{\mathcal{D}}\hat{\mathcal{U}}^T - \mathcal{U}\mathcal{D}\mathcal{U}^T\). Recall the definition of the orthogonal matrix \(\Xi\) which minimizes \(\|W - \mathcal{U}^T\hat{\mathcal{U}}\|_F\) among all \(d \times d\) orthogonal matrices \(W\). We then have

\[
\begin{align*}
\hat{\mathcal{U}}\hat{\mathcal{D}}\hat{\mathcal{U}}^T - \mathcal{U}\mathcal{D}\mathcal{U}^T &= (\hat{\mathcal{U}} - \hat{\mathcal{U}}^T\Xi)^T\hat{\mathcal{D}}\hat{\mathcal{U}}^T + \hat{\mathcal{U}}^T\hat{\mathcal{D}}\hat{\mathcal{U}}^T - \mathcal{U}\mathcal{D}\mathcal{U}^T \\
&= \left[(\hat{\mathcal{U}} - \mathcal{U}\Xi) - \mathcal{U}(\mathcal{U}^T\hat{\mathcal{U}} - \Xi)\right]\hat{\mathcal{D}}\hat{\mathcal{U}}^T + \hat{\mathcal{U}}^T\hat{\mathcal{D}}\hat{\mathcal{U}}^T - \mathcal{U}\mathcal{D}\mathcal{U}^T
\end{align*}
\]

We first recall a few elementary but useful algebraic facts that are used frequently in the subsequent derivations.

**Fact 1.**

\[
\begin{align*}
\|\mathcal{U}^T\hat{\mathcal{U}} - \Xi\|_2 &\leq \|\sin \Theta(\hat{\mathcal{U}}, \mathcal{U})\|_2^2, \tag{B.24} \\
\|\mathcal{U}^T\mathcal{U}_{\perp}\mathcal{U}_{\perp}^T\|_2 &\leq \|\mathcal{U}^T\mathcal{U}_{\perp}\mathcal{U}_{\perp}^T\|_2 = \|\mathcal{U}^T\mathcal{U}_{\perp}\mathcal{U}_{\perp}^T\|_2 = \|\sin \Theta(\hat{\mathcal{U}}, \mathcal{U})\|_2, \tag{B.25} \\
\|\sin \Theta(\hat{\mathcal{U}}, \mathcal{U})\|_2 &\leq \|\mathcal{U}^T - \mathcal{U}^T\|_2 \leq 2\|\sin \Theta(\hat{\mathcal{U}}, \mathcal{U})\|_2, \tag{B.26} \\
\|\mathcal{U}^T\hat{\mathcal{D}} - \mathcal{U}^T\mathcal{D}\|_2 &\leq \|\mathcal{U}^T(\Sigma - \hat{\Sigma})\|_2 \|\mathcal{H}\|_2. \tag{B.27}
\end{align*}
\]
where $H = (H_{ij})$ is a $d \times d$ matrix with entries

$$H_{ij} = (\lambda_j + \delta^2)^{-1/2}(\lambda_i + \sigma^2)^{-1/2}((\lambda_j + \delta^2)^{1/2} + (\lambda_i + \sigma^2)^{1/2})^{-1}.$$

Eq. (B.24) is from Lemma 6.7 in Cape et al. (2019) while Eq. (B.25) and Eq. (B.26) are standard results for the sin-$\Theta$ distance between subspaces; see for example Lemma 1 in Cai and Zhang (2016). Eq. (B.27) follows from the following observation

$$(U^T \hat{U} \hat{D} - D U^T \hat{U})_{ij} = (U^T \hat{U})_{ij} (\hat{D}_{jj} - D_{ii})$$

We thus have $U^T \hat{U} \hat{D} - D U^T \hat{U} = (U^T (\Sigma - \hat{\Sigma}) \hat{U}) \circ H$. Therefore, by Schur inequality for Hadamard product (see e.g., Theorem 5.5.1 of Horn and Johnson (1991)), we have

$$\|(U^T (\Sigma - \hat{\Sigma}) \hat{U}) \circ H\|_2 \leq \|(U^T (\Sigma - \hat{\Sigma}) \hat{U})\|_2 \times \|H\|_2.$$

We next state a technical lemma for bounding several terms that appears frequently in our analysis.

