De-Biasing Covariance-Regularized Discriminant Analysis

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Abstract

Fisher's Linear Discriminant Analysis (FLD) is a well-known technique for linear classification, feature extraction and dimension reduction. The empirical FLD relies on two key estimations from the data – the mean vector for each class and the (inverse) covariance matrix. To improve the accuracy of FLD under the High Dimension Low Sample Size (HDLSS) settings, *Covariance-Regularized FLD* (CRLD) has been proposed to use shrunken covariance estimators, such as Graphical Lasso, to strike a balance between biases and variances. Though CRLD could obtain better classification accuracy, it usually incurs bias and converges to the optimal result with a slower asymptotic rate. Inspired by the recent progress in de-biased Lasso, we propose a novel FLD classifier, **DBLD**, which improves classification accuracy of CRLD through *de-biasing*. Theoretical analysis shows that **DBLD** possesses better asymptotic properties than CRLD. We conduct experiments on both synthetic datasets and real application datasets to confirm the correctness of our theoretical analysis and demonstrate the superiority of **DBLD** over classical FLD, CRLD and other downstream competitors under HDLSS settings.

1 Introduction

Fisher's Linear Discriminant Analysis (FLD) [Duda *et al.*, 2001] is a well-known technique for feature extraction and dimension reduction [Kulis and others, 2013]. It has been widely used in many applications, such as face recognition [Peck and Van Ness, 1982], image retrieval, etc. An intrinsic limitation of classical FLD is that its objective function relies on the *well-estimated* and *non-singular* covariance matrices. For many applications, such as the micro-array data analysis, all scatter matrices can be *singular* or *ill-posed* since the data is often with high dimension but low sample size (HDLSS) [Cai *et al.*, 2016].

The classical FLD classifier relies on two key parameters – the mean vector of each type and the precision matrix. Under the HDLSS settings, the sample precision matrix (a.k.a., the inverse of sample covariance matrix) used in FLD is usually ill-estimated and quite different from the inverse of population/true covariance matrix [Cai *et al.*, 2016]. For example, the largest eigenvalue of the sample covariance matrix is not a consistent estimate of the largest eigenvalue of the population covariance matrix, and the eigenvectors of the sample covariance matrix can be nearly orthogonal to the truth when the number of dimensions is greater than the number of samples [Marčenko and Pastur, 1967]. Such inconsistency between the true and the estimated precision matrices degrades the accuracy of FLD classifiers under the HDLSS settings [Zollanvari and Dougherty, 2013].

A plethora of excellent work has been conducted to address such HDLSS data classification problem for FLD. For example, Krzanowski et al. [Krzanowski *et al.*, 1995] suggested to use pseudo-inverse to approximate the inverse covariance matrix, when the sample covariance matrix is singular. However, the precision of pseudo-inverse FLD is usually low and not well guaranteed. Other techniques include the two-stage algorithm PCA+FLD [Ye *et al.*, 2004], FLD based on Kernels [Zhang and others, 2003] and/or other non-parametric statistics [Kaski and Peltonen, 2003]. To overcome the singularity of the sample covariance matrices, instead of estimating inverse covariance matrix and mean vectors separately, [Cai and Liu, 2011] proposed to estimate the projection vector for discrimination directly. More popularly, regularized FLD approaches [Krzanowski *et al.*, 1995; Witten and Tibshirani, 2009] are proposed to solve the problem. These methods can improve the performance of FLD either empirically or theoretically [Durrant and Kabán, 2015; Bickel *et al.*, 2004], while few of them can directly address the ill-estimated inverse covariance matrix estimation issue.

One representative regularization approach is *Covariance-Regularized FLD* [Witten and Tibshirani, 2009] that replaces the precision matrix used in FLD with a shrunken estimator, such as Graphical Lasso [Friedman *et al.*, 2008], so as to achieve a *"superior prediction"*. Intuitively, through replacing precision matrix used in FLD with a sparse regularized estimation, the ill-posed problem caused by the HDLSS settings can be well addressed. The sparse estimators usually converge to the inverse of true/population covariance matrix faster than the sample estimators [Cai *et al.*, 2016]. With the asymptotic properties, the sparse FLD should be close to the optimal FLD. However, the way that the sparsity and the convergence rate of the precision matrix estimator would affect the classification

accuracy is not well studied in literature.

Further, with induced sparsity, the inverse covariance estimator becomes biased [Zhang and Zhang, 2014]. The performance of sparse FLD is frequently bottlenecked due to the bias of the sparse estimators. Recently, researchers tried to de-bias the Lasso estimator [Zhang and Zhang, 2014], through adjusting the ℓ_1-penalty for the regularized estimation, so as to achieve a better regression performance. Inspired by this line of research, we propose to improve sparse FLD through de-biasing (i.e., de-sparsifing) in this paper.

Our Contributions. With respect to the aforementioned issues, in this paper, we made the following contributions.

1. Inspired by De-biased Lasso [Javanmard and Montanari, 2014], we study the problem of de-biasing the Covariance-Regularized FLD (CRLD), which has been widely-used for empirical sparse FLD estimation, for performance improvement. To the best of our knowledge, this is the first work aiming at de-biasing CRLD.
2. We propose a novel algorithm **DBLD** – De-Biased Fisher's Linear Discriminant Analysis on top of CRLD. **DBLD** leverages yet-another De-Biased Estimator for *linear classification* problem, to re-balance the variances and biases of the estimation, through de-sparsifying the projection vector obtained by CRLD.
3. Our theoretical analysis shows, under certain mild assumptions, **DBLD** converges faster than CRLD with sharp asymptotic rate. We also conduct extensive experiments to demonstrate the advantage of the proposed algorithms over other competitors. The results validate the correctness of our theoretical analysis.

