ABSTRACT

Linear discriminant analysis (LDA) is a popular technique to learn the most discriminative features for multi-class classification. A vast majority of existing LDA algorithms are prone to be dominated by the class with very large deviation from the others, i.e., edge class, which occurs frequently in multi-class classification. First, the existence of edge classes often makes the total mean biased in the calculation of between-class scatter matrix. Second, the exploitation of $\ell_2$-norm based between-class distance criterion magnifies the extremely large distance corresponding to edge class. In this regard, a novel self-weighted robust LDA with $\ell_{2,1}$-norm based pairwise between-class distance criterion, called SWRLDA, is proposed for multi-class classification especially with edge classes. SWRLDA can automatically avoid the optimal mean calculation and simultaneously learn adaptive weights for each class pair without setting any additional parameter. An efficient re-weighted algorithm is exploited to derive the global optimum of the challenging $\ell_{2,1}$-norm maximization problem. The proposed SWRLDA is easy to implement, and converges fast in practice. Extensive experiments demonstrate that SWRLDA performs favorably against other compared methods on both synthetic and real-world datasets, while presenting superior computational efficiency in comparison with other techniques.

Keywords Robust linear discriminant analysis · dimension reduction · multi-class classification · edge class

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1 Introduction

As one of the most fundamental problems in data mining, multi-class classification has attracted a surge of research interests [1, 2]. Various models for multi-class classification have been proposed in literature, such as decision trees [3], k-Nearest Neighbor [4], Naive Bayes [5], and Support Vector Machines [6]. However, the efficiency and effectiveness of these methods usually drop exponentially as the feature dimensionality increases due to the “curse of dimensionality" problem [7, 8]. The original data in real-world applications usually possess very large dimension and contain redundant or noisy features which are useless and even harmful to the separation of multiple categories [9]. Linear Discriminant Analysis (LDA) is thus developed to address this problem by selecting and extracting the most discriminative features for multi-class classification in a supervised way [10, 11, 12, 13, 14]. The basic idea of LDA is to learn an optimal projection matrix which minimizes the variability within each class and simultaneously maximizes the discrepancy between different classes in the embedding space. In such a way, the original high-dimensional data can be transformed into a low-dimensional subspace with high class separability.

However, gradient method is adopted to solve the proposed challenging problems in [29, 30, 31, 32, 33], which converge very slowly in many cases. Bian et al. [34] also presented a max-min distance analysis to guarantee the separation of all class pairs by maximizing the minimum between-class distance. However, this method needs to solve a challenging non-smooth min-max problem with orthonormal constraints, which can only obtain an approximate solution by using a sequential convex relaxation algorithm.

Several earlier LDA variants have been proposed to address this issue by taking the estimation of optimal mean into consideration, including M-estimator [23], S-estimators [24], Minimum Covariance Determinant (MCD) [25] and Minimum Volume Ellipsoid (MVE) [26]. However, these methods usually suffer from intractable computational complexity and still cannot guarantee a better solution to the class separation problem. Other researchers have approached the problem by maximizing the pairwise distance between every two class means. As a result, the original \( c \)-class fisher criterion is decomposed into \( \frac{1}{2} c(c - 1) \) pairwise between-class distances, corresponding to the worst case between-class separation criterion [27]. However, the class pairs with extreme large distance can still dominant the whole classification due to the exploitation of \( \ell_2 \)-norm distance criterion. To focus more on the closer ones, many weighting methods have been proposed to learn different weights for each class pair. Loog et al. [28] proposed an approximate pairwise accuracy criterion such that the importance of each class pair depends on the approximation of Bayes error rate. This method can be easily solved by eigenvalue decomposition as traditional LDA; however, the learned approximate pairwise weights may not be the optimal ones because it is calculated in the original high-dimensional space. Tao et al. [29] assumed that all the classes are sampled from homoscedastic Gaussians with identical covariance matrices and developed three new criteria to maximize the geometric mean of Kullback-Leibler (KL) divergences between different pairs of classes. Bian et al. [30] proposed to maximize the harmonic mean of all pairs of symmetric KL divergences under the homoscedastic Gaussian assumption. However, gradient method is adopted to solve the proposed challenging problems in [29, 30, 31, 32, 33], which converge very slowly in many cases. Bian et al. [34] also presented a max-min distance analysis to guarantee the separation of all class pairs by maximizing the minimum between-class distance. However, this method needs to solve a challenging non-smooth min-max problem with orthonormal constraints, which can only obtain an approximate solution by using a sequential convex relaxation algorithm.

Taking all the discussed challenges into consideration, we propose a novel formulation of self-weighted robust LDA for multi-class classification with edge classes, termed as SWRLDA. The optimal mean estimation is automatically avoided by maximizing the sum of distances between every two class centers, rather than that between each class center and the total mean. Considering the fact that \( \ell_2 \)-norm is prone to be dominated by large between-class distances corresponding to edge class, \( \ell_2 \)-norm is exploited to further reduce the effect of edge classes and simultaneously enhance the robustness. An efficient re-weighted algorithm is adopted to optimize all the projection directions simultaneously without increasing the time complexity in contrast to the state-of-the-art LDA methods [35, 9, 36, 37, 38, 39]. By optimizing the objective function of SWRLDA, the self-adaptive weights of each class pair can be learned implicitly in the embedding space. In this way, SWRLDA is capable of investigating the contribution of each class pair to
classification automatically, instead of tuning additional parameters. Besides, the optimal weight corresponding to each class pair is learned based on their distances in the desired subspace such that it is more robust when the original data contain large noise. Extensive experiments on both synthetic and real-world datasets demonstrate the superior classification performance and high computational efficiency of the proposed method.

