

Sparse Discriminant Analysis

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Abstract

We consider the problem of performing interpretable classification in the high-dimensional setting, in which the number of features is very large and the number of observations is limited. This setting has been studied extensively in the chemometrics literature, and more recently has become commonplace in biological and medical applications. In this setting, a traditional approach involves performing feature selection before classification. We propose sparse discriminant analysis, a method for performing linear discriminant analysis with a sparseness criterion imposed such that classification and feature selection are performed simultaneously. Sparse discriminant analysis is based on the optimal scoring interpretation of linear discriminant analysis, and can be extended to perform sparse discrimination via mixtures of Gaussians if boundaries between classes are non-linear or if subgroups are present within each class. Our proposal also provides low-dimensional views of the discriminative directions.

1 Introduction

Linear discriminant analysis (LDA) is a favored tool for supervised classification in many applications, due to its simplicity, robustness, and predictive accuracy (Hand, 2006). LDA also provides low-dimensional projections of the data onto the most discriminative directions, which can be useful for data interpretation. There are three distinct arguments that result in the LDA classifier: the multivariate Gaussian model, Fisher’s discriminant problem, and the optimal scoring problem. These are reviewed in Section 2.1.

Though LDA often performs quite well in simple, low-dimensional settings, it is known to fail in the following cases:

- When the number of predictor variables p is large relative to the number of observations n . In this case, LDA cannot be applied directly because the within-class covariance matrix of the features is singular.
- When a single prototype per class is insufficient.
- When linear boundaries cannot separate the classes.

Moreover, in some cases where $p \gg n$, one may wish for a classifier that performs feature selection - that is, a classifier that involves only a subset of the p features. Such a *sparse* classifier ensures easier model interpretation and may reduce overfitting of the training data.

In this paper, we develop a sparse version of LDA using an ℓ_1 or *lasso* penalty (Tibshirani, 1996). The use of an ℓ_1 penalty to achieve sparsity has been studied extensively in the regression framework (Tibshirani, 1996; Efron et al., 2004; Zou and Hastie, 2005; Zou et al., 2006). If \mathbf{X} is a $n \times p$ data matrix and \mathbf{y} is an outcome vector of length n , then the lasso solves the problem

$$\text{minimize}_{\boldsymbol{\beta}} \{ \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda \|\boldsymbol{\beta}\|_1 \} \tag{1}$$

and the elastic net (Zou and Hastie, 2005) solves the problem

$$\text{minimize}_{\boldsymbol{\beta}}\{\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda\|\boldsymbol{\beta}\|_1 + \gamma\|\boldsymbol{\beta}\|^2\} \quad (2)$$

where λ and γ are nonnegative tuning parameters. When λ is large, then both the lasso and the elastic net will yield sparse coefficient vector estimates. Through the additional use of an ℓ_2 penalty, the elastic net provides some advantages over the lasso: correlated features tend to be assigned similar regression coefficients, and more than $\min(n, p)$ features can be included in the model. In this paper, we apply an elastic net penalty to the coefficient vectors in the optimal scoring interpretation of LDA in order to develop a sparse version of discriminant analysis. This is related to proposals by Grosenick et al. (2008) and Leng (2008). Since our proposal is based on the optimal scoring framework, we are able to extend it to mixtures of Gaussians (Hastie and Tibshirani, 1996).

There already exist a number of proposals to extend LDA to the high-dimensional setting. Some of these proposals involve non-sparse classifiers. For instance, within the multivariate Gaussian model for LDA, Dudoit et al. (2001) and Bickel and Levina (2004) assume independence of the features (naive Bayes), and Friedman (1989) suggests applying a ridge penalty to the within-class covariance matrix. Other positive definite estimates of the within-class covariance matrix are considered by Krzanowski et al. (1995) and Xu et al. (2009). Some proposals that lead to sparse classifiers have also been considered: Tibshirani et al. (2002) adapt the naive Bayes classifier by soft-thresholding the mean vectors, and Guo et al. (2007) combine a ridge-type penalty on the within-class covariance matrix with a soft-thresholding operation. Witten and Tibshirani (2011) apply ℓ_1 penalties to Fisher’s discriminant problem in order to obtain sparse discriminant vectors, but this approach cannot be extended to the Gaussian mixture setting and lacks the simplicity of the regression-based optimal

scoring approach that we take in this paper.

The rest of this paper is organized as follows. In Section 2, we review LDA and we present our proposals for sparse discriminant analysis and sparse mixture discriminant analysis. Section 3 briefly describes three methods to which we will compare our proposal: shrunken centroids regularized discriminant analysis, sparse partial least squares, and elastic net regression of dummy variables. Section 4 contains experimental results, and the discussion is in Section 5.

2 Methodology

2.1 A review of linear discriminant analysis

Let \mathbf{X} be a $n \times p$ data matrix, and suppose that each of the n observations falls into one of K classes. Assume that each of the p features has been centered to have mean zero, and that the features have been standardized to have equal variance if they are not measured on the same scale. Let \mathbf{x}_i denote the i th observation, and let C_k denote the indices of the observations in the k th class. Consider a very simple multivariate Gaussian model for the data, in which we assume that an observation in class k is distributed $N(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_w)$ where $\boldsymbol{\mu}_k \in \mathbb{R}^p$ is the mean vector for class k and $\boldsymbol{\Sigma}_w$ is a $p \times p$ pooled *within-class covariance matrix* common to all K classes. We use $\frac{1}{|C_k|} \sum_{i \in C_k} \mathbf{x}_i$ as an estimate for $\boldsymbol{\mu}_k$, and we use $\frac{1}{n} \sum_{k=1}^K \sum_{i \in C_k} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T$ as an estimate for $\boldsymbol{\Sigma}_w$ (see e.g. Hastie et al., 2009). The LDA classification rule then results from applying Bayes' rule to estimate the most likely class for a test observation.