Notations. Following key notations are used in the rest of this paper: Given a p-dimensional vector $\mathbf{v} \in \mathbb{R}^p$, we denote the $\ell_{\mathcal{P}}$ vector-norm as $|\mathbf{v}|_{\mathcal{P}} = (\sum_{i=1}^{m} |\mathbf{v}_i|^{\mathcal{P}})^{1/\mathcal{P}}$ ($\mathcal{P}$ is a non-negative integer) and the ℓ_∞ vector-norm as $|\mathbf{v}|_\infty = \max_{1\leq i\leq m}\{|\mathbf{v}_i|\}$. Given a matrix $\mathbf{A} \in \mathbb{R}^{m_1\times m_2}$, we denote the $\ell_{\mathcal{P}}$ matrix-norm as $||\mathbf{A}||_{\mathcal{P}} = \max_{\mathbf{v}\in\mathbb{R}^p}\{|\mathbf{A}\mathbf{v}|_{\mathcal{P}}/|\mathbf{v}|_{\mathcal{P}}\}$. Note that the symbol p refers to the number of dimensions of the data while m refers to the number of samples. The operator $\mathcal{O}_p(\cdot)$ refers to the big-O-notation in high probability.

2 Preliminaries

In this section, we first briefly introduce the binary classifier using FLD, then present the practice of CRLD based on Graphical Lasso.

2.1 FLD for Binary Classification

To use the Fisher's Linear Discriminant Analysis (FLD), given the $i.i.d.$ labeled data pairs $(x_1, \ell_1) \dots (x_m, \ell_m)$, we first estimate the sample covariance matrix $\bar{\Sigma}$ using the pooled sample covariance matrix estimator with respect to the two classes [Duda *et al.*, 2001], then estimate the sample precision matrix as $\bar{\Theta} = \bar{\Sigma}^{-1}$. Further, $\bar{\mu}_+$ and $\bar{\mu}_-$ are estimated as the mean vectors of the positive samples and the negative samples in the m training samples, respectively.

Given all estimated parameters $\bar{\Sigma}$ (and $\bar{\Theta} = \bar{\Sigma}^{-1}$), $\bar{\mu}_+$ and $\bar{\mu}_-$, the FLD model classifies a new data vector x as the result of:

$$\begin{aligned} \bar{f}(x) &= \underset{\ell\in\{-,+\}}{\operatorname{argmax}}\ \delta(x, \bar{\Theta}, \bar{\mu}_\ell, \pi_\ell), \ \textbf{where} \\ \delta(x,\bar{\Theta}, \bar{\mu}_\ell, \pi_\ell) &= x^\top \bar{\Theta}\bar{\mu}_\ell - \frac{1}{2}\bar{\mu}_\ell^\top \bar{\Theta}\bar{\mu}_\ell + \log \pi_\ell, \end{aligned} \tag{1}$$

where π_+ and π_- refer to the (foreknown) frequencies of positive samples and negative samples in the whole population, respectively.

2.2 Covariance-Regularized FLD via Graphical Lasso

This algorithm, referred to as the Covariance-Regularized FLD (CRLD) via Graphical Lasso, was derived from the *Scout family* of FLD introduced by *Witten et al.* in [Witten and Tibshirani, 2009]. Compared to the classical FLD, this baseline algorithm leverages Graphical Lasso estimator to replace the precision matrix estimated using sample covariance matrix. The proposed algorithm is implemented using the discriminant function defined in Eq. 1, as:

$$\widehat{f}(x) = \underset{\ell\in\{-,+\}}{\operatorname{argmax}}\ \delta(x, \widehat{\Theta}, \bar{\mu}_\ell, \pi_\ell), \tag{2}$$

where $\widehat{\Theta}$ refers to the Graphical Lasso estimator based on the sample covariance matrix $\bar{\Sigma}$:

$$\widehat{\Theta} = \underset{\Theta>0}{\operatorname{argmin}} \left(\operatorname{tr}(\bar{\Sigma}\Theta) - \log\det(\Theta) + \lambda \sum_{j\neq k} |\Theta_{jk}| \right). \tag{3}$$

Note that, as a linear classifier, the CRLD decision rule introduced in Eq. 2 can be re-formulated in a linear model, such as:

$$\begin{aligned} \widehat{f}(x) &= \operatorname{sign}\left(\delta(x, \widehat{\Theta}, \bar{\mu}_+, \pi_+) - \delta(x, \widehat{\Theta}, \bar{\mu}_-, \pi_-)\right) \\ &= \operatorname{sign}\left(x^\top \widehat{\beta}^G + c^g\right), \end{aligned} \tag{4}$$

where $\operatorname{sign}(\cdot)$ function returns $+1$ if the input is non-negative, and -1 when the input is negative. The vector $\widehat{\beta}^G = \widehat{\Theta}(\bar{\mu}_+ - \bar{\mu}_-)$ and the scalar $c^g = -\frac{1}{2}\cdot(\bar{\mu}_+ + \bar{\mu}_-)^\top \widehat{\beta}^G + log(\pi_+/\pi_-)$. Obviously, $\widehat{\beta}^G$ is the vector of projection coefficients for linear classification.

In this paper, we present the analytical results (i.e., statistical rate of convergence that $\widehat{\beta}^G$ approximates to the optimal projection vector with varying number of samples n and dimensions p) of CRLD in **Theorem 1**.

3 The Proposed Algorithm

In this section, we introduce our proposed algorithm **DBLD**—$\mathcal{D}$e-$\mathcal{B}$iased Fisher's $\mathcal{L}$inear $\mathcal{D}$iscriminant Analysis (via Graphical Lasso), then present the theoretical analysis on the theoretical properties of the proposed algorithms.

3.1 DBLD: The De-Biased Estimation for Covariance-Regularized FLD

Given the $i.i.d.$ labeled data pairs $(x_1, \ell_1) \dots (x_m, \ell_m)$ drawn from the two classes with certain priors, as shown in Algorithm 1. The algorithm first **(i)** estimates the sample estimation

of covariance matrices and the mean vectors, then **(ii)** leverages CRLD to estimate the shrunken projection vector $\widehat{\beta}^G$. Further, **DBLD (iii)** proposes a de-biased estimator (denoted as DeBias function) to de-bias $\widehat{\beta}^G$ and obtain the projection vector $\widehat{\beta}^D$. Finally, we introduce a decision rule that enables classification using the estimated $\widehat{\beta}^D$.