**Lemma 2.** Suppose that Condition 1 through Condition 4 are satisfied. Then with probability at least $1 - O(p^{-1})$, the following bounds hold simultaneously

$$\|H\|_2 = O(d^{3/2}p^{-3/2}), \quad \|U^T (\Sigma - \hat{\Sigma}) \hat{U}\|_2 = O(p^{1/2} \ln p), \quad \|U^T (\Sigma - \hat{\Sigma}) \hat{U}\|_2 = O(p^{1/2} \ln p), \quad \|U^T \hat{U} \hat{D} - D U^T \hat{U}\|_2 = O(n^{-1/2}p^{-1/2} \ln p), \quad \|\hat{U} U^T - U U^T\|_2 = O(\sqrt{n^{-1} \ln p}).$$

Eq. (B.29) and Eq. (B.30) follows from the sub-multiplicativity of the spectral norm together with bounds for $\|\Sigma_0 - \Sigma\|$ from Lounici (2014) and Koltchinskii and Lounici (2017). Eq. (B.32) is a consequence of Eq. (B.26) and the Davis-Kahan theorem. Eq. (B.28) follows from Weyl’s inequality and the bound for $\|\Sigma - \hat{\Sigma}\|$. Finally, Eq. (B.27), Eq. (B.28), and Eq. (B.30) together imply Eq. (B.31).

With the above preparations in place, we now resume our proof of Theorem 2. For part 1 of the term (B)-(I), we have, with probability at least $1 - O(p^{-2})$,

$$\left\| \left( \hat{U} - U \Xi \right) - U U^T \hat{U} \left( \Xi - \hat{\Xi} \right) \hat{D} U^T \delta \right\|_\infty \leq (\|U - U\Xi\|_2 \to \infty + \|U\|_2 \to \infty) \|U^T \hat{U} - \Xi\|_2 (\|\hat{D} - D\|_2 + \|\hat{D} - D\|_2) \|U^T \delta\|_2 \leq C \left( \frac{\ln p}{\sqrt{n}} \frac{d^3}{p} + \sqrt{\frac{d \ln p}{n}} \left( \frac{1}{\sqrt{\lambda_1 + \sigma^2}} + \frac{1}{\sqrt{\lambda_2 + \sigma^2}} \right) \sqrt{n} \left( \frac{1}{n_1} + \frac{1}{n_2} \right) \ln p \right)$$

$$= O \left( \frac{\ln p}{\sqrt{n}} \right)$$
For the above inequality, we have used Lemma 1 to bound $\|\mathbf{D}-\mathbf{D}\|_2$ and used Theorem 1 to bound $\|\hat{U}-U\mathbf{D}\|_2 \rightarrow \infty$. Finally we used Eq. (B.24), Eq. (B.26) and Eq. (B.32) to bound $\|\hat{U}^T\mathbf{U}-\Xi\|_2$.

For Part 2 of the term $(B)-(I)$, we have, with probability at least $1-O(p^{-2})$,

$$
\begin{align*}
\|\hat{U}(U^T\hat{U}\hat{D}-DU^T\hat{u})\hat{u}\delta+UDU^T(U\hat{u}^T-I_p)\delta\|_\infty \\
\leq \|U(U^T\hat{U}\hat{D}-DU^T\hat{u})\hat{u}\delta\|_\infty + \|UDU^T(U\hat{u}^T-I_p)\delta\|_\infty \\
\leq \|U\|_{2 \rightarrow \infty} \|U^T\hat{U}\hat{D}-DU^T\hat{u}\|_2 \|\hat{u}\|_2 + \|U\|_{2 \rightarrow \infty} \|D\|_2 \|U^T(U\hat{u}^T-I_p)\|_2 \|\delta\|_2 \\
\leq C \sqrt{\frac{d}{p} \left( \frac{\ln p}{\sqrt{p}} \right)} \sqrt{p \left( \frac{1}{n_1} + \frac{1}{n_2} \right) \ln p} + C \sqrt{\frac{d}{p} \left( \frac{\ln p}{\sqrt{p}} \right) \sqrt{p \left( \frac{1}{n_1} + \frac{1}{n_2} \right) \ln p}} \\
= O(\frac{1}{\sqrt{p}} \ln p)
\end{align*}
$$