LDA can also be seen as arising from Fisher's discriminant problem. Define the *between-class covariance matrix* $\boldsymbol{\Sigma}_b = \sum_{k=1}^K \pi_k \boldsymbol{\mu}_k \boldsymbol{\mu}_k^T$, where π_k is the prior probability for class k (generally estimated as the fraction of observations belonging to class k). Fisher's discriminant problem involves seeking *discriminant vectors* $\boldsymbol{\beta}_1, \dots, \boldsymbol{\beta}_{K-1}$

that successively maximize

$$\text{maximize}_{\beta_k} \{\beta_k^T \Sigma_b \beta_k\} \text{ subject to } \beta_k^T \Sigma_w \beta_k = 1, \beta_k^T \Sigma_w \beta_l = 0 \forall l < k. \quad (3)$$

Since Σ_b has rank at most $K - 1$, there are at most $K - 1$ non-trivial solutions to the generalized eigen problem (3), and hence at most $K - 1$ discriminant vectors. These solutions are directions upon which the data has maximal between-class variance relative to its within-class variance. One can show that nearest centroid classification on the matrix $(\mathbf{X}\beta_1 \dots \mathbf{X}\beta_{K-1})$ yields the same LDA classification rule as the multivariate Gaussian model described previously (see e.g. Hastie et al., 2009). Fisher’s discriminant problem has an advantage over the multivariate Gaussian interpretation of LDA, in that one can perform *reduced-rank* classification by performing nearest centroid classification on the matrix $(\mathbf{X}\beta_1 \dots \mathbf{X}\beta_q)$ with $q < K - 1$. One can show that performing nearest centroid classification on this $n \times q$ matrix is exactly equivalent to performing full-rank LDA on this $n \times q$ matrix. We will make use of this fact later. Fisher’s discriminant problem also leads to a tool for data visualization, since it can be informative to plot the vectors $\mathbf{X}\beta_1$, $\mathbf{X}\beta_2$, and so on.

In this paper, we will make use of *optimal scoring*, a third formulation that yields the LDA classification rule and is discussed in detail in Hastie et al. (1995). It involves recasting the classification problem as a regression problem by turning categorical variables into quantitative variables, via a sequence of *scorings*. Let \mathbf{Y} denote a $n \times K$ matrix of dummy variables for the K classes; Y_{ik} is an indicator variable for whether the i th observation belongs to the k th class. The optimal scoring criterion takes the form

$$\text{minimize}_{\beta_k, \theta_k} \{ \|\mathbf{Y}\theta_k - \mathbf{X}\beta_k\|^2 \} \text{ subject to } \frac{1}{n} \theta_k^T \mathbf{Y}^T \mathbf{Y} \theta_k = 1, \theta_k^T \mathbf{Y}^T \mathbf{Y} \theta_l = 0 \forall l < k, \quad (4)$$

where θ_k is a K -vector of scores, and β_k is a p -vector of variable coefficients. Since

the columns of \mathbf{X} are centered to have mean zero, we can see that the constant score vector $\mathbf{1}$ is trivial, since $\mathbf{Y}\mathbf{1} = \mathbf{1}$ is an n -vector of 1's and is orthogonal to all of the columns of \mathbf{X} . Hence there are at most $K - 1$ non-trivial solutions to (4). Letting $\mathbf{D}_\pi = \frac{1}{n}\mathbf{Y}^T\mathbf{Y}$ be a diagonal matrix of class proportions, the constraints in (4) can be written as $\boldsymbol{\theta}_k^T\mathbf{D}_\pi\boldsymbol{\theta}_k = 1$ and $\boldsymbol{\theta}_k^T\mathbf{D}_\pi\boldsymbol{\theta}_l = 0$ for $l < k$. One can show that the p -vector $\boldsymbol{\beta}_k$ that solves (4) is proportional to the solution to (3), and hence we will also refer to the vector $\boldsymbol{\beta}_k$ that solves (4) as the k th discriminant vector. Therefore, performing full-rank LDA on the $n \times q$ matrix $\left(\mathbf{X}\boldsymbol{\beta}_1 \dots \mathbf{X}\boldsymbol{\beta}_q\right)$ yields the rank- q classification rule obtained from Fisher's discriminant problem.