Algorithm 1 **DBLD** Estimation Algorithm

1: **procedure** **DBLD**$((x_1, \ell_1) \dots (x_m, \ell_m))$
2: /*(i) Sample Estimators for Mean and Covariance */
3: $\mathbb{X}_+ \leftarrow \text{PositiveSampleSet}((x_1, \ell_1)..(x_m, \ell_m))$;
4: $\mathbb{X}_- \leftarrow \text{NegativeSampleSet}((x_1, \ell_1)..(x_m, \ell_m))$;
5: $\bar{\mu}_+ \leftarrow \frac{1}{|\mathbb{X}_+|} \cdot \sum_{x \in \mathbb{X}_+} x$, $\bar{\mu}_- \leftarrow \frac{1}{|\mathbb{X}_-|} \cdot \sum_{x \in \mathbb{X}_-} x$;
6: $\bar{\Sigma}_+ \leftarrow \frac{1}{|\mathbb{X}_+|} \cdot \sum_{x \in \mathbb{X}_+} (x - \bar{\mu}_+)(x - \bar{\mu}_+)^\top$;
7: $\bar{\Sigma}_- \leftarrow \frac{1}{|\mathbb{X}_-|} \cdot \sum_{x \in \mathbb{X}_-} (x - \bar{\mu}_-)(x - \bar{\mu}_-)^\top$;
8: $\bar{\mu} \leftarrow \frac{|\mathbb{X}_+| \cdot \bar{\mu}_+ + |\mathbb{X}_-| \cdot \bar{\mu}_-}{|\mathbb{X}_+| + |\mathbb{X}_-|}$, $\bar{\Sigma} \leftarrow \frac{|\mathbb{X}_+| \cdot \bar{\Sigma}_+ + |\mathbb{X}_-| \cdot \bar{\Sigma}_-}{|\mathbb{X}_+| + |\mathbb{X}_-|}$;
9: /*(ii) CRLD Estimator (to obtain $\widehat{\beta}^G$) */
10: $\widehat{\Theta} \leftarrow \text{GraphicalLasso}(\bar{\Sigma}, \lambda)$;
11: $\widehat{\beta}^G \leftarrow \widehat{\Theta}(\bar{\mu}_+ - \bar{\mu}_-)$;
12: /*(iii) **DBLD** Estimator (to obtain $\widehat{\beta}^D$) */
13: $\mathbf{X} \leftarrow [x_1, x_2, ...x_m]$; /*$p \times m$ matrix */
14: $\mathbf{L} \leftarrow [\ell_1, \ell_2, \dots \ell_m]^\top$; /*$m \times 1$ matrix */
15: $\mathbf{U} \leftarrow [\bar{\mu}, \bar{\mu}, \dots \bar{\mu}]$;
16: /*$\mathbf{U}$ is an $m \times p$ matrix, every column is $\bar{\mu}$*/
17: $c \leftarrow -\bar{\mu}^\top \widehat{\beta}^G$;
18: $\mathbf{C} \leftarrow [c, c, \dots, c]^\top$;
19: /*$\mathbf{C}$ is a $m \times 1$ matrix, every row is c*/
20: $\widehat{\beta}^D \leftarrow \widehat{\beta}^G + \frac{1}{m} \cdot \widehat{\Theta}(\mathbf{X} - \mathbf{U}) \left(2 \cdot \mathbf{L} - \mathbf{X}^\top \widehat{\beta}^G - \mathbf{C}\right)$
21: **return** $\widehat{\beta}^D$;

In the following section, we present the design of the De-Biased Estimator (denoted as DeBiasing function in Algorithm 1) to obtain $\widehat{\beta}^D$, then introduce the decision rule for optimal classification. Later we analyze the theoretical properties of $\widehat{\beta}^D$.

The De-Biased Estimator

Inspired by the De-biased Lasso [Javanmard and Montanari, 2014], we propose to improve the performance of CRLD through de-biasing β^G. Given m labeled training data $(x_1, \ell_1), (x_2, \ell_2), \dots (x_m, \ell_m)$ with balanced labels, the Graphical Lasso estimator $\widehat{\Theta}$ on the data and the CRLD model (i.e., $\hat{\beta}^G$), we propose a novel de-biased estimator of $\hat{\beta}^D$ that takes the form as

$$\widehat{\beta}^D \leftarrow \widehat{\beta}^G + \frac{1}{m} \cdot \widehat{\Theta}(\mathbf{X} - \mathbf{U}) \left(2 \cdot \mathbf{L} - \mathbf{X}^\top \widehat{\beta}^G - \mathbf{C}\right), \quad (5)$$

where we denote $\mathbf{X}$ as an $p \times m$ matrix where $1 \leq i \leq m$ and the i^{th} column is x_i; $\mathbf{L}$ as an $m \times 1$ matrix (i.e., vector) whose i^{th} row is $\ell_i \in \{\pm 1\}$; $\mathbf{U}$ is a $p \times m$ matrix where each column is $\bar{\mu}$ (as line 7 in Algorithm 1); and $\mathbf{C}$ is an $m \times 1$ matrix where each row is c (as line 16 in Algorithm 1).

The DBLD Classifier.

Given the de-biased estimator $\widehat{\beta}^D$, the **DBLD** classifies the input vector x using the following rule:

$$\widehat{f}^D(x) = \text{sign}\left(\left(x^\top - \frac{\bar{\mu}_+ + \bar{\mu}_-}{2}\right)^\top \widehat{\beta}^D + \log(\pi_+/\pi_-)\right). \quad (6)$$

In the following section, we present the analytical results of **DBLD**, including the computational complexity of de-biasing and statistical rate of convergence.

3.2 Complexity Analysis of DBLD

In this section, we analyze the computational complexity for the three steps of **Algorithm** 1. The step (i) estimates the sample covariance matrices and mean vectors, which consumes at most $\mathcal{O}(p^2 \cdot m)$ operations. The step (ii) performs Graphical Lasso and matrix multiplication, where the complexity based on standard implementation [Friedman *et al.*, 2008] is upper-bounded by $\mathcal{O}(p^3)$. The step (iii) de-biasing is implemented as an exact formula with $\mathcal{O}(p^2)$ complexity.

Remark 1. All three steps of **Algorithm** 1 are scalable on both the number of dimensions (p) and the number of training samples (m). The overall complexity of the three steps is $\mathcal{O}(p^3 + p^2 \cdot m)$. Under the HDLSS setting $p > m$, the computational complexity of **DBLD** is upper-bounded by $\mathcal{O}(p^3)$. On the other hand, with large sample setting where $m \geq p$, the worst case computational complexity of **DBLD** is bounded by $\mathcal{O}(p^2 \cdot m)$. Obviously, the proposed de-biasing estimator (i.e., step (iii)) with complexity $\mathcal{O}(p^2)$ would not bound the performance, when compared to the first two steps.