2 Related Work

2.1 Linear Discriminant Analysis

In previous literature, various extensions of naive LDA have been developed for further enhancement. For example, orthogonal LDA (OLDA) [40], uncorrelated LDA (ULDA) [41] were proposed to address the small sample size problem of naive LDA. To capture the geometric structure of data, discriminant locality preserving projection (ℓ2,1-DLPP) [42], discriminative locality alignment (DLA) [43], and manifold partition discriminant analysis (MPDA) [44] were proposed. To classify high-dimensional data without feature selection, Peng et al. [45, 46] introduced LDA based discriminant ridge models to classification. However, all those methods maximize the sum of distances between each class mean and the total data mean [47, 48, 49, 50, 51, 52], instead of explicitly maximizing the distance between every two class pairs. In such a way, it is inevitable that several classes are totally overlapped in the learned subspace, especially in multi-class classification with edge classes. To achieve the separability of every binary classes, FLDA is proposed to maximize the pairwise distance between every two class means, but not just the average distances [53]. Specifically, the between-class scatter matrix of FLDA is usually rewritten as $S_b = \sum_{i=1}^{c} \sum_{j=i+1}^{c} \frac{n_i n_j}{n_i + n_j} (x_i - x_j)(x_i - x_j)^T$, which is measured by distances between each class pair instead of that between each class center and the total mean. Based on this reformulation, the c-class fisher criterion can be decomposed to $\frac{1}{2}c(c-1)$ two-class fisher criterion. FLDA is typically solved by a two-step algorithm, which first learns a whitened space to obtain the optimal distance metric, and then conducts dimension reduction in the learned whitened space. However, FLDA still cannot directly address the class separation problem. First, there is no guarantee that FLDA can prevent the incompatibility and information loss between the two independent stages, making the final result unreliable. Second, the quadratic distances between all the class pairs are maximized with equal weights, which is easily dominated by the classes located remotely from the others.

2.2 Weighted Pairwise Distance Criterion

To attach more importance to the closer class pairs, many weighting schemes have been proposed to learn different weights for different class pairs. For example, Loog et al. [28] developed a weighting function based on the Mahanalobis distance between the $i$th and $j$th class in the original space, which can be efficiently solved by
eigen-decomposition as in traditional LDA. However, the weights are simply calculated according to the distances in the original space, but not calculated according to the distances in the optimal subspace. Therefore, the calculated weights might not the optimal weights, especially when the data distribution in the optimal subspace changes largely from the original space or when the data contain large noise. GMSS \cite{29} and HMSS \cite{30} are also weighting methods to reduce the class separation problem. GMSS \cite{29} was proposed to maximize the weighted geometric mean of between-class distances under the homoscedastic Gaussian assumption, i.e., \( \text{let@tokeneonedot} \), Bian and Tao et al \cite{30} presented HMSS to further reduce the class separation problem by maximizing the weighted harmonic mean, i.e., \( \text{let@tokeneonedot} \). To guarantee the separation of all the class pairs, Abou-Moustafa et al \cite{57} further proposed to maximize all the pairwise distances simultaneously. Although these methods have reported improved performance compared with FLDA, they are all based on some complex iterative optimization procedures to solve the models, which makes them not scalable for large-scale dimension reduction problems.

3 The Proposed Methodology

In this section, we will elaborate the formulation of the proposed self-weighted robust LDA model for multi-class classification. The notations used in this paper are introduced as follows. Following the standard notation, we denote vector and matrix by bold lowercase letters (e.g., \( \text{let@tokeneonedot} \)) and bold uppercase letters (e.g., \( \text{let@tokeneonedot} \)) respectively. The \( \ell_2 \)-norm of vector \( a \in \mathbb{R}^n \) is written as \( \| a \|_2^2 = \sum_{i=1}^{n} a_i^2 \) and the \( \ell_{2,1} \)-norm of matrix \( A \in \mathbb{R}^{m \times n} \) is defined as \( \| A \|_{2,1} = \sum_{i=1}^{m} \sqrt{\sum_{j=1}^{n} A_{i,j}^2} \), where \( a_i \) refers to the \( i \)-th element of vector \( a \) and \( A_{i,j} \) denotes the element corresponding to the \( i \)-th row and \( j \)-th column of matrix \( A \).

3.1 Problem Formulation

Given training data \( X = [x_1, x_2, \ldots, x_n] \in \mathbb{R}^{d \times n} \) belonging to \( c \) classes for dimension reduction, where \( n \) refers to the number of data points and each data point is represented by a \( d \)-dimensional feature vector. The goal of LDA is to learn a linear projection matrix \( W \in \mathbb{R}^{d \times m} (m \ll d) \), which can transform original \( d \)-dimensional data to a \( m \)-dimensional embedding subspace with higher class separability. This is achieved by maximizing the between-class difference and meanwhile minimizing the within-class variability in the projected space, which can be formulated as the maximization of Fisher’s criterion:

\[
\max_{W} \text{Tr}(W^\top S_b W (W^\top S_w W)^{-1}).
\]

Specifically, \( S_w \in \mathbb{R}^{d \times d} \) and \( S_b \in \mathbb{R}^{d \times d} \) refer to the within-class and between-class scatter matrix respectively, which are defined as

\[
S_w = \sum_{i=1}^{c} \frac{n_i}{n} (x_i - \bar{x})(x_i - \bar{x})^\top,
\]

\[
S_b = \sum_{i=1}^{c} \frac{n_i}{n} (x_i - \bar{x})(x_i - \bar{x})^\top,
\]

where \( n_i \) refers to the number of data points belonging to the \( i \)-th class. Moreover, \( \bar{x} = \frac{1}{n} \sum_{i=1}^{c} n_i x_i \) is the total mean of \( X \) and \( \bar{x}_i = \frac{1}{n_i} \sum_{j=1}^{n_i} x_j \) is the mean of the \( i \)-th class. To guarantee the uniqueness of optimal solution, optimization problem (1) can be reformulated by replacing the denominator with an equality constraint as:

\[
\max_{W} \sum_{i=1}^{c} \frac{n_i}{n} \| W^\top (x_i - \bar{x}) \|^2_{2}, \quad \text{s.t.} \quad W^\top S_w W = I,
\]