2.2 Sparse discriminant analysis

Since $\boldsymbol{\Sigma}_w$ does not have full rank when the number of features is large relative to the number of observations, LDA cannot be performed. One approach to overcome this problem involves using a regularized estimate of the within-class covariance matrix in Fisher's discriminant problem (3). For instance, one possibility is

$$\text{maximize}_{\boldsymbol{\beta}_k} \{\boldsymbol{\beta}_k^T \boldsymbol{\Sigma}_b \boldsymbol{\beta}_k\} \text{ subject to } \boldsymbol{\beta}_k^T (\boldsymbol{\Sigma}_w + \boldsymbol{\Omega}) \boldsymbol{\beta}_k = 1, \boldsymbol{\beta}_k^T (\boldsymbol{\Sigma}_w + \boldsymbol{\Omega}) \boldsymbol{\beta}_l = 0 \forall l < k \quad (5)$$

with $\boldsymbol{\Omega}$ a positive definite matrix. This approach is taken in Hastie et al. (1995). Then $\boldsymbol{\Sigma}_w + \boldsymbol{\Omega}$ is positive definite and so the discriminant vectors in (5) can be calculated even if $p \gg n$. Moreover, for an appropriate choice of $\boldsymbol{\Omega}$, (5) can result in smooth discriminant vectors. However, in this paper, we are instead interested in a technique for obtaining *sparse* discriminant vectors. One way to do this is by applying a ℓ_1 penalty in (5), resulting in the optimization problem

$$\text{maximize}_{\boldsymbol{\beta}_k} \{\boldsymbol{\beta}_k^T \boldsymbol{\Sigma}_b \boldsymbol{\beta}_k - \gamma \|\boldsymbol{\beta}_k\|_1\} \text{ subject to } \boldsymbol{\beta}_k^T (\boldsymbol{\Sigma}_w + \boldsymbol{\Omega}) \boldsymbol{\beta}_k = 1, \boldsymbol{\beta}_k^T (\boldsymbol{\Sigma}_w + \boldsymbol{\Omega}) \boldsymbol{\beta}_l = 0 \forall l < k. \quad (6)$$

Indeed, this approach is taken in Witten and Tibshirani (2011). Solving (6) is challenging, since it is not a convex problem and so specialized techniques, such as the minorization-maximization approach pursued in Witten and Tibshirani (2011), must be applied. In this paper, we instead apply ℓ_1 penalties to the optimal scoring formulation for LDA (4).

Our sparse discriminant analysis (SDA) criterion is defined sequentially. The k th SDA solution pair $(\boldsymbol{\theta}_k, \boldsymbol{\beta}_k)$ solves the problem

$$\begin{aligned} & \text{minimize}_{\boldsymbol{\beta}_k, \boldsymbol{\theta}_k} \quad \{ \|\mathbf{Y}\boldsymbol{\theta}_k - \mathbf{X}\boldsymbol{\beta}_k\|^2 + \gamma \boldsymbol{\beta}_k^T \boldsymbol{\Omega} \boldsymbol{\beta}_k + \lambda \|\boldsymbol{\beta}_k\|_1 \} \\ & \text{subject to} \quad \frac{1}{n} \boldsymbol{\theta}_k^T \mathbf{Y}^T \mathbf{Y} \boldsymbol{\theta}_k = 1, \boldsymbol{\theta}_k^T \mathbf{Y}^T \mathbf{Y} \boldsymbol{\theta}_l = 0 \quad \forall l < k, \end{aligned} \quad (7)$$

where $\boldsymbol{\Omega}$ is a positive definite matrix as in (5), and λ and γ are nonnegative tuning parameters. The ℓ_1 penalty on $\boldsymbol{\beta}_k$ results in sparsity when λ is large. We will refer to the $\boldsymbol{\beta}_k$ that solves (7) as the k th SDA discriminant vector. It is shown in Witten and Tibshirani (2011) that critical points of (7) are also critical points of (6). Since neither criterion is convex, we cannot claim these are local minima, but the result does establish an equivalence at this level.

We now consider the problem of solving (7). We propose the use of a simple iterative algorithm for finding a local optimum to (7). The algorithm involves holding $\boldsymbol{\theta}_k$ fixed and optimizing with respect to $\boldsymbol{\beta}_k$, and holding $\boldsymbol{\beta}_k$ fixed and optimizing with respect to $\boldsymbol{\theta}_k$. For fixed $\boldsymbol{\theta}_k$, we obtain

$$\text{minimize}_{\boldsymbol{\beta}_k} \{ \|\mathbf{Y}\boldsymbol{\theta}_k - \mathbf{X}\boldsymbol{\beta}_k\|^2 + \gamma \boldsymbol{\beta}_k^T \boldsymbol{\Omega} \boldsymbol{\beta}_k + \lambda \|\boldsymbol{\beta}_k\|_1 \}, \quad (8)$$

which is an elastic net problem if $\boldsymbol{\Omega} = \mathbf{I}$ and a generalized elastic net problem for an arbitrary symmetric positive semidefinite matrix $\boldsymbol{\Omega}$. (8) can be solved using the algorithm proposed in Zou and Hastie (2005), or using a coordinate descent approach

(Friedman et al., 2007). For fixed β_k , the optimal scores θ_k solve

$$\text{minimize}_{\theta_k} \{ \|\mathbf{Y}\theta_k - \mathbf{X}\beta_k\|^2 \} \text{ subject to } \theta_k^T \mathbf{D}_\pi \theta_k = 1, \theta_k^T \mathbf{D}_\pi \theta_l = 0 \quad \forall l < k \quad (9)$$

where $\mathbf{D}_\pi = \frac{1}{n} \mathbf{Y}^T \mathbf{Y}$. Let \mathbf{Q}_k be the $K \times k$ matrix consisting of the previous $k - 1$ solutions θ_k , as well as the trivial solution vector of all 1's. One can show that the solution to (9) is given by $\theta_k = s \cdot (\mathbf{I} - \mathbf{Q}_k \mathbf{Q}_k^T \mathbf{D}_\pi) \mathbf{D}_\pi^{-1} \mathbf{Y}^T \mathbf{X} \beta_k$, where s is a proportionality constant such that $\theta_k^T \mathbf{D}_\pi \theta_k = 1$. Note that $\mathbf{D}_\pi^{-1} \mathbf{Y}^T \mathbf{X} \beta_k$ is the unconstrained estimate for θ_k , and the term $(\mathbf{I} - \mathbf{Q}_k \mathbf{Q}_k^T \mathbf{D}_\pi)$ is the orthogonal projector (in \mathbf{D}_π) onto the subspace of \mathbb{R}^K orthogonal to \mathbf{Q}_k .