3.3 Convergence Analysis of DBLD

In order to analyze the performance of **DBLD**, we first define the linear projection vector of the optimal FLD as β^*. Given m samples $(x_1, \ell_1), \dots (x_m, \ell_m)$ drawn i.i.d. from $\mathcal{N}(\mu_+^*, \Sigma^*)$ and $\mathcal{N}(\mu_-^*, \Sigma^*)$ with the equal priors for training, the optimal projection vector should be $\beta^* = \Theta^*(\mu_+^* - \mu_-^*)$ and $\Theta^* = \Sigma^{*-1}$. We intend to understand how close $\widehat{\beta}^G$ and $\widehat{\beta}^D$ approximate to the optimal estimation β^*.

Assumption 1. *We follow the assumptions made in [Rothman* et al.*, 2010] that a positive constant K having*

$$1/\mathcal{K} \leq \lambda_{min}(\Sigma^*) \leq \lambda_{max}(\Sigma^*) \leq \mathcal{K}$$

exists. The operators $\lambda_{min}(\cdot)$ and $\lambda_{max}(\cdot)$ denote the smallest and largest eigenvalues respectively. In this way, there exists $\|\Sigma^*\|_2 \leq \mathcal{K}$ and $\|\Theta^*\|_2 \leq \mathcal{K}$.

Assumption 2. *We further follow the assumption that, the data vectors for training are all realized from a random vector X and there exists an constant $\mathcal{B}$ having $|X|_2 \leq \mathcal{B}$. Thus there has $|\bar{\mu}_+|_2 \leq \mathcal{B}$ and $|\bar{\mu}_-|_2 \leq \mathcal{B}$.*

Theorem 1. *With appropriate setting of tuning parameter $\lambda \asymp \sqrt{\log p/m}$ (in Eq 3), the ℓ_2-vector-norm convergence rate of CRLD $\widehat{\beta}^G$ approximating to the optimal estimation β^* is:*

$$|\widehat{\beta}^G - \beta^*|_2 = \mathcal{O}_p\left(\sqrt{\frac{(p+d)\log p}{m}}\right), \quad (7)$$

where $d = max_{1\leq i\leq p}|\{j : \Sigma^{*^{-1}}_{i,j} \neq 0\}|$ refers to the maximal degree of the graph (i.e., population inverse covariance matrix).

Proof. Here, we first prove the upper bound of $|\widehat{\beta}^G - \beta^*|_\infty$. As was defined $\widehat{\beta}^G = \widehat{\Theta}(\bar{\mu}_+ - \bar{\mu}_-)$, then we have:

$$|\widehat{\beta}^G - \beta^*|_2 = |\widehat{\Theta}(\bar{\mu}_+ - \bar{\mu}_-) - \Theta^*(\mu^*_+ - \mu^*_-)|_2. \quad (8)$$

Considering the inequities $|x+y|_2 \leq |x|_2 + |y|_2$ and $|Ax|_2 \leq ||A||_2 \cdot |x|_2$, we have

$$\begin{aligned} |\widehat{\beta}^G - \beta^*|_2 \leq & ||(\widehat{\Theta} - \Theta^*)||_2 \cdot |\bar{\mu}_+ - \bar{\mu}_-|_2 \\ & + \|\Theta^*\|_2 \left(|\bar{\mu}_+ - \mu^*_+|_2 + |\bar{\mu}_- - \mu^*_-|_2\right). \end{aligned} \quad (9)$$

According to [Rothman *et al.*, 2010], when $\lambda \asymp \sqrt{\log p/m}$, we consider the spectral-norm convergence rate $\|\widehat{\Theta} - \Theta^*\|_2 \leq \|\widehat{\Theta} - \Theta^*\|_F = \mathcal{O}_p(\sqrt{(p+d)\cdot \log\ p/m})$, the asymptotic rate of sample mean vector [DasGupta, 2008] is $|\bar{\mu}_+ - \mu^*_+|_2 = \mathcal{O}_p(\sqrt{p/m})$ and $|\bar{\mu}_- - \mu^*_-|_2 = \mathcal{O}_p(\sqrt{p/m})$, with the increasing number of dimensions p and number of samples m.

Further, there has $\|\Theta^*\|_2 \leq \mathcal{K}$ (**Assumption 1**) and ℓ_2-norms of all mean vectors are bounded by $\mathcal{B}$. In this way, there must exist positive constants C_1 and C_2 having:

$$|\widehat{\beta}^G - \beta^*|_2 \leq C_1 \cdot 2\mathcal{B}\sqrt{\frac{(p+d)\log\ p}{m}} + C_2\mathcal{K}\sqrt{\frac{p}{m}}. \quad (10)$$

Thus, according to the definition of asymptotic rate, we conclude the convergence rate as:

$$|\widehat{\beta}^G - \beta^*|_2 = \mathcal{O}_p\left(\sqrt{\frac{(p+d)\log\ p}{m}}\right). \quad (11)$$

□

Theorem 2. *With appropriate setting of tuning parameter λ (in Eq 3), the ℓ_2-vector-norm convergence rate of* **DBLD** $\widehat{\beta}^G$ *approximating to the optimal estimation β^* is:*

$$|\widehat{\beta}^D - \beta^*|_2 = \mathcal{O}_p\left(\sqrt{\frac{p\log\ p}{m}}\right). \quad (12)$$

Proof. Here, we prove the upper bound of $|\widehat{\beta}^D - \beta^*|_\infty$. Consider the definition of the de-biased FLD estimator $\widehat{\beta}^D$ introduced in Eq. 5, we have

$$\begin{aligned} \widehat{\beta}^D = & \widehat{\beta}^G + \frac{2}{m}\cdot\widehat{\Theta}\mathbf{XL} \\ & - \frac{2}{m}\cdot\widehat{\Theta}\mathbf{UL} - \frac{1}{m}\cdot\widehat{\Theta}(\mathbf{X}-\mathbf{U})(\mathbf{X}-\mathbf{U})^\top\widehat{\beta}^G. \end{aligned} \quad (13)$$