(B.34)

In the above derivations, we used eq. (B.31) to bound $\|U^T\hat{U}\hat{D}-DU^T\hat{u}\|_2$ and Eq. (B.25), Eq. (B.26) and Eq. (B.32) to bound $\|U^T(I_p-U\hat{u}^T)\|_2$. The bound for $\|U\|_{2 \rightarrow \infty}$ and $\|D\|_2$ follows from bounded coherence in Condition 4 and the spiked eigenvalues growth rate in Condition 3, respectively.

Combining the bounds in Eq. (B.33) and Eq. (B.34), we obtain $(B)-(I)$ as

$$
\|\hat{U}\hat{D}\hat{u}^T - UD\hat{u}^T\|_\infty = O\left( \frac{1}{\sqrt{p}} \ln \frac{p}{n} \right)
$$

(B.35)

with probability at least $1-O(p^{-2})$. For the term in $(B)-(III)$, similar arguments to that used in bounding $(B)-(I)$ yield

$$
\begin{align*}
\|\hat{\sigma}^{-1}(\hat{u}\hat{u}^T - U\hat{u}^T)\delta\|_\infty \\
\leq \|\hat{\sigma}^{-1}((\hat{u} - U\mathbf{D}) - U(U^T\hat{u} - \Xi))\hat{u}^T\delta\|_\infty + \|\hat{\sigma}^{-1}U\hat{u}^T(U\hat{u}^T-I_p)\delta\|_\infty \\
\leq C \sqrt{\left( \frac{\ln p \cdot \frac{d^3}{p}}{n} + \sqrt{\frac{d \cdot \ln p}{p \cdot n}} \right) \sqrt{p \left( \frac{1}{n_1} + \frac{1}{n_2} \right) \ln p} + C \sqrt{\frac{d}{p} \left( \frac{\ln p}{\sqrt{p}} \right) \sqrt{p \left( \frac{1}{n_1} + \frac{1}{n_2} \right) \ln p}} \\
= O\left( \frac{\ln p}{n} \right)
\end{align*}
$$

(B.36)

with probability at least $1-O(p^{-2})$. In the above derivations we have used Lemma 1 to show that $\hat{\sigma}^{-1}$ is bounded away from 0 by some constant not depending on $p$ and $n$.

Recall that $\Delta \mu = \mu_2 - \mu_1 = \Sigma^{1/2} \zeta$. We now replace $\delta$ with $\Sigma^{1/2} \zeta$ in the arguments to derive Eq. (B.33), Eq. (B.34) and Eq. (B.36), the terms $(C)-(I)$ and $(C)-(III)$ are obtained as

$$
\|\hat{U}\hat{D}\hat{u}^T - UD\hat{u}^T\|_{\Sigma^{1/2} \zeta} = O\left( \frac{1}{\sqrt{p}} \sqrt{\ln \frac{p}{n} \|\zeta\|_2} \right)
$$