where \( I \in \mathbb{R}^{m \times m} \) is an identity matrix. In Eq. (4), the between-class distance is measured by subtracting the total mean from each class center, while the average of data is directly regarded as the optimal mean. In this way, the between-class scatter matrix calculation can be easily dominated by edge classes, which decreases the robustness of LDA model. To this end, we equivalently reformulate the between-class distance criterion in traditional LDA to avoid the optimal mean calculation by introducing the following lemma and theorem.
Lemma 3.1. If \( p \in \mathbb{R}^c \geq 0, p^T 1 = 1, u = \sum_{j=1}^c p_j u_j \in \mathbb{R}^d \), then the following equation holds:

\[
\sum_{i=1}^c p_i (u_i - \overline{u})^T (u_i - \overline{u}) = \sum_{i,j=1}^c \frac{p_ip_j}{2} (u_i - u_j)^T (u_i - u_j),
\]

(5)

where \( p_i \) and \( p_j \) refer to the \( i \)th and \( j \)th element of \( p \).

**Proof.** Based on the fact that \( u = \sum_{j=1}^c p_j u_j \), the left side of Eq. (5) can be derived as \( \sum_{i=1}^c p_i(u_i - \sum_{j=1}^c p_j u_j)^T(u_i - \sum_{j=1}^c p_j u_j) \), which can be further decomposed into the sum of three items, i.e.,

\[
\sum_{i=1}^c p_i u_i^T u_i - 2 \sum_{i=1}^c p_i u_i^T \sum_{j=1}^c p_j u_j + \sum_{j=1}^c p_j u_j^T \sum_{j=1}^c p_j u_j.
\]

(6)

By combining the second and third terms of Eq. (6), we can arrive at

\[
\sum_{i=1}^c p_i u_i^T u_i - \sum_{i=1}^c p_i u_i^T \sum_{j=1}^c p_j u_j.
\]

(7)

Subsequently, the right side of Eq. (5) can be reformulated as

\[
\frac{1}{2} \sum_{i,j=1}^c (p_ip_j u_i^T u_i + p_ip_j u_j^T u_j - 2p_ip_j u_i^T u_j).
\]

(8)

By combining the first two items, it reduces to Eq. (7). The proof is completed. \( \square \)

**Theorem 3.2.** The optimization problem (4) is equivalent to

\[
\max_{W} \sum_{i=1}^c \sum_{j=1}^c \frac{n_in_j}{2n^2} \|W^T(x_i - x_j)\|_2^2, \quad \text{s.t.} \quad W^T S_u W = I.
\]

(9)

**Proof.** Let \( p, u, \) and \( u \) in Lemma 3.1 denote the vector \( \begin{bmatrix} \frac{n_1}{n}, \frac{n_2}{n}, \ldots, \frac{n_c}{n} \end{bmatrix} \in \mathbb{R}^c, W^T x_i \in \mathbb{R}^m (\forall i) \) and \( W^T x \in \mathbb{R}^m \) respectively. Based on this denotation, the optimization problem (4) is equivalent to the left side of Eq. (5), while the optimization problem (9) is equivalent to the right side of Eq. (6). It’s evident that the optimization problem (4) and (9) equal to each other according to Lemma 3.1. The proof is completed. \( \square \)

Different from traditional LDA formulation based on \( c \)-class fisher criterion in (4), the optimal mean calculation can be automatically avoided in (9), where the between-class variability is measured by the sum of distances between every two class centers, instead of that between each class center and the total mean. However, with the exploitation of \( \ell_2 \)-norm based distance criterion, the learned projection directions are still easily dominated by the class pairs with very large deviation. For this issue, we further reformulate problem (9) via \( \ell_{2,1} \)-norm maximization as

\[
\max_{W} \sum_{i=1}^c \sum_{j=1}^c \frac{n_in_j}{2n^2} \|W^T(x_i - x_j)\|_2, \quad \text{s.t.} \quad W^T S_u W = I,
\]

(10)

where \( \sum_{i=1}^c \sum_{j=1}^c \|W^T(x_i - x_j)\|_2 \) is essentially the sum of multiple matrix \( \ell_{2,1} \)-norms. Intuitively, the distance criterion \( \|W^T(x_i - x_j)\|_2 \) is not quadratic and thus edge classes would have less importance to it than the squared distance criterion in (9). Whenever edge class occurs in a classification problem, the projection direction of traditional LDA would be completely destroyed because its between-class distance criterion depends entirely on the biased mean calculation and at the same time overemphasizes the effect of class pairs with large deviation. In terms of SWRLDA, only the distance calculation corresponding to the edge class will be affected with the exploitation of “avoiding optimal mean” strategy and this effect is further reduced via \( \ell_{2,1} \)-norm based distance criterion. Note that no extra weight factor for each class pair is explicitly included in this objective function. However, by solving problem (10) with a re-weighted optimization algorithm, we will demonstrate that this formulation of self-weighted robust LDA can indeed adaptively learn an optimal weight for each class pair without additional parameters.
3.2 Optimization Procedure

Considering the complexity of directly solving the proposed non-smooth problem, we adopt an efficient iterative re-weighted algorithm to reformulate the proposed optimization problem \([10]\) as

\[
\max_W \sum_{i=1}^{c} \sum_{j=1}^{c} \frac{w_{ij}}{2\|w_{ij}\|_2^2} s_{ij}^T (x_i - x_j), \quad s.t. \quad W^T S_w W = I,
\]

(11)

where \(s_{ij}\) is set to be stationary, i.e., let @tokenedot,

\[
s_{ij} = \begin{cases} \frac{w_{ij}^T (x_i - x_j)}{\|w_{ij}^T (x_i - x_j)\|_2}, & \text{if } \|w_{ij}^T (x_i - x_j)\|_2 \neq 0; \\ 0, & \text{if } \|w_{ij}^T (x_i - x_j)\|_2 = 0. \end{cases}
\]

(12)