With the assumption of equal priors ($\pi_+ = \pi_- = 0.5$), $\mathbf{L}$ is a $m \times 1$ label matrix that half of its elements are $+1$ while the rest are all -1. $\mathbf{X}$ refers to a $p \times m$ matrix, where each column is a sample of data e.g., $x_1, x_2, \ldots, x_m$. As was defined $\widehat{\beta}^G = \widehat{\Theta}(\bar{\mu}_+ - \bar{\mu}_-) = \frac{2}{m}\cdot\widehat{\Theta}\mathbf{XL}$. As $\mathbf{U}$ is a matrix in which each column is a constant vector $(\bar{\mu}_+ + \bar{\mu}_-)/2$ and $\mathbf{L}$ is a vector with half elements as 1 and half elements as -1, thus $\frac{2}{m}\cdot\widehat{\Theta}\mathbf{UL} = \frac{2}{m}\cdot\widehat{\Theta}(\mathbf{UL}) = \mathbf{0}$. As each column of $\mathbf{X}$ refers to a sample drawn from the original data distribution, thus $\frac{1}{m}(\mathbf{X}-\mathbf{U})(\mathbf{X}-\mathbf{U})^\top = \bar{\Sigma}_s$ is the sample covariance matrix estimator. With all above in mind, we have

$$\widehat{\beta}^D = \widehat{\beta}^G + \left(\mathbf{I} - \widehat{\Theta}\bar{\Sigma}_s\right)\widehat{\beta}^G, \quad (14)$$

where $\mathbf{I}$ refers to a $p \times p$ identity matrix. Note that $\left(\mathbf{I} - \widehat{\Theta}\bar{\Sigma}\right)\widehat{\beta}^G$ can be considered as the de-sparsification term that de-biases $\widehat{\beta}^G$. Thus, considering the asymptotic rate of sample mean vector [DasGupta, 2008] is $|\bar{\mu}_+ - \mu^*_+|_2 = \mathcal{O}_p(\sqrt{p/m})$ and $|\bar{\mu}_- - \mu^*_-|_2 = \mathcal{O}_p(\sqrt{p/m})$, we have

$$\begin{aligned} |\widehat{\beta}^D - \beta^*|_2 &\leq \left|\left|\left(2\cdot\mathbf{I} - \widehat{\Theta}\bar{\Sigma}_s\right)\widehat{\Theta} - \Theta^*\right|\right|_2 |\bar{\mu}_+ - \bar{\mu}_-|_2 \\ &\quad + |\Theta^*(\bar{\mu}_+ - \mu^*_+ - \bar{\mu}_- + \mu^*_-)|_2 \\ &\leq 2\mathcal{B}\left|\left|\left(2\cdot\mathbf{I} - \widehat{\Theta}\bar{\Sigma}_s\right)\widehat{\Theta} - \Theta^*\right|\right|_2 + C_2\mathcal{K}\sqrt{\frac{p}{m}}. \end{aligned} \quad (15)$$

According to [Jankova *et al.*, 2015], with appropriate setting of λ, the spectral-norm convergence rate of the de-sparisified estimator $\widehat{\Theta}^D = \left(2\cdot\widehat{\Theta} - \widehat{\Theta}\bar{\Sigma}_s\widehat{\Theta}\right)$ under mild conditions should be $\|\widehat{\Theta}^D - \Theta^*\|_\infty = \mathcal{O}_p(\sqrt{\log\ p/m})$, then there exists $\|\widehat{\Theta}^D - \Theta^*\|_2 = \mathcal{O}_p(\sqrt{p\log\ p/m})$, with the varying number of dimensions p and number of samples m. In this way, with high probability, we conclude the convergence rate:

$$|\widehat{\beta}^D - \beta^*|_2 = \mathcal{O}_p\left(\sqrt{\frac{p\log\ p}{m}}\right). \quad (16)$$

□

Remark 2. Compared to CRLD's projection vector $\widehat{\beta}^G$, our method **DBLD** recovers the linear projection vector $\widehat{\beta}^D$ with a faster asymptotic rate, i.e., $\sqrt{p\log\ p/m}$ v.s. $\sqrt{(p+d)\log\ p/m}$ in a mild condition. Thus, it would benefit to some applications, such as dimensionality reduction and feature selection. Our later experimental results show that **DBLD** outperforms CRLD with higher classification accuracy, due to the faster statistical rate of convergence.

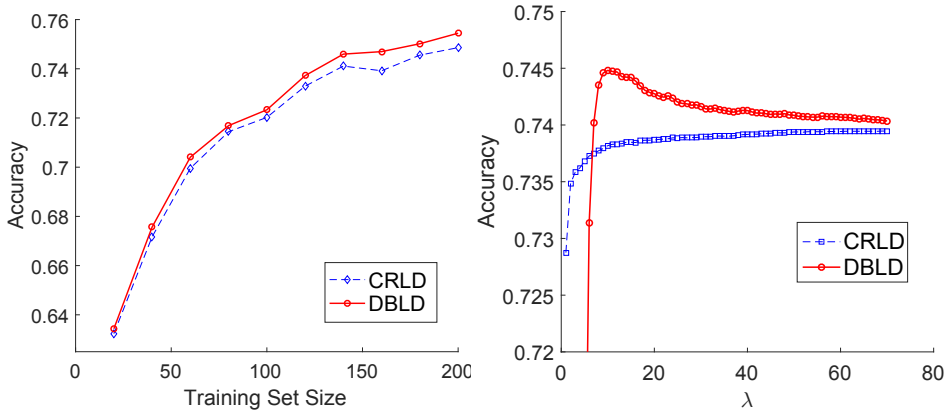
Remark 3. The proposed algorithm provides a *sub-optimal* solution, when compared to [Cai and Liu, 2011]. Our work intend to propose an estimator of β^* through approximating Σ^*, μ^*_+ and μ^*_- separately, while [Cai and Liu, 2011] approximates $\widehat{\beta}^*$ straightforwardly via so-called "direct estimation".

4 Experiments

In this section, we first validate different properties of **DBLD** on the synthesized data. Then, we experimentally evaluate the performance of **DBLD** using several real-world datasets. Experiments show the superiority of **DBLD**.