(B.37)
Table 14. Asymptotic Order of Each Term:

| Expression | $\mathbf{v} = \delta$ | $\mathbf{v} = \Sigma^{1/2} \zeta$ | Corresponding Terms |
|------------|----------------------|-------------------------------|---------------------|
| $\|\mathbf{W}\mathbf{v}\|_\infty$ | $\sqrt{\ln \frac{p}{n}}$ | n.a. | (A) |
| $\|\mathbf{[U}^T \tilde{U} - \mathbf{U} \tilde{U}^T]\mathbf{v}\|_\infty$ | $\frac{1}{\sqrt{p}} \ln \frac{p}{n}$ | $\frac{1}{\sqrt{p}} \sqrt{\ln \frac{p}{n}} \|\zeta\|_2$ | (B)-(I) and (C)-(I) |
| $\|\mathbf{[\bar{\sigma}^{-1} - \sigma^{-1}(\mathcal{I}_p - \mathbf{U} \tilde{U}^T)\mathbf{v}\|_\infty}$ | $\frac{1}{\sqrt{p}} \ln \frac{p}{n}$ | $\sqrt{\ln \frac{p}{n}} \|\zeta\|_\infty$ | (B)-(III) and (C)-(II) |
| $\|\tilde{\mathbf{U}}^T - \mathbf{U}^T\mathbf{v}\|_\infty$ | $\frac{1}{\sqrt{p}} \ln \frac{p}{n} \sqrt{\ln \frac{p}{n}} \|\zeta\|_2$ | (B)-(III) and (C)-(III) |

and

$$|\tilde{\sigma}^{-1}(\tilde{\mathbf{U}}^T - \mathbf{U}^T)\Sigma^{1/2} \zeta\|_\infty = \mathcal{O}\left(\sqrt{\ln \frac{p}{n}} \|\zeta\|_2\right)$$

(B.38)

with probability at least $1 - \mathcal{O}(p^{-2})$. A brief summary of the asymptotic order for the terms (A), (B)-(I) through (B)-(III) and (C)-(I) through (C)-(III) are provided in Table B.3.

**Corollary 1.** Suppose that Condition 1 through Condition 4 are satisfied. Let $\mathbf{v}$ be either a fixed vector in $\mathbb{R}^p$ or a $p$-variate sub-Gaussian random vector with $\mathbb{E}[\mathbf{v}] = \mathbf{0}$. We then have

$$\|\mathbf{W} - \mathbf{W}\|_{\mathbb{F}} = \begin{cases} \mathcal{O}\left(\ln p \sqrt{n^{-1}} \max_i [\text{Var}[\mathbf{v}]]_{ii}\right) & \text{if } \mathbf{v} \text{ is a sub-Gaussian vector} \\ \mathcal{O}\left(\sqrt{n^{-1} \ln p} \|\Sigma^{-1/2} \mathbf{v}\|_2\right) & \text{if } \mathbf{v} \text{ is a constant vector} \end{cases}$$

with probability at least $1 - \mathcal{O}(p^{-2})$, where $[\text{Var}[\mathbf{v}]]_{ii}$ is the variance of the $i^{th}$ coordinate of $\mathbf{v}$.

**Corollary 2.** Suppose that Condition 1 through Condition 4 are satisfied. Let $\mathbf{v}$ be a $p$-variate sub-Gaussian random vector with $\text{Var}[\mathbf{v}] = c n^{-1} \Sigma$ for some finite $c > 0$. We then have

$$\|\mathbf{W} - \mathbf{W}\|_{\mathbb{F}} = \mathcal{O}\left(\sqrt{n^{-1} \ln p}\right)$$

with probability at least $1 - \mathcal{O}(p^{-2})$.

Corollary 1 and Corollary 2 summarize the results in the proof of Theorem 2 for more general sub-Gaussian vector. The proofs follow analogously.

**B.4. Proof of Theorem 3**

For simplicity of notation we will write $\tilde{S}$ instead of $\tilde{S}_\zeta$ since Theorem 3 only depends on the whitened vector $\zeta$. Now recall the definition of $\tilde{S}$ as

$$\tilde{S} = \{j : |\tilde{\zeta}_j| > t_n\}$$

where $t_n$ satisfies $t_n = C(n^{-1} \ln p)^\alpha$ for some constants $C > 0$ and $0 < \alpha < \frac{1}{2}$. We first show that $\tilde{S} = \tilde{S}$ asymptotically almost surely.
By Theorem 2 there exists a choice of \( C \) such that if \( \beta_n = C \sqrt{n^{-1} \ln p} \) then

\[
\Pr\left( \bigcup_{j=1}^{p} \{|\zeta_j - \hat{\zeta}_j| > \beta_n\} \right) = O(p^{-2}).
\]