Note that an unknown variable \(s_{ij}\) depending on \(W\) is introduced into the optimization problem. Thus, alternating optimization scheme is exploited to update the two variables iteratively. In each iteration, \(s_{ij}\) is updated with the current solution of \(W\), and then \(W\) is recalculated with the updated \(s_{ij}\). This iterative procedure is repeated until the objective function converges to a certain value. Note that \(\frac{w_{ij}^T (x_i - x_j)}{\|w_{ij}^T (x_i - x_j)\|_2}\) can be naturally treated as the weight corresponding to the distance between the \(i\)th and \(j\)th class pair, i.e., let @tokenedot, \(\|w_{ij}^T (x_i - x_j)\|_2^2\), which constitutes the symmetric weighted matrix. It’s noteworthy that the smaller distance corresponds to a larger weight, which indicates that more attention will be paid to the class pairs with high similarities in the learned subspace. Besides, the weight is self-adaptive and can be derived automatically without additional parameters. For notation simplicity, we introduce a matrix \(M = \sum_{i,j=1}^{c} \frac{w_{ij}^T (x_i - x_j)}{2\|w_{ij}\|_2^2} s_{ij}^T\) to transform the problem \([11]\) as:

\[
\max_W \text{Tr}(W^T M), \quad s.t. \quad W^T S_w W = I.
\]

(13)

To determine the closed-form solution of optimal projection matrix \(W\) in problem \([13]\), we introduce the following theorem.

**Theorem 3.3.** The SVD of matrix \(A = S_w^{-\frac{1}{2}} M \in \mathbb{R}^{d \times m}\) is \(U[A; 0]V^T\), where \(U \in \mathbb{R}^{d \times d}\) and \(V \in \mathbb{R}^{m \times m}\) are both orthonormal matrices and \(A = \text{diag}(\lambda_{11}, \lambda_{22}, \ldots, \lambda_{mm}) \in \mathbb{R}^{m \times m}\) is a diagonal matrix with \(\lambda_{kk} \geq 0\) for \(\forall k\). Then the optimal solution of the optimization problem \(\max_{W \in \mathbb{R}^m} \text{Tr}(W^T M)\) can be derived as \(S_w^{-\frac{1}{2}} U [I; 0] V^T\).

**Proof.** Since the matrix \(A\) equals to \(S_w^{-\frac{1}{2}} M\), the objective function in \([13]\) can be rewritten as \(\text{Tr}(W^T S_w^{-\frac{1}{2}} A)\). Based on the SVD result of \(A\), we can further transform it into

\[
\text{Tr}([A; 0] V^T W^T S_w^{-\frac{1}{2}} U) = \text{Tr}([A; 0] Z) = \sum_{i=1}^{m} \lambda_{ii} z_{ii},
\]

where \(Z = V^T W^T S_w^{-\frac{1}{2}} U\), \(\lambda_{ii}\) and \(z_{ii}\) are the \((i, i)\)-th element of matrix \(A\) and \(Z\) respectively. Note that \(Z\) is an orthonormal matrix, i.e., let @tokenedot, \(Z^T Z = I\), thus \(z_{ii} \leq 1\) holds for each \(i\). Since \(\lambda_{ii}\) is the singular value of \(A\), \(\lambda_{ii} \geq 0\) satisfies for each \(i\), and thus we can derive the following inequality:

\[
\text{Tr}(W^T M) = \sum_{i=1}^{m} \lambda_{ii} z_{ii} \leq \sum_{i=1}^{m} \lambda_{ii},
\]

(14)

When \(z_{ii} = 1(\forall i)\), i.e., let @tokenedot, \(Z = I\), the equality in \([14]\) holds and at the same time \(\text{Tr}(W^T M)\) reaches its maximum. Recall that \(Z = V^T W^T S_w^{-\frac{1}{2}} U\), the optimal solution of problem \(\max_{W \in \mathbb{R}^m} \text{Tr}(W^T M)\) is \(S_w^{-\frac{1}{2}} U [I; 0] V^T\). The proof is completed.

The key steps of SWRLDA are summarized in Algorithm [1]. We will theoretically analyze its computational complexity and convergence in the following parts.

3.3 Computational Complexity Reduction Analysis

Despite the fact that SWRLDA traverses the distance between all the class pairs, its computational complexity is \(O(cnmdt)\) which doesn’t increase in contrast to the state-of-the-art LDA methods [35, 9, 37].
The multiplication of matrix $W^T$ and $X$, i.e., $tokenetonedot$, $W^T X$, is computed as $P = [p_1, p_2, \ldots, p_n] \in \mathbb{R}^{m \times c}$ with computational complexity $O(cd m)$, where $X = [x_1, x_2, \ldots, x_c] \in \mathbb{R}^{d \times c}$ collects all the class mean vectors. According to Eq. (12), $s_{ij}(i, j = 1, 2, \ldots, c)$ can be updated with the entire time complexity $O(mc^2)$, which is further exploited to calculate the matrix $M$. It seems that the computational cost of $M$ is $O(c^2 dm)$. Actually, it can be accelerated by considering the computation of $s_{ij}$ and $M$ in a comprehensive way. The computation of $M = \sum_{i,j=1}^{c} \frac{n_i n_j}{2n^2} (x_i - x_j)^T s_{ij} x_j$ can be reformulated as $\frac{1}{2n^2} \sum_{i=1}^{c} n_i x_i (\sum_{j=1}^{c} n_j s_{ij}^T - \frac{1}{2n^2} \sum_{i,j=1}^{c} n_i n_j x_j) \sum_{i=1}^{c} n_i s_{ij}^T$. Under the condition that $s_{ij}^T = \sum_{i=1}^{c} n_i s_{ij}$ and $s_{ij}^T = \sum_{i=1}^{c} n_i s_{ij}$, it reduces to $\frac{1}{2n^2} \sum_{i=1}^{c} n_i x_i (s_i^T - s_i^T)$. Thus, when $s_i$ and $s_j$ are given, the matrix $M$ can be computed with time complexity $O(cd m)$. Based on Eq. (12), we can derive $s_i = \sum_{j=1}^{c} n_j s_{ij} = \sum_{j=1}^{c} n_j \frac{p_i - d}{n_i - p_i - d}$ and $s_j = \sum_{i=1}^{c} n_i s_{ij} = \sum_{i=1}^{c} n_i \frac{p_i - d}{n_i - p_i - d}$, where $\|p_i - d\|_2 \neq 0$. Therefore, $s_i$ and $s_j(\forall i)$ can be calculated with time complexity $O(c^2 m^3)$. Next, the computational cost of the following steps mainly lies in the SVD of matrix $A \in \mathbb{R}^{d \times m} = U \Sigma V$. Note that the left singular vectors of $A$, $i.e.,tokenetonedot$, the column vectors of $U$, are the eigenvectors of $A A^T$ and the right singular vectors of $A$, $i.e.,tokenetonedot$, the column vectors of $V$, are the eigenvectors of $A^T A$. If $U$ or $V$ is given, the other one can be recovered by the equation $A V = U \Sigma$ and $U^T A = \Sigma V^T$. Due to the fact that $d \geq m$, we only need to compute the eigenvectors of $A^T A$ as $V$, and then recover $U$ from $V$, whose total computational complexity is $O(dm^2 + d^3)$.