4.1 Synthesized Data Evaluation

To validate our algorithms, we evaluate our algorithms on a synthesized dataset (imported from [Cai and Liu, 2011]), which is obtained through a pseudo-random simulation. The



(a) **DBLD** vs. CRLD (b) λ Tuning

Figure 1: Classification Accuracy of **DBLD** vs. CRLD on Pseudo-Random Synthesized Data

synthetic data are generated by two predefined Gaussian distributions $\mathcal{N}(\mu_+^*, \Sigma^*)$ and $\mathcal{N}(\mu_-^*, \Sigma^*)$ with equal priors. The settings of μ_+^*, μ_-^* and Σ^* are as follows: Σ^* is a $p \times p$ symmetric and positive-definite matrix, where each element $\Sigma_{i,j}^* = 0.8^{|i-j|}$, $1 \leq i \leq p$ and $1 \leq j \leq p$. μ_+^* and μ_-^* are both p-dimensional vectors, where $\mu_+^* = \langle 1, 1, \ldots, 1, 0, 0, \ldots, 0 \rangle^T$ (the first 10 elements are all 1's, while the rest $p-10$ elements are 0's) and $\mu_-^* = \mathbf{0}$. In our experiment, we set $p = 200$. To simulate the HDLSS settings, we train CRLD and **DBLD**, with 20 to 200 samples randomly drawn from the distributions with equal priors, and test the two algorithms using 500 randomly generated samples. For each settings, we repeat the experiments for 100 times and report the averaged results, in a cross-validation manner.

In this experiment, we compare **DBLD**, CRLD and FLD (with pseudo inverse). The results of FLD is not included here, as it performs extremely worse than both CRLD and **DBLD** under the HDLSS settings. Figure. 1(a) presents the comparison between **DBLD** and CRLD, in terms of accuracy, where each algorithm is fine tuned with the best parameter λ. A detailed example of parameter tuning is reported in Figure. 1(b), where we run both algorithms, with training set size as 160, when varying λ from 1 to 70. From Figure. 1(a), it is obvious that **DBLD** outperforms CRLD marginally. The λ tuning comparison addressed in Figure. 1(b) shows that, given a small λ, both CRLD and **DBLD** cannot perform well, as the sparse approximation of $\widehat{\beta}^G$ and $\widehat{\beta}^D$ cannot be well recovered in such case [Witten and Tibshirani, 2009]. When $\lambda \geq 6$, **DBLD** starts outperforming CRLD, while the advantage of **DBLD** to CRLD decreases when increasing λ. However, even with an extremely large λ, **DBLD** still outperforms CRLD. In Figure 2(a), we present the evaluation results based on unbalanced datasets, where the accuracy of algorithms using $m = 160$ training samples drawn with varying priors is illustrated. The proportion of positive training samples is varying from 10% to 40%. It is obvious that all algorithms achieve their best performance when the proportion of positive training sample is 10% (the most unbalanced case).

To further verify our algorithms, we propose the optimal FLD classifier $\beta^* = \Theta^*(\mu_+^* - \mu_-^*)$, which is all based on the population parameters. We compare the $\widehat{\beta}^D$, $\widehat{\beta}^G$ and $\bar{\beta}$ estimated by **DBLD**, CRLD and FLD (with pseudo-inverse) to β^*. Figure. 2(b) presents the comparison among $|\widehat{\beta}^D - \beta^*|_\infty$, $|\widehat{\beta}^G - \beta^*|_\infty$ and $|\bar{\beta} - \beta^*|_\infty$. It is obvious that $\widehat{\beta}^D$ is more close to β^* than $\widehat{\beta}^G$ and $\bar{\beta}$. This observation further verifies the **Theorem 1** and **2**. We also compare the accuracy of β^* to CRLD, **DBLD** and FLD. β^* outperforms these algorithms and the accuracy of β^* is around 84.4% It is reasonable to conclude that **DBLD** outperforms CRLD, because $\widehat{\beta}^D$ is more close to β^*.

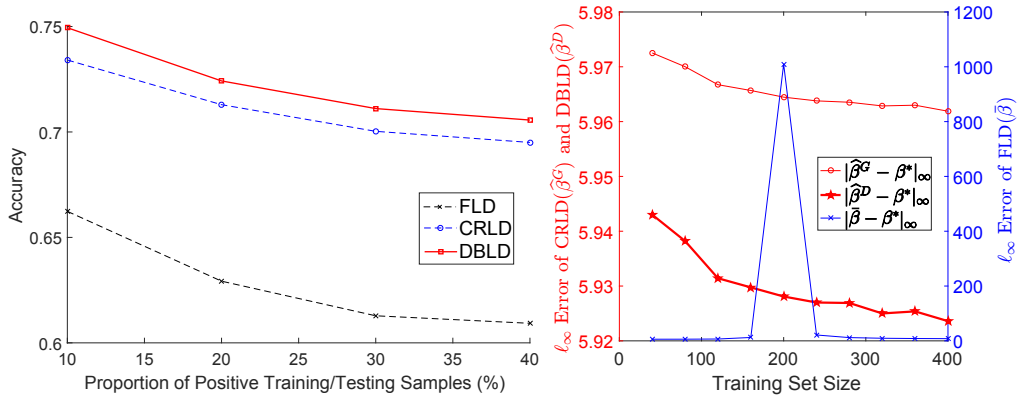
4.2 Benchmark Evaluation Results

In Figure. 3(a), we compare **DBLD** and other FLD algorithms, including FLD with pseudo-inverse, Sparse FLD via Graphical Lasso (CRLD) and Ye-FLD derived from [Ye *et al.*, 2004], on the Web datasets [Lin, 2017]. To simulate the HDLSS settings ($p \gg m$), we vary the training sample sizes from 30 to 120 while using 400 samples for testing. The numbers of dimensions p is 300. For each algorithm, reported result is averaged over 100 randomly selected subsets of the training/testing data with equal priors. CRLD and **DBLD** are fine-tuned with the best λ. The experimental settings show that **DBLD** consistently outperforms other competitors in different settings. The non-monotonic trend of FLD with the increasing training set size is partially due to the poor performance of pseudo inverse used in FLD.

In addition to FLD classifiers, we also compared **DBLD** with other downstream algorithms including *Decision Tree*, *Random Forest*, *Linear Support Vector Machine (SVM)* and *Kernel SVM with Gaussian Kernel*. The comparison results are listed in Figure. 3(b). All algorithms are fine-tuned with the best parameters under our experiment settings.