Once sparse discriminant vectors have been obtained, we can plot the vectors $\mathbf{X}\beta_1, \mathbf{X}\beta_2$, and so on in order to perform data visualization in the reduced subspace. The classification rule is obtained by performing standard LDA on the the $n \times q$ reduced data matrix $\begin{pmatrix} \mathbf{X}\beta_1 & \dots & \mathbf{X}\beta_q \end{pmatrix}$ with $q < K$. In summary, the SDA algorithm is given in Algorithm 1.

2.3 Sparse mixture of Gaussians

2.3.1 A review of mixture discriminant analysis

LDA will tend to perform well if there truly are K distinct classes separated by linear decision boundaries. However, if a single prototype per class is insufficient for capturing the class structure, then LDA will perform poorly. Hastie and Tibshirani (1996) proposed *mixture discriminant analysis* (MDA) to overcome the shortcomings of LDA in this setting. We review the MDA proposal here.

Rather than modeling the observations within each class as multivariate Gaussian with a class-specific mean vector and a common within-class covariance matrix, in MDA one instead models each class as a mixture of Gaussians in order to achieve increased flexibility. The k th class, $k = 1, \dots, K$, is divided into R_k subclasses,

Algorithm 1 Sparse Discriminant Analysis

1. Let \mathbf{Y} be a $n \times K$ matrix of indicator variables, $Y_{ij} = 1_{i \in C_k}$.
 2. Let $\mathbf{D}_\pi = \frac{1}{n} \mathbf{Y}^T \mathbf{Y}$.
 3. Initialize $k = 1$, and let \mathbf{Q}_1 be a $K \times 1$ matrix of 1's.
 4. For $k = 1, \dots, q$, compute a new SDA direction pair $(\boldsymbol{\theta}_k, \boldsymbol{\beta}_k)$ as follows:
 - (a) Initialize $\boldsymbol{\theta}_k = (\mathbf{I} - \mathbf{Q}_k \mathbf{Q}_k^T \mathbf{D}_\pi) \boldsymbol{\theta}_*$, where $\boldsymbol{\theta}_*$ is a random K -vector, and then normalize $\boldsymbol{\theta}_k$ so that $\boldsymbol{\theta}_k^T \mathbf{D}_\pi \boldsymbol{\theta}_k = 1$.
 - (b) Iterate until convergence or until a maximum number of iterations is reached:
 - i. Let $\boldsymbol{\beta}_k$ be the solution to the generalized elastic net problem

$$\text{minimize}_{\boldsymbol{\beta}_k} \left\{ \frac{1}{n} \|\mathbf{Y} \boldsymbol{\theta}_k - \mathbf{X} \boldsymbol{\beta}_k\|^2 + \gamma \boldsymbol{\beta}_k^T \boldsymbol{\Omega} \boldsymbol{\beta}_k + \lambda \|\boldsymbol{\beta}_k\|_1 \right\}. \quad (10)$$
 - ii. For fixed $\boldsymbol{\beta}_k$ let

$$\tilde{\boldsymbol{\theta}}_k = (\mathbf{I} - \mathbf{Q}_k \mathbf{Q}_k^T \mathbf{D}_\pi) \mathbf{D}_\pi^{-1} \mathbf{Y}^T \mathbf{X} \boldsymbol{\beta}_k, \quad \boldsymbol{\theta}_k = \tilde{\boldsymbol{\theta}}_k / \sqrt{\tilde{\boldsymbol{\theta}}_k^T \mathbf{D}_\pi \tilde{\boldsymbol{\theta}}_k}. \quad (11)$$
 - (c) If $k < q$, set $\mathbf{Q}_{k+1} = (\mathbf{Q}_k : \boldsymbol{\theta}_k)$.
 5. The classification rule results from performing standard LDA with the $n \times q$ matrix $(\mathbf{X} \boldsymbol{\beta}_1 \mathbf{X} \boldsymbol{\beta}_2 \cdots \mathbf{X} \boldsymbol{\beta}_q)$.
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and we define $R = \sum_{k=1}^K R_k$. It is assumed that the r th subclass in class k , $r = 1, 2, \dots, R_k$, has a multivariate Gaussian distribution with a subclass-specific mean vector $\boldsymbol{\mu}_{kr} \in \mathbb{R}^p$ and a common $p \times p$ covariance matrix $\boldsymbol{\Sigma}_w$. We let Π_k denote the prior probability for the k th class, and π_{kr} the mixing probability for the r th subclass, with $\sum_{r=1}^{R_k} \pi_{kr} = 1$. The Π_k can be easily estimated from the data, but the π_{kr} are unknown model parameters.