Now suppose \( S^c \cap \tilde{S} \neq \emptyset \). Then there exists a \( j \) such that \( \zeta_j = 0 \) and \( |\hat{\zeta}_j| > t_n \) and for this \( j \) we have \( |\zeta_j - \hat{\zeta}_j| > t_n > \beta_n \), provided that \( n \) is sufficiently large. We thus have

\[
\Pr(S^c \cap \tilde{S} \neq \emptyset) \leq \Pr\left( \bigcup_{j=1}^{p} \{|\zeta_j - \hat{\zeta}_j| > \beta_n\} \right) = O(p^{-2}). \tag{B.39}
\]

Similarly, if \( S \cap \tilde{S}^c \neq \emptyset \) then there exist a \( j \) such that \( |\zeta_j| > C_0 \) and \( |\hat{\zeta}_j| \leq t_n \). Recall that \( C_0 > 0 \) is the constant appearing in Condition 2; in particular \( K \) does not depend on \( n \) and \( p \). By the reverse triangle inequality, \( |\zeta_j - \hat{\zeta}_j| > C_0 - t_n > \beta_n \) for some \( j \) and hence

\[
\Pr(S \cap \tilde{S}^c \neq \emptyset) \leq \Pr\left( \bigcup_{j=1}^{p} \{|\zeta_j - \hat{\zeta}_j| > \beta_n\} \right) = O(p^{-2}). \tag{B.40}
\]

Combining Eq. (B.39) and Eq. (B.40) yields \( \Pr(S \neq \tilde{S}) = O(p^{-2}) \) and hence, as \( p \to \infty \), \( S = \tilde{S} \) asymptotically almost surely.

We now show that the error rate for the PCLDA rule converges to the Bayes error rate \( R_F \) asymptotically almost surely. Recall the definition of the PCLDA rule in Eq. (2.8). Then to show that \( R_{PCLDA} \to R_F \), it is sufficient to show that

\[
\hat{\zeta}_S^\top [\hat{W}(\mathbf{Z} - \bar{X}_1 + \bar{X}_2)] S - \zeta_S^\top [W(\mathbf{Z} - \frac{\mu_1 + \mu_2}{2})] S \to 0, \tag{B.41}
\]

\[
\ln \frac{n_1}{n_2} \to \ln \frac{\pi_1}{1 - \pi_1}. \tag{B.42}
\]

Here the convergence in Eq. (B.41) is with respect to a random testing data point \( \mathbf{Z} \sim \pi_1 \mathcal{N}(\mu_1, \Sigma) + (1 - \pi_1) \mathcal{N}(\mu_2, \Sigma) \) together with the training data and the convergence in Eq. (B.42) is with respect to the training data only. Note that Eq. (B.42) follows directly from the strong law of large numbers. We thus focus our effort on showing Eq. (B.41).

Let us now condition on the event \( \tilde{S} = S \). We then have

\[
|\hat{\zeta}_S^\top [\hat{W}(\mathbf{Z} - \bar{X}_1 + \bar{X}_2)] S - \zeta_S^\top [W(\mathbf{Z} - \frac{\mu_1 + \mu_2}{2})] S| \leq s_0 \| [\hat{W}(\mathbf{Z} - \bar{X}_1 + \bar{X}_2)] S - W(\mathbf{Z} - \frac{\mu_1 + \mu_2}{2})] S \|_\infty \| \zeta - \hat{\zeta} \|_\infty + s_0 \| [W(\mathbf{Z} - \frac{\mu_1 + \mu_2}{2})] S \|_\infty \| \zeta - \hat{\zeta} \|_\infty. \tag{B.43}
\]