In conclusion, the whole time complexity of the proposed method is $O((cd + c^2 + md + m^2)mt)$, where $t$ is the iteration number. Since the feature dimensionality $d$ is usually much larger than the number of classes $c$ and the reduced dimensionality $m$, the computational complexity of Algorithm 1 can be simplified as $O(cmd t)$.

### 3.4 Convergence Analysis

In this section, we will analyze the convergence of the proposed SWRLDA by introducing the following lemma and theorem.

#### Lemma 3.4

The objective function in optimization problem (10) is upper bounded.

**Proof.** For a given $i$, the subproblem of (10) can reduce to $\sum_{j=1}^{c} ||W^T (x_i - x_j)||_2$ by not considering the constants in $\frac{n_i n_j}{2n^2}$. It can be further derived as $\sum_{j=1}^{c} ||B^T d_{ij}||_2$, where $B = S_w^{-1} W$ with $B^T B = I$ and $d_{ij} = S_w^{-1} (x_i - x_j)$. According to Cauchy-Schwarz inequality, we have the following derivations:

$$\sum_{j=1}^{c} ||B^T d_{ij}||_2 \leq \sum_{j=1}^{c} ||B^T d_{ij}||_1 = \sum_{k=1}^{m} ||B^T||_2 ||d_{ij}||_2 \leq (\sum_{k=1}^{m} \lambda_1 ||B^T||_2 ||d_{ij}||_2 = \sum_{j=1}^{c} \lambda ||d_{ij}||_2,$$

where $b_k$ is the $k$th column of matrix $B$. For a given dataset, $\sum_{j=1}^{c} \lambda ||d_{ij}||_2$ is a constant, which indicates the objective function in optimization problem (10) has an upper bound. The proof is completed. □
Theorem 3.5. The objective in optimization problem (10) will monotonically increase and converge to its maximum with Algorithm 7.

Proof. For simplicity, let \( v_{ij} \) denote the vector \( \mathbf{x}_i - \mathbf{x}_j \). With the fixed \( s_{ij(t)} \) in the \( t \)th iteration, the optimal \( W(t) \) can be obtained when the objective function in (11) reaches its maximum, such that

\[
\sum_{i,j} \frac{n_i n_j}{2n^2} s_{ij(t)}^T W(t)^T W_{ij} W_{ij}^T v_{ij} = \sum_{i,j} \frac{n_i n_j}{2n^2} s_{ij(t)}^T W_{ij} W_{ij}^T v_{ij},
\]

According to Cauchy-Schwarz inequality, it's easily to get \( \|W(t)^T v_{ij}\|_2 \|W(t)^T v_{ij}\|_2 \geq \langle W(t)^T v_{ij} , W(t)^T v_{ij} \rangle \).

Based on this inequality and Eq. (12), we have \( \|W(t)^T v_{ij}\|_2 - s_{ij(t)}^T W(t)^T v_{ij} \geq 0 \), and Eq. (12) can be reformulated as \( \|W_{(t-1)}^T v_{ij}\|_2 - s_{ij(t)}^T W_{(t-1)}^T v_{ij} = 0 \). Combining the above two equations, we can arrive at \( \|W_{(t-1)}^T v_{ij}\|_2 \geq \|W_{(t-1)}^T v_{ij}\|_2 - s_{ij(t)}^T W_{(t-1)}^T v_{ij} \). Since the above inequality holds for each \( i \) and \( j \), we can derive that

\[
\sum_{i,j} \frac{n_i n_j}{2n^2} (\|W_{(t)}^T v_{ij}\|_2 - s_{ij(t)}^T W_{(t)}^T v_{ij}) \geq \sum_{i,j} \frac{n_i n_j}{2n^2} (\|W_{(t-1)}^T v_{ij}\|_2 - s_{ij(t)}^T W_{(t-1)}^T v_{ij}).
\]

Summing the two inequalities in (15) and (16) on both sides, we obtain

\[
\sum_{i,j} \frac{n_i n_j}{2n^2} \|W_{(t)}^T v_{ij}\|_2 \geq \sum_{i,j} \frac{n_i n_j}{2n^2} \|W_{(t-1)}^T v_{ij}\|_2.
\]

Thus, the objective value in problem (10) monotonically increases with Algorithm 7 and is bounded above by a supremum based on Lemma 3.4; then it will converge to its maximum. The proof is completed.