Hastie and Tibshirani (1996) suggest employing the expectation-maximization (EM) algorithm in order to estimate the subclass-specific mean vectors, the within-class covariance matrix, and the subclass mixing probabilities. In the expectation step, one estimates the probability that the i th observation belongs to the r th sub-

class of the k th class, given that it belongs to the k th class:

$$p(c_{kr}|\mathbf{x}_i, i \in C_k) = \frac{\pi_{kr} \exp(-(\mathbf{x}_i - \boldsymbol{\mu}_{kr})^T \boldsymbol{\Sigma}_w^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_{kr})/2)}{\sum_{r'=1}^{R_k} \pi_{kr'} \exp(-(\mathbf{x}_i - \boldsymbol{\mu}_{kr'})^T \boldsymbol{\Sigma}_w^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_{kr'})/2)}, r = 1, \dots, R_k. \quad (12)$$

In (12), c_{kr} is shorthand for the event that the observation \mathbf{x}_i is in the r th subclass of the k th class. In the maximization step, estimates are updated for the subclass mixing probabilities as well as the subclass-specific mean vectors and the pooled within-class covariance matrices:

$$\pi_{kr} = \frac{\sum_{i \in C_k} p(c_{kr}|\mathbf{x}_i, i \in C_k)}{\sum_{r'=1}^{R_k} \sum_{i \in C_k} p(c_{kr'}|\mathbf{x}_i, i \in C_k)}, \quad (13)$$

$$\boldsymbol{\mu}_{kr} = \frac{\sum_{i \in C_k} \mathbf{x}_i p(c_{kr}|\mathbf{x}_i, i \in C_k)}{\sum_{i \in C_k} p(c_{kr}|\mathbf{x}_i, i \in C_k)}, \quad (14)$$

$$\boldsymbol{\Sigma}_w = \frac{1}{n} \sum_{k=1}^K \sum_{i \in C_k} \sum_{r=1}^{R_k} p(c_{kr}|\mathbf{x}_i, i \in C_k) (\mathbf{x}_i - \boldsymbol{\mu}_{kr})(\mathbf{x}_i - \boldsymbol{\mu}_{kr})^T. \quad (15)$$

The EM algorithm proceeds by iterating between equations (12)-(15) until convergence. Hastie and Tibshirani (1996) also present an extension of this EM approach to accommodate a reduced-rank LDA solution via optimal scoring, which we extend in the next section.

2.3.2 The sparse mixture discriminant analysis proposal

We now describe our *sparse mixture discriminant analysis* (SMDA) proposal. We define \mathbf{Z} , a $n \times R$ *blurred response matrix*, which is a matrix of subclass probabilities. If the i th observation belongs to the k th class, then the i th row of \mathbf{Z} contains the values $p(c_{k1}|\mathbf{x}_i, i \in C_k), \dots, p(c_{kR_k}|\mathbf{x}_i, i \in C_k)$ in the k th block of R_k entries, and 0's elsewhere. \mathbf{Z} is the mixture analog of the indicator response matrix \mathbf{Y} . We extend the MDA algorithm presented in Section 2.3.1 by performing SDA using \mathbf{Z} , rather than \mathbf{Y} , as the indicator response matrix. Then rather than using the raw data \mathbf{X}

in performing the EM updates (12)-(15), we instead use the transformed data \mathbf{XB} where $\mathbf{B} = \begin{pmatrix} \beta_1 & \dots & \beta_q \end{pmatrix}$ and where $q < R$. Details are provided in Algorithm 2. This algorithm yields a classification rule for assigning class membership to a test observation. Moreover, the matrix \mathbf{XB} serves as a q -dimensional graphical projection of the data.

3 Methods for comparison

In Section 4, we will compare SDA to shrunken centroids regularized discriminant analysis (RDA; Guo et al., 2007), sparse partial least squares regression (SPLS; Chun and Keles, 2010), and elastic net (EN) regression of dummy variables.

3.1 Shrunken centroids regularized discriminant analysis

Shrunken centroids regularized discriminant analysis (RDA) is based on the same underlying model as LDA, i.e. normally distributed data with equal dispersion (Guo et al., 2007). The method regularizes the within-class covariance matrix used by LDA,

$$\tilde{\Sigma}_w = \alpha \hat{\Sigma}_w + (1 - \alpha)\mathbf{I} \quad (21)$$

for some α , $0 \leq \alpha \leq 1$, where $\hat{\Sigma}_w$ is the standard estimate of the within-class covariance matrix used in LDA. In order to perform feature selection, one can perform soft-thresholding of the quantity $\tilde{\Sigma}_w^{-1} \boldsymbol{\mu}_k$, where $\boldsymbol{\mu}_k$ is the observed mean vector for the k th class. That is, we compute

$$\text{sgn}(\tilde{\Sigma}_w^{-1} \boldsymbol{\mu}_k)(|\tilde{\Sigma}_w^{-1} \boldsymbol{\mu}_k| - \Delta)_+, \quad (22)$$

and use (22) instead of $\Sigma_w^{-1} \boldsymbol{\mu}_k$ in the Bayes' classification rule arising from the multivariate Gaussian model. The R package `rda` is available from CRAN (2009).