The bounds for \( \ell_\infty \) norm of \( \zeta \) and \( \hat{\zeta} - \zeta \) have been addressed in Condition 2 and it suffices to bound two pieces

\[
(D) = \| [\hat{W}(\mathbf{Z} - \bar{X}_1 + \bar{X}_2)] S \|_\infty
\]

\[
(E) = \| W(\mathbf{Z} - \frac{\mu_1 + \mu_2}{2})] S \|_\infty
\]
in Eq.(B.44), Eq.(B.45) and Eq.(B.46). Now write $Z = \mu_z + \Sigma^{1/2}\epsilon_z$ where $\mu_z = \mu_1$ if $Z$ is sampled from class 1 and $\mu_z = \mu_2$ otherwise.

Firstly, the term $\|[(\hat{W} - W)\Sigma^{1/2}\epsilon_z]_S\|_\infty$ can be analyzed using the decomposition for $\hat{W} - W$ given in (B.21) together with similar arguments to that for deriving (B.23), (B.33), (B.34) and (B.36). We therefore have, with probability at least $1 - \mathcal{O}(n^{-2})$, that

$$
\|[(\hat{W} - W)\Sigma^{1/2}\epsilon_z]_S\|_\infty = \mathcal{O}\left(\sqrt{\frac{\ln n \ln p}{n}}\right) \quad (B.47)
$$

Secondly, for the term $(D)$, using Corollary 1, Corollary 2 and (B.47), we have, with probability at least $1 - \mathcal{O}(n^{-2})$

$$
\left\|\hat{W}(Z - \bar{X}_1 + \bar{X}_2) - W(Z - \mu_1 + \mu_2)\right\|_\infty \\
\leq \left\|[(\hat{W} - W)\Sigma^{1/2}\epsilon_z]_S\|_\infty + \|W\mu_1\|_\infty + \frac{1}{2}\|W\mu_2\|_\infty + \frac{1}{2}\|W\mu_2 - W\mu_1\|_\infty
\leq C\left(\sqrt{\frac{\ln n \ln p}{n}} + \sqrt{\frac{\ln p}{n}} + \sqrt{\frac{\ln p}{n}}\right)
= \mathcal{O}\left(\sqrt{\frac{\ln n \ln p}{n}}\right).
$$

Thirdly, by Condition 2, the term $(E)$ can be bounded as

$$
\left\|[W(Z - \frac{\mu_1 + \mu_2}{2})]_S\|_\infty \leq \|W(\mu_z - \frac{\mu_1 + \mu_2}{2})\|_\infty + \left\|[W(Z - \mu_z)]_S\|_\infty
\leq \frac{1}{2}\|\zeta\|_\infty + \|\epsilon_z\|_\infty
= \vartheta(Z)
$$

where $[\epsilon_z]_S$ is a mean 0 sub-Gaussian vector in $\mathbb{R}^{s_0}$ and $\text{Var}[\epsilon_z]_S = I_{s_0}$. The term $\vartheta(Z)$ is thus bounded in probability.

Combining the above bounds, we conclude that with probability at least $1 - \mathcal{O}(n^{-2})$, $\tilde{S} = S$ and simultaneously

$$
\left|\hat{\zeta}^T_S \left[(\hat{W}(Z - \frac{\bar{X}_1 + \bar{X}_2}{2})]_S - \zeta^T_S \left[W(Z - \frac{\mu_1 + \mu_2}{2})\right]_S\right]\right| \leq C_{S_0}\left(\sqrt{\frac{\ln n \ln p}{n}}\|\zeta\|_\infty + \vartheta(Z)\sqrt{\frac{\ln p}{n}}\right),
$$

and hence, for $\ln n \ln p = o(n)$, we have

$$
\left|\hat{\zeta}^T_S \left[(\hat{W}(Z - \frac{\bar{X}_1 + \bar{X}_2}{2})]_S - \zeta^T_S \left[W(Z - \frac{\mu_1 + \mu_2}{2})\right]_S\right]\right| \to 0
$$
as desired.