4 Experiments

In this section, extensive experiments on both synthetic and real-world datasets are conducted to evaluate the effectiveness of the proposed method. The proposed SWRLDA is developed in the Matlab environment. All experiments are performed on the Windows-10 operating system (Intel Core i5-6200U CPU @ 2.40 GHz, 16 GB RAM). In addition, seven state-of-the-art algorithms are selected for comparison, which are briefly introduced as follows:

- \( c \)-class fisher criterion based LDA models rely on the total mean calculation, whose between-class distance is calculated by subtracting the total mean from each class center. Specifically, LDA \[29\] corresponds to the traditional LDA model and RSLDA \[2\] is a robust version of LDA by introducing the \( \ell_{2,1} \)-norm minimization of projection matrix.
- Weighted pairwise fisher criterion based methods decompose the original \( c \)-class fisher criterion into \( \frac{1}{2}c(c-1) \) two-class fisher criterion, and then attach certain weight to each class pair to characterize its importance. aPAC \[28\] assigned different weights according to their Mahalanobis distance in the original space. GMSS \[29\] and HMSS \[30\] learned weights by maximizing the weighted geometric mean and weighted harmonic mean of KL divergences of class pairs respectively. STRDA \[59\] was proposed to maximize the weighted harmonic mean of pairwise trace ratios. MMDA \[34\] maximized the minimal pairwise distance by introducing a local SDP relaxation.

4.1 Experiments on Synthetic Datasets

4.1.1 Experimental Setup

Considering that the projection directions may be different in the presence and absence of edge class, we design an experiment to evaluate each method on two 2D synthetic datasets, denoted as syn1 and syn2 respectively. The first dataset syn1 contains three classes, \( \{1.e1\} @ \{tokenednot\}, \) class 1, 2 and 3, which are located very closely to each other. The second dataset syn2 is constructed by adding an extra class far away from class 1, 2 and 3, denoted as class 4, which can be regarded as an edge class. Each class is composed of 200 data points generated from Gaussian distribution with the same standard deviation \([1, 0; 0, 1]\). The data means corresponding to class 1, 2, 3 and 4 are \([-5, -4], [-3, 1], [-1, 6] \) and \([10, -2] \) respectively. The scatter plots of syn1 and syn2 are illustrated in Figure 2(a) and Figure 2(b).
Figure 2: Projection directions learned by different methods on 2D synthetic data.

Figure 3: The histograms of two synthetic datasets projected onto the optimal direction learned by different methods. Specifically, the histogram below and above the zero ordinate corresponds to syn1 and syn2 respectively.

4.1.2 Performance Comparison

Figure 2 demonstrates the projection directions learned by different methods over syn1 and syn2. Under each direction, the original data points can be projected into a new embedding space as shown in Figure 3(a) to Figure 3(h) corresponding to different methods respectively. For syn1 without edge class, each comparative method can learn a satisfying projection direction to classify them correctly. However, the four classes of syn2 with edge class overlap with each other in varying degrees under the projection directions learned by most comparisons. According to Figure 2(b), all the methods can be arranged by sorting their slopes in descending order as MMDA, aPAC, SWRLDA, GMSS, HMSS, RSLDA, LDA and STRDA. Based on their sensitivity to edge class, we roughly divide them into three categories, i.e., over-sensitive, middle and under-sensitive. From the projected histograms of syn2, we can observe that all of LDA, RSLDA, HMSS, GMSS and STRDA fall into the over-sensitive category. Consequently, class 1, 2 and 3 overlap with each other in varying degrees and class 4 is far away from them under the directions learned by these methods. This phenomenon indicates that the existence of edge class can indeed dominate the projection direction learned by most LDA methods. The classification of the edge and non-edge class is over-emphasized while the distinction between multiple non-edge classes is neglected, which fails to obtain desirable classification results of the whole data. On the contrary, MMDA belongs to the under-sensitive category, since it only maximizes the class pair with minimum distance while completely ignoring the edge class. Although class 1, 2 and 3 can be separated well, class 4 suffers from a large overlap with others. Compared with these methods, aPAC and SWRLDA can much better
Table 1: Summary of the benchmark datasets used for classification in our experiments.

| Dataset     | Samples\((n)\) | Dimension\((d)\) | Classes\((c)\) | Type    |
|-------------|----------------|-----------------|----------------|---------|
| COIL20      | 1440           | 1024            | 20             | Image   |
| COIL100     | 7200           | 1024            | 100            | Image   |
| Isolet      | 7797           | 617             | 26             | Speech  |
| Wine        | 178            | 13              | 3              | UCI     |
| CMU PIE     | 11554          | 1024            | 68             | Image   |
| YaleB       | 2414           | 1024            | 38             | Image   |
| 20Newsgroups| 18846          | 26214           | 20             | Document|

Table 2: Performance comparison in terms of ACC ± std% for different methods over six benchmark datasets.

| Method   | COIL20  | COIL100 | Isolet  | 20Newsgroups | CMU PIE | YaleB   |
|----------|---------|---------|---------|--------------|---------|---------|
| LDA      | 93.19±0.121 | 87.62±0.085 | 93.91±0.066 | -    | 93.44±0.052 | 99.13±0.027 |
| RSLDA    | 97.35±0.167 | 89.08±0.049 | 85.62±0.025 | -    | 94.89±0.040 | 95.38±0.034 |
| aPAC     | 94.93±0.176 | 88.36±0.061 | 93.63±0.085 | -    | 94.34±0.039 | 99.58±0.035 |
| GMSS     | 95.14±0.097 | 87.76±0.099 | 93.76±0.032 | -    | 94.72±0.036 | 99.63±0.051 |
| HMSS     | 95.35±0.089 | 87.95±0.143 | 93.49±0.094 | -    | 94.72±0.030 | 99.12±0.020 |
| STRDA    | 90.69±0.108 | 87.45±0.065 | 92.68±0.070 | -    | 90.37±0.078 | 99.45±0.028 |
| MMDA     | 95.69±0.061 | 88.36±0.101 | 94.07±0.029 | -    | 94.95±0.064 | 99.21±0.079 |
| SWRLDA   | **99.65±0.042** | **95.01±0.045** | **96.64±0.033** | **89.81±0.058** | **97.02±0.041** | **99.75±0.027** |

results on the dataset with edge class. As illustrated in Figure 3(c) and 3(h), class 3 and 4 still suffer from a relatively large overlap on the projection direction learned by aPAC, while SWRLDA can find a projection that provides a better overall trade-off between all the classes. This phenomenon indicates the superiority of our method in classification and discrimination between classes, even though the training set contains edge class.