Algorithm 2 Sparse Mixture Discriminant Analysis

1. Initialize the subclass probabilities, $p(c_{kr}|\mathbf{x}_i, i \in C_k)$, for instance by performing R_k -means clustering within the k th class.
2. Use the subclass probabilities to create the $n \times R$ blurred response matrix \mathbf{Z} .
3. Iterate until convergence or until a maximum number of iterations is reached:
 - (a) Using \mathbf{Z} instead of \mathbf{Y} , perform SDA in order to find a sequence of $q < R$ pairs of score vectors and discriminant vectors, $\{\boldsymbol{\theta}_k, \boldsymbol{\beta}_k\}_{k=1}^q$.
 - (b) Compute $\tilde{\mathbf{X}} = \mathbf{X}\mathbf{B}$, where $\mathbf{B} = (\boldsymbol{\beta}_1 \cdots \boldsymbol{\beta}_q)$.
 - (c) Compute the weighted means, covariance, and mixing probabilities using equations (13)-(15), substituting $\tilde{\mathbf{X}}$ instead of \mathbf{X} . That is,

$$\pi_{kr} = \frac{\sum_{i \in C_k} p(c_{kr}|\tilde{\mathbf{x}}_i, i \in C_k)}{\sum_{r'=1}^{R_k} \sum_{i \in C_k} p(c_{kr'}|\tilde{\mathbf{x}}_i, i \in C_k)}, \quad (16)$$

$$\tilde{\boldsymbol{\mu}}_{kr} = \frac{\sum_{i \in C_k} \tilde{\mathbf{x}}_i p(c_{kr}|\tilde{\mathbf{x}}_i, i \in C_k)}{\sum_{i \in C_k} p(c_{kr}|\tilde{\mathbf{x}}_i, i \in C_k)}, \quad (17)$$

$$\tilde{\boldsymbol{\Sigma}}_w = \frac{1}{n} \sum_{k=1}^K \sum_{i \in C_k} \sum_{r=1}^{R_k} p(c_{kr}|\tilde{\mathbf{x}}_i, i \in C_k) (\tilde{\mathbf{x}}_i - \tilde{\boldsymbol{\mu}}_{kr})(\tilde{\mathbf{x}}_i - \tilde{\boldsymbol{\mu}}_{kr})^T. \quad (18)$$

- (d) Compute the subclass probabilities using equation (12), substituting $\tilde{\mathbf{X}}$ instead of \mathbf{X} and using the current estimates for the weighted means, covariance, and mixing probabilities, as follows:

$$p(c_{kr}|\tilde{\mathbf{x}}_i, i \in C_k) = \frac{\pi_{kr} \exp(-(\tilde{\mathbf{x}}_i - \tilde{\boldsymbol{\mu}}_{kr})^T \tilde{\boldsymbol{\Sigma}}_w^{-1} (\tilde{\mathbf{x}}_i - \tilde{\boldsymbol{\mu}}_{kr})/2)}{\sum_{r'=1}^{R_k} \pi_{kr'} \exp(-(\tilde{\mathbf{x}}_i - \tilde{\boldsymbol{\mu}}_{kr'})^T \tilde{\boldsymbol{\Sigma}}_w^{-1} (\tilde{\mathbf{x}}_i - \tilde{\boldsymbol{\mu}}_{kr'})/2)}. \quad (19)$$

- (e) Using the subclass probabilities, update the blurred response matrix \mathbf{Z} .
4. The classification rule results from assigning a test observation $\mathbf{x}_{test} \in \mathbb{R}^p$ to the class for which

$$\Pi_k \sum_{r=1}^{R_k} \pi_{kr} \exp(-(\tilde{\mathbf{x}}_i - \tilde{\boldsymbol{\mu}}_{kr})^T \tilde{\boldsymbol{\Sigma}}_w^{-1} (\tilde{\mathbf{x}}_i - \tilde{\boldsymbol{\mu}}_{kr})/2) \quad (20)$$

is largest.

3.2 Sparse partial least squares

In the chemometrics literature, partial least squares (PLS) is a widely used regression method in the $p \gg n$ setting (see for instance Indahl et al., 2009; Barker and Rayens,

2003; Indahl et al., 2007). Sparse PLS (SPLS) is an extension of PLS that uses the lasso to promote sparsity of a surrogate direction vector \mathbf{c} instead of the original latent direction vector $\boldsymbol{\alpha}$, while keeping $\boldsymbol{\alpha}$ and \mathbf{c} close (Chun and Keles, 2010). That is, the first SPLS direction vector solves

$$\text{minimize}_{\boldsymbol{\alpha} \in \mathbb{R}^p, \mathbf{c} \in \mathbb{R}^p} \{-\kappa \boldsymbol{\alpha}^T \mathbf{M} \boldsymbol{\alpha} + (1-\kappa)(\mathbf{c}-\boldsymbol{\alpha})^T \mathbf{M}(\mathbf{c}-\boldsymbol{\alpha}) + \lambda \|\mathbf{c}\|_1 + \gamma \|\mathbf{c}\|^2\} \text{ subject to } \boldsymbol{\alpha}^T \boldsymbol{\alpha} = 1 \quad (23)$$

where $\mathbf{M} = \mathbf{X}^T \mathbf{Y} \mathbf{Y}^T \mathbf{X}$, κ is a tuning parameter with $0 \leq \kappa \leq 1$, and γ and λ are nonnegative tuning parameters. A simple extension of (23) allows for the computation of additional latent direction vectors. Letting $\mathbf{c}_1, \dots, \mathbf{c}_q \in \mathbb{R}^p$ denote the sparse surrogate direction vectors resulting from the SPLS method, we obtained a classification rule by performing standard LDA on the matrix $(\mathbf{X}_{\mathbf{c}_1} \dots \mathbf{X}_{\mathbf{c}_q})$. The R package `spls` is available from CRAN (2009).