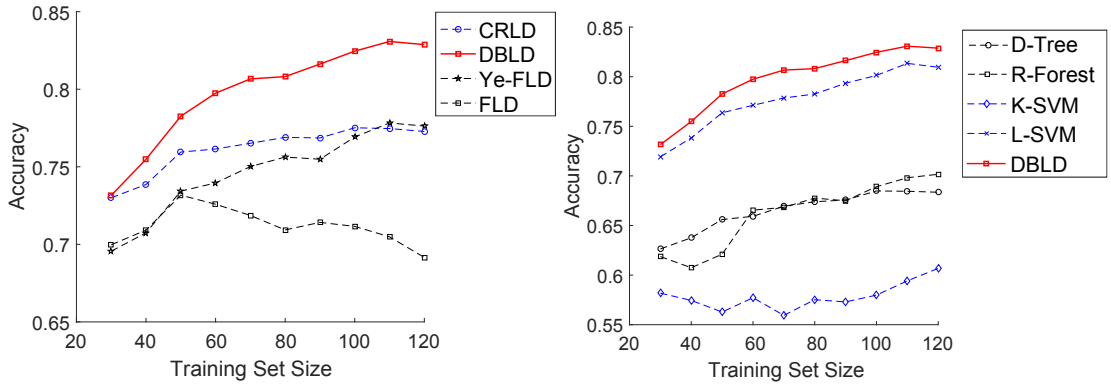
4.3 Early Detection of Diseases on EHR Datasets

To demonstrate the effectiveness of **DBLD** in handling the real problems, we evaluate **DBLD** on the real-world Electronic Health Records (EHR) data for early detection of dis-



(a) Accuracy on Unbalanced Datasets ($m = 160$) (b) Asymptoticity

Figure 2: More Performance Comparison based on Pseudo-Random Synthesized Data



(a) **DBLD** vs. FLDs (b) **DBLD** vs. Downstream

Figure 3: Performance Comparison on Benchmark Datasets ($p = 300$ and $p \gg m$, D-Tree: Decision Tree, R-Forest: Random Forest, K-SVM: Kernel SVM, and L-SVM:Linear SVM)

	Training Set Size						
Algorithm	100	200	300	400	500	600	700
DBLD	**0.659±0.022**	**0.677±0.028**	**0.691±0.024**	**0.692±0.023**	**0.690±0.021**	**0.696±0.024**	**0.701±0.023**
FLD	0.543±0.034	0.586±0.033	0.616±0.022	0.642±0.029	0.642±0.022	0.657±0.025	0.658±0.026
Ye-FLD	0.627±0.050	0.620±0.077	0.652±0.063	0.620±0.067	0.655±0.062	0.637±0.064	0.670±0.045
Decision Tree	0.621±0.046	0.649±0.031	0.652±0.041	0.655±0.030	0.671±0.028	0.665±0.031	0.668±0.040
Linear SVM	0.615±0.026	0.628±0.030	0.647±0.023	0.666±0.029	0.666±0.021	0.670±0.030	0.675±0.029
Kernel SVM	0.635±0.032	0.669±0.027	0.674±0.039	0.678±0.021	0.668±0.038	0.688±0.024	0.682±0.029
AdaBoost	0.631±0.035	0.630±0.039	0.620±0.028	0.622±0.027	0.621±0.022	0.617±0.025	0.626±0.070
CRLD	0.658±0.023	0.676±0.024	0.682±0.028	0.686±0.022	0.683±0.021	0.692±0.025	0.695±0.018
Random Forest	0.590±0.035	0.602±0.035	0.653±0.031	0.602±0.040	0.674±0.024	0.666±0.026	0.658±0.032

Table 1: Early Detection of Diseases Accuracy Comparison between **DBLD** and Baselines.

eases [Zhang *et al.*, 2015]. In this application, each patient's EHR data is represented by a $p = 295$ dimensional vector, referring to the outpatient record on the physical disorders diagnosed. Patients are labeled with either "positive" or "neg-

	Training Set						
Algorithm	100	200	300	400	500	600	700
DBLD	0.690±0.028	0.708±0.027	**0.722±0.024**	**0.729±0.018**	**0.727±0.0118**	**0.736±0.018**	**0.734±0.022**
FLD	0.539±0.048	0.580±0.044	0.611±0.030	0.646±0.027	0.644±0.025	0.662±0.028	0.663±0.032
Ye-FLD	0.644±0.100	0.657±0.124	0.688±0.071	0.678±0.057	0.698±0.035	0.698±0.035	0.712±0.027
Decision Tree	0.626±0.120	0.671±0.074	0.675±0.088	0.703±0.032	0.695±0.034	0.676±0.078	0.690±0.097
Linear SVM	0.616±0.031	0.627±0.041	0.651±0.026	0.675±0.031	0.675±0.026	0.680±0.035	0.690±0.031
Kernel SVM	**0.701±0.063**	**0.723±0.022**	0.702±0.115	0.726±0.016	0.681±0.115	0.734±0.019	0.715±0.071
AdaBoost	0.560±0.081	0.533±0.107	0.498±0.065	0.503±0.078	0.500±0.080	0.482±0.066	0.503±0.070
CRLD	0.696±0.021	0.716±0.021	0.719±0.024	0.725±0.018	0.721±0.015	0.733±0.021	0.734±0.016
Random Forest	0.419±0.126	0.509±0.102	0.613±0.067	0.509±0.110	0.661±0.036	0.640±0.058	0.603±0.063

Table 2: Early Detection of Diseases F1-Score Comparison between **DBLD** and other Baselines.

Datasets	# Features	# Samples
Leukemia	7,128	72 (47 / 25)
Colon	2,000	62 (40 / 22)

Table 3: Description of Datasets for Classification

ative", indicating whether he/she was diagnosed with depression & anxiety disorders. Through supervised learning on the datasets, the trained binary classifier is expected to predict whether a (new) patient is at-risk or would develop to the depression & anxiety disorders from their historical outpatient records (physical disorder records) [Zhang *et al.*, 2015].