4.2 Experiments on Real-World Datasets

We adopt seven real-world datasets widely used in the previous research to evaluate the performance of the proposed SWRLDA, including COIL20 [60], COIL100 [61], Isolet [62], 20Newsgroups [63], Wine [64] [65], CMU PIE [66] and YaleB [67]. Among them, COIL100 is an image library of 100 objects viewed from varying angles and COIL20 is a subset of COIL100 with 20 classes. Isolet is a spoken letter database with 150 subjects who spoke the name of each letter of the alphabet twice. 20Newsgroups is a large-scale dataset collected and originally used for document classification by Lang [63] with 18,846 documents, evenly distributed across 20 classes. The CMU PIE contains face images under 5 poses(C05, C07, C09, C27, C29), 43 illumination conditions, and 4 expressions for each person. The YaleB consists of 2414 frontal-face images of 38 individuals captured under various lighting conditions. Wine is a dataset from UCI machine learning repository [64], which consists of 178 samples with 13 attributes from 3 classes. The statistics for each dataset are summarized in Table 1.

4.2.1 Experimental Setup

According to the standard 5-fold cross validation, each dataset is randomly partitioned into 5 sets with 4 parts for training and the remaining part for testing in each round. During the training period, the optimal projection matrix can be obtained when the relative change of objective function is below \(10^{-6}\). Once the optimal projection matrix is obtained, we use \(k\)-Nearest Neighbor (\(k\)-NN) method (\(k = 1\) is used in this work) to classify the data points in the projected space. In \(k\)-NN, we use the most widely used Euclidean distance as the distance metric. For a comprehensive comparison, the following five performance evaluation metrics are considered to evaluate the quality of different LDA methods for classification: (a) average classification accuracy with standard deviation; (b) minimum pairwise distance in the projected low-dimensional subspace; (c) two-dimensional data visualization; (d) average running time; (e) robustness of models.
4.2.2 Classification Accuracy

The classification accuracy and standard deviation are the most widely used evaluation metrics for discriminant dimension reduction methods. For fair comparison, the mean classification accuracy (ACC) and standard deviation (std) of 5-fold cross validation with the same projection dimension $c - 1$ corresponding to each method are reported in Table 2. Notably, we only report the results on 20Newsgroups achieved by our method, because all the comparison methods fail to deal with this large-scale dataset with affordable cost (>24h). Figure 4 demonstrates the classification accuracy with respect to various reduced dimensions over three datasets. From these results, we can make the following observations:

- The proposed SWRLDA achieves the highest classification accuracy among all the comparisons over all the datasets. Specifically, the classification accuracy improves 2.4% on COIL20, 6.7% on COIL100, 2.7% on Isolet, 2.2% on CMU PIE and 0.1% on YaleB respectively. We can attribute this improvement to the combination of “avoiding optimal mean” strategy and self-weighted between-class distance criterion based on $\ell_{2,1}$-norm.

- As shown in Figure 4, SWRLDA obtains the best performance in most dimensions over all the datasets. With the decrease of projection dimension $m$, the classification accuracy of comparative methods decreases significantly, while the proposed approach is more stable except when $m$ is too small (e.g., $m = 1$). This suggests that SWRLDA is more robust to the selection of projected feature dimensions.

4.2.3 Average Minimum Pairwise Distance

In general, a larger minimum pairwise distance indicates a better separation of all class pairs in the low-dimensional subspace. For each projected dimension, we calculate the minimum pairwise distance in the projected subspace by averaging 100 independent runnings. The experimental results on COIL20 and Isolet dataset are demonstrated in Figure 5(a) and Figure 5(b) respectively. As shown in Figure 5(a) and Figure 5(b), the average minimum pairwise distance of each method increases continuously with the increasing of projected dimensions. Specifically, when
projecting to 1-dimensional subspace, almost all the compared algorithms obtain the same result. However, as the dimension increases, the proposed algorithm gains more significant performance improvements compared with other methods.

### 4.2.4 Two-Dimensional Visualization of Wine Dataset

For qualitative analysis, the two-dimensional scatter plot in the embedding subspace is exploited to visualize the separability of each model over Wine dataset. Specifically, a two-dimensional subspace is first learned with all the samples of Wine dataset, and then all of them are projected onto the two-dimensional subspace. From the graphical representations shown in Figure 6, we can see that LDA, RSLDA and aPAC achieve the worst separation results, since all the three classes overlap with each other seriously. Compared with them, the samples are almost separable in the subspace generated by GMSS, HMSS, STRDA, MMDA and SWRLDA. While there are still slight overlaps among the results of these methods, the proposed SWRLDA is able to learn a separation of no overlapped samples with the largest minimum between-class distance. This indicates that SWRLDA can still make a good trade-off among all the classes by learning appropriate weights even though the training data do not contain edge class.