3.3 Elastic net regression of dummy variables

As a simple alternative to SDA, we consider performing an elastic net (EN) regression of the matrix of dummy variables \mathbf{Y} onto the data matrix \mathbf{X} , in order to compute a $n \times K$ matrix of fitted values $\hat{\mathbf{Y}}$. This is followed by a (possibly reduced-rank) LDA, treating the fitted value matrix $\hat{\mathbf{Y}}$ as the predictors. The resulting classification rule involves only a subset of the features if the lasso tuning parameter in the elastic net regression is sufficiently large. If the elastic net regression is replaced with standard linear regression, then this approach amounts to standard LDA (see for instance Indahl et al., 2007).

4 Experimental results

This section illustrates results on a number of data sets. In these examples, SDA arrived at a stable solution in fewer than 30 iterations. The tuning parameters for all of the methods considered were chosen using leave-one-out cross-validation on the training data (Hastie et al., 2009). Subsequently, the models with the chosen parameters were evaluated on the test data. Unless otherwise specified, the features were centered to have mean zero and standard deviation one, and the penalty matrix $\Omega = \mathbf{I}$ was used in the SDA formulation.

4.1 Female and male silhouettes

In order to illustrate the sparsity of the SDA discriminant vectors, we consider a shape-based data set consisting of 20 male and 19 female adult face silhouettes. A minimum description length (MDL) approach to annotate the silhouettes was used (Thodberg and Ólafsdóttir, 2003), and Procrustes' alignment was performed on the resulting 65 MDL (x, y) -coordinates. The training set consisted of 22 silhouettes (11 female and 11 male), and there were 17 silhouettes in the test set (8 female and 9 male). Panels (a) and (b) of Figure 1 illustrate the two classes of silhouettes.

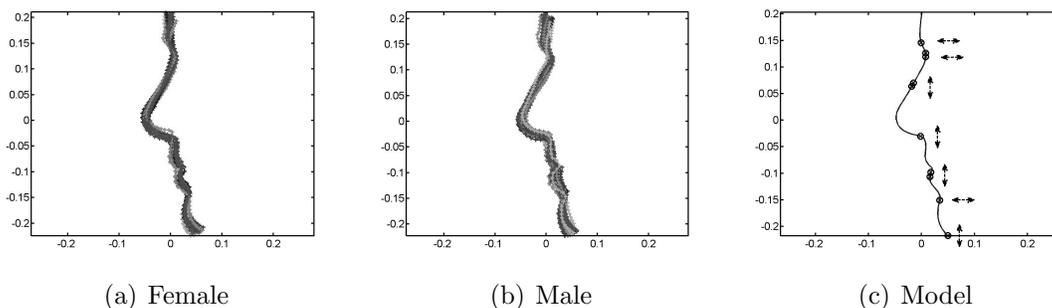


Figure 1: (a) and (b): The silhouettes and the 65 (x, y) -coordinates for the two classes. (c): The mean shape of the silhouettes, and the 10 (x, y) -coordinates in the SDA model. The arrows illustrate the directions of the differences between male and female observations.

We performed SDA in order to classify the observations into male versus female.

Leave-one-out cross validation on the training data resulted in the selection of 10 non-zero features. The SDA results are illustrated in Figure 1(c). Since there are two classes in this problem, there was only one SDA discriminant vector. Note that the non-zero features included in the model were placed near high curvature points in the silhouettes. The training and test classification rates (fraction of observations correctly classified) were both 82%. In the original paper, a logistic regression was performed on a subset of the principal components of the data, where the subset was determined by backwards elimination using a classical statistical test for significance. This resulted in an 85% classification rate on the test set (Thodberg and Ólafsdóttir, 2003). The SDA model has an interpretational advantage, since it reveals the exact locations of the main differences between the two genders.

4.2 Leukemia microarray data

We now consider a leukemia microarray data set published in Yeoh et al. (2002) and available at <http://sdmc.i2r.a-star.edu.sg/rp/>. The study aimed to classify subtypes of pediatric acute lymphoblastic leukemia. The data consisted of 12,558 gene expression measurements for 163 training samples and 85 test samples belonging to 6 cancer classes: BCR-ABL, E2A-PBX1, Hyperdiploid (>50 chromosomes), MLL rearrangement, T-ALL, and TEL-AML1. Analyses were performed on non-normalized data for comparison with the original analysis of Yeoh et al. (2002). In Yeoh et al. (2002), the data were analyzed in two steps: a feature selection step was followed by a classification step, using a decision tree structure such that one group was separated using a support vector machine at each tree node. On this data, SDA resulted in a model with only 30 non-zero features in each of the SDA discriminant vectors. The classification rates obtained by SDA were comparable to or slightly better than those in Yeoh et al. (2002). The results are summarized in Table 1. In comparison, EN resulted in overall classification rates of 98% on both the training

and test sets, with 20 features in the model. Figure 2 displays scatter plots of the six groups projected onto the SDA discriminant vectors.

Table 1: Training and test classification rates using SDA with 30 non-zero features on the leukemia data.