We evaluate **DBLD** and other competitors, including Linear Support Vector Machine, Nonlinear SVM with Gaussian Kernel, Decision Tree, AdaBoost, Random Forest and other FLD baselines, with varying training dataset size m from 100 to 700. Table 1 presents the comparison results. To simplify the comparison, we only present the results of the algorithm with fine-tuned parameter, which is selected through 10-fold cross-validation. It is obvious that **DBLD** and CRLD outperform other baseline algorithms significantly, while **DBLD** performs better than CRLD. The advantage of **DBLD** over other algorithms, such as SVM, is extremely obvious when the size of training dataset m is small. With the increasing sample size, though the margins of **DBLD** over the rest of algorithms decrease, **DBLD** still outperforms other algorithms. We also measured the F1-score of all algorithms, **DBLD** still outperforms other competitors in the most cases. Please refer to Table 2 for details.

4.4 Leukemia and Colon Cancer Datasets

We evaluate **DBLD**, CRLD and other baseline algorithms, including Decision Tree, Random Forest and SVM, using leukemia and colon cancer datasets (derived from [Lin, 2017; Tibshirani *et al.*, 2002]) under HDLSS settings (i.e., $p = 7,128$ and $2,000$ vs. $m = 20$).

Table **??** presents the description of two datasets [Lin, 2017; Tibshirani *et al.*, 2002] that we used to evaluate the proposed and baseline algorithms. "Leukemia" refers to the leukemia cancer dataset [Tibshirani *et al.*, 2002] that includes 7,128 features and totally 72 samples (for training and testing). In this datasets, 47 samples are labeled as "ALL" class while 25 samples are identified as "AML". On the other hand, "Colon" refers to the colon cancer datasets [Lin, 2017] that are with 2,000 features and totally 62 samples, where 40 samples are negative and 22 samples are identified as positive. Both datasets are with a ultra-large number of dimensions but with extremely low sample sizes (i.e., $p \gg m$).

To accurately estimate the performance of algorithms using these datasets under HDLSS settings, we use cross-validation to limit the potential over-fitting. In each round of cross-validation, we first randomly drawn 20 samples with equal prior from the datasets as the training set, and randomly drawn 20 samples with equal prior from the disjoint set of training set as the testing set. For each round of cross validation, there are no common samples shared by the two sets. We use the training set to train each classifier (i.e., $p = 7,128$ or $2,000$ and $m = 20$), so as to simulate the extremely HDLSS settings, then test the trained classifiers using the testing set. For each experiment, we repeat the cross-validation for 100 rounds. All algorithms (including baselines and **DBLD**) are tuned to have the best accuracy. The experiment results are shown in Table **??**. All results show that **DBLD** significantly improves CRLD, and it outperforms all baseline algorithms with the highest accuracy and F1-score. Please note that though we trained classifiers using less training data, baselines in our experiments perform comparably with the test errors reported in [Tibshirani *et al.*, 2002].

4.5 Summary of Experiment Results

We evaluate **DBLD** with a limited number of samples for training i.e., $p > m$ or $m \not\gg p$, to understand its performance under HDLSS setting. For large sample scenario, i.e., when $m \gg p$, the sample-based estimators may provide a robust estimation of LDA. In this case, singularity issues might not exist, then regularization and further the de-biasing procedures are not mandatory.

	Colon		Leukemia	
Algorithm	Accuracy	F1 Score	Accuracy	F1 Score
DBLD	**0.803**	**0.802**	**0.964**	**0.964**
CRLD	0.633	0.630	0.690	0.690
Decision Tree	0.669	0.658	0.804	0.800
Random Forest	0.801	0.798	0.957	0.956
SVM	0.797	0.812	0.906	0.914

Table 4: Accuracy and F1-Score Comparison between **DBLD** and other Baselines Based on Colonar and Leuk Cancer Datasets.

5 Related Work and Discussion

In this section, we review several most relevant studies of our research. To address the HDLSS issues for FLD, a line of research [Shao *et al.*, 2011; Cai and Liu, 2011] proposed to directly estimate a sparse projection vector without estimating the inverse covariance matrix (sample covariance matrix is not invertible) and mean vectors separately. On the other hand, [Peck and Van Ness, 1982; Bickel and Levina, 2008; Witten and Tibshirani, 2009] proposed to first estimate the inverse covariance matrix through shrunken covariance estimators, then estimate the projection vector with sample mean vectors. Through regularizing the (inverse) covariance matrix estimation, these algorithms are expected to estimate a sparse projection vector with (sub-)optimal discrimination power [Zollanvari and Dougherty, 2013]. Moreover, the performance of FLD has been previously studied in [Durrant and Kabán, 2015; Bickel *et al.*, 2004].

In our paper, we focus on improving covariance-regularized FLD [Witten and Tibshirani, 2009], through de-biasing the projection vector estimated with Graphical Lasso [Witten *et al.*, 2011]. Our work is distinct due to the following reasons: **(1)** Our work is the first to study the problem of de-biasing the sparse FLD [Zhang and Zhang, 2014]; **(2)** Compared to the existing solution to the de-biased linear regression models [Javanmard and Montanari, 2014], we proposed a novel de-biased estimator (using a different formulate in Eq 5) for the *covariance-regularized sparse Linear Discriminant Analysis* [Witten and Tibshirani, 2009; Witten *et al.*, 2011]; **(3)** We analyzed the de-biased estimator and obtained its asymptotic properties; **(4)** We validate our algorithms through comparing a wide range of baselines on both synthesized and real-world datasets, where the evaluation result endorses our theory (e.g., asymptotic properties proved in **Theorem 1** and **2** vs. the curve shown in Fig 2(b)).

Discussion and Future Work. In this research, we compare **DBLD** with CRLD, and common FLD (sample FLD, pseudo-inverse FLD, Ye-FLD). We do not make further comparison with other sparse FLD [Cai and Liu, 2011], as we focus on the covariance-regularization. In future work, we plan to study the de-biased estimators for these sparse FLD.

6 Conclusion

In this paper, we studied the problem of improving the performance of covariance-regularized FLD (CRLD) through re-balancing the biases and variances of the projection vector estimation. Inspired by the de-biased estimator of Lasso [Javanmard and Montanari, 2014], we proposed **DBLD** – a novel De-Biased estimator for CRLD that lowers the estimation error with faster asymptotic rate, through de-biasing the projection vector obtained by CRLD. Our analysis shows that **DBLD** is with better asymptotic properties, compared to CRLD, and can obtain higher classification accuracy, under HDLSS settings. The experimental results on synthesized and real-world datasets show that **DBLD** outperformed all baseline algorithms. Further, the empirical studies on estimator comparison validate our theoretical analysis.

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