### 4.2.5 Average Running Time

All the comparison methods need to solve a time-consuming eigen-decomposition problem in each iteration with time complexity $O(d^3)$. By contrast, the proposed SWRLDA naturally avoids the eigen-decomposition and only needs to conduct SVD with time complexity $O(dm^2 + m^3)$. Due to the fact that the original feature dimensionality $d$ is much larger than the reduced dimensionality $m$, the proposed SWRLDA is guaranteed to be much more efficient than the

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**Table 3: Average running times with respect to different methods over six benchmark datasets.**

| Method   | COIL20  | COIL100 | Isolet  | 20Newsgroups | PIE     | YaleB    |
|----------|---------|---------|---------|---------------|---------|----------|
| LDA      | 18.95s  | 57.13s  | 12.70s  | >24h          | 12.18s  | 5.94s    |
| RSLDA    | 10.61s  | 47.95s  | 22.43s  | >24h          | 27.39s  | 6.81s    |
| aPAC     | 14.94s  | 54.11s  | 2.286s  | >24h          | 7.95s   | 5.49s    |
| GMSS     | 20.31s  | 57.90s  | 11.97s  | >24h          | 13.14s  | 6.38s    |
| HMSS     | 21.24s  | 60.30s  | 12.48s  | >24h          | 13.25s  | 6.37s    |
| STRDA    | 29.47s  | 143.22s | 30.94s  | >24h          | 126.38s | 106.26s  |
| MMDA     | 25.17s  | 90.94s  | 18.29s  | >24h          | 71.26s  | 40.01s   |
| SWRLDA   | 0.63s   | 2.11s   | 0.36s   | 51.25s        | 0.65s   | 0.37s    |

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Figure 6: Visualization of Wine dataset projected onto a two-dimensional subspace learned by different methods.
with different random initializations, which indicates that the solution obtained by our iterative algorithm is a global optimum on these data sets in practice.

In this part, we test the convergence speed of the proposed SWRLDA on all the employed datasets in Fig. 8. Specifically, we use 50 times different random initializations of $W$ to calculate objective function value in each iteration until converge. For each employed dataset, the mean and standard deviation of the objective function value in each iteration are illustrated in Fig. 8. Notably, the objective function value of our method converges in 13 iterations on all the datasets, which can be regarded as an attempt to simulate an edge class to some extent. With 20, 40, 60 and 80 percentage of images corrupted in each class, the recognition accuracy with respect to varying number of corrupted classes ranging from 0 to 15 over CMU PIE and YaleB is demonstrated in Figure 7. Note that SWRLDA only achieves slightly better performance than the comparisons without corrupted class. As the number of corrupted classes increases, all the comparisons have varying degrees of performance degradation, while the superiority of SWRLDA becomes more obvious. The performance of competitors decreases dramatically while the performance of our method keeps more stable, which demonstrates the strong robustness of SWRLDA.

4.2.7 Convergence Analysis

In this part, we test the convergence speed of the proposed SWRLDA on all the employed datasets in Fig. 8. Specifically, we use 50 times different random initializations of $W$ to calculate objective function value in each iteration until converge. For each employed dataset, the mean and standard deviation of the objective function value in each iteration are illustrated in Fig. 8. Notably, the objective function value of our method converges in 4 iterations on all the datasets, and thus the convergence speed is very fast. Moreover, the objective function value will converge to a stable value with different random initializations, which indicates that the solution obtained by our iterative algorithm is a global optimum on these data sets in practice.

Experimental results on both synthetic and real-world datasets demonstrate that the proposed method achieves comparable or even better performance than other methods. We can attribute this improvement to the combination of avoiding

Figure 7: Recognition accuracy with (a) 20% (b) 40% (c) 60% (d) 80% corrupted samples in each corrupted class over CMU PIE and (e) 20% (f) 40% (g) 60% (h) 80% corrupted samples in each corrupted class over YaleB.

comparison methods. For fair comparison, the average running times of each method over each dataset with $c - 1$ reduced dimension are demonstrated in Table 3. From Table 3, we can make the following two observations:

- For 20Newsgroups with a very large number of samples and features, all the comparison methods become infeasible due to the intractable computation complexity ($> 24$ h). This is because they need to produce and store large matrices that cannot be fit into the memory when both sample number and feature dimension are large.
- The proposed SWRLDA only takes several seconds to finish the run over the large-scale 20Newsgroups dataset, which presents its high efficiency for handling large-scale dimensionality reduction problems. For the other smaller datasets, the calculation time of SWRLDA is also noticeably shorter (15 times) than other algorithms.

4.2.6 The Evaluation of Robustness

To evaluate the robustness of the proposed SWRLDA, we further design a face recognition experiment over CMU PIE and YaleB with pixel corruption. Specifically, a certain proportion of samples are randomly selected from a class to be corrupted with “salt and pepper” noise and the corruption degree of each image is 30%, which can be regarded as an attempt to simulate an edge class to some extent. With 20, 40, 60 and 80 percentage of images corrupted in each class, the recognition accuracy with respect to varying number of corrupted classes ranging from 0 to 15 over CMU PIE and YaleB is demonstrated in Figure 7. Note that SWRLDA only achieves slightly better performance than the comparisons without corrupted class. As the number of corrupted classes increases, all the comparisons have varying degrees of performance degradation, while the superiority of SWRLDA becomes more obvious. The performance of competitors decreases dramatically while the performance of our method keeps more stable, which demonstrates the strong robustness of SWRLDA.
optimal mean strategy and self-weighted between-class distance criterion based on $\ell_{2,1}$-norm. Benefiting from the efficient re-weighted optimization algorithm, SWRLDA enjoys a very fast convergence speed and is able to obtain the global optimal solution after optimization. Particularly, with a reduced computation complexity superior to most other methods, SWRLDA is more efficient for dealing with large-scale dimension reduction problems.

5 Conclusion

In this paper, we propose a novel formulation of self-weighted robust LDA for multi-class classification with edge classes, termed as SWRLDA. Considering the fact that the total mean of data is easily dominated by edge classes, the between-class scatter matrix is equivalently redefined as the difference between every two class centers to automatically avoid the calculation of optimal mean. Since the $\ell_2$-norm based distance criterion is prone to overemphasize the class pairs with large distances and neglects the small ones, a $\ell_{2,1}$-norm based between-class distance criterion is exploited in SWRLDA to further enhance its robustness to edge classes. By optimizing the objective function of SWRLDA with an effective re-weighted algorithm, self-adaptive weights are learned for each class pair to characterize its contribution to classification without tuning additional parameters. Extensive experiments on two synthetic and six real-world datasets demonstrate the effectiveness and superiority of the proposed approach.

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