Group	Train	Test
All groups	99%	99%
BCR-ABL	89%	83%
E2A-PBX1	100%	100%
Hyperdiploid	100%	100%
T-ALL	100%	100%
TEL-AML1	100%	100%
MLL	100%	100%

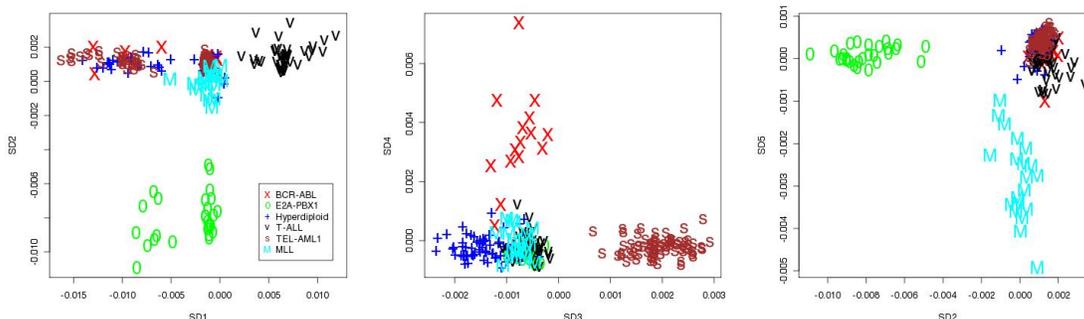


Figure 2: SDA discriminant vectors for the leukemia data set.

4.3 Spectral identification of fungal species

Next, we consider a high-dimensional data set consisting of multi-spectral imaging of three *Penicillium* species: *Melanconodium*, *polonicum*, and *venetum*. The three species all have green/blue conidia (spores) and are therefore visually difficult to distinguish. For each of the three species, four strains were injected onto yeast extract sucrose agar in triplicate, resulting in 36 samples. 3,542 variables were extracted from multi-spectral images with 18 spectral bands – ten in the visual range, and eight in the near infrared range. More details can be found in Clemmensen et al. (2007). The data was partitioned into a training set (24 samples) and a test set (12 samples); one

of the three replicates of each strain was included in the test set. Table 2 summarizes the results. The SDA discriminant vectors are displayed in Figure 3.

Table 2: Classification rates on the *Penicillium* data.

Method	Train	Test	Nonzero loadings
RDA	100%	100%	3502
SPLS	100%	100%	3810
EN	100%	100%	3
SDA	100%	100%	2

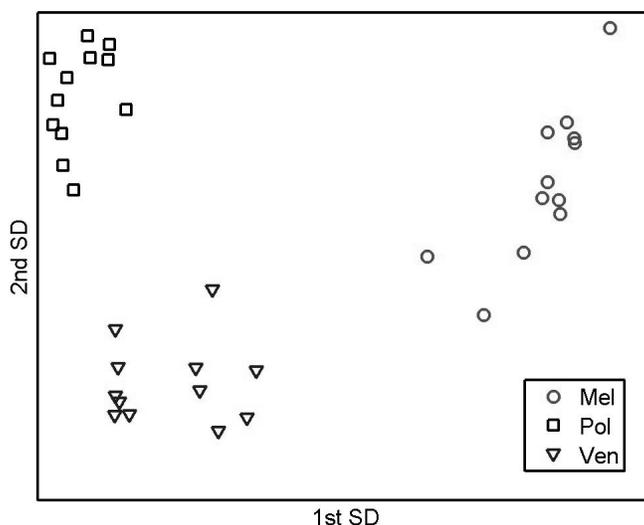


Figure 3: The *Penicillium* data set projected onto the SDA discriminant vectors.

4.4 Classification of fish species based on shape and texture

Here we consider classification of three fish species – cod, haddock, and whiting – on the basis of shape and texture features. The data were taken from Larsen et al. (2009), and consist of texture and shape measurements for 20 cod, 58 haddock, and 30 whiting. The shapes of the fish are represented with coordinates based on MDL. There were 700 coordinates for the contours of the fish, 300 for the mid line, and one for the eye. The shapes were Procrustes aligned to have full correspondence. The

texture features were simply the red, green, and blue intensity values from digitized color images taken with a standard camera under white light illumination. They were annotated to the shapes using a Delauney triangulation approach. In total, there were 103,348 shape and texture features. In Larsen et al. (2009), classification was performed via principal components analysis followed by LDA; this led to a 76% leave-one-out classification rate. Here, we split the data in two: 76 fish for training, and 32 fish for testing. The results are listed in Table 3. In this case, SDA gives the

Table 3: Classification rates for the fish data. RDA (n) and (u) indicate the procedure applied to the normalized and unnormalized data. SPLS was excluded from comparisons for computational reasons.

Method	Train	Test	Nonzero loadings
RDA(n)	100%	41%	103084
RDA(u)	100%	94%	103348
EN	100%	94%	90
SDA	100%	97%	60

most sparse solution and the best test classification rate. Only one of the whiting was misclassified as haddock.

The SDA discriminant vectors are displayed in Figure 4. The first SDA discriminant vector is mainly dominated by blue intensities, and reflects the fact that cod are in general less blue than haddock and whiting around the mid line and mid fin (Larsen et al., 2009). The second SDA discriminant vector suggests that relative to cod and whiting, haddock tends to have more blue around the head and tail, less green around the mid line, more red around the tail, and less red around the eye, the lower part, and the mid line.

5 Discussion

Linear discriminant analysis is a commonly-used method for classification. However, it is known to fail if the true decision boundary between the classes is nonlinear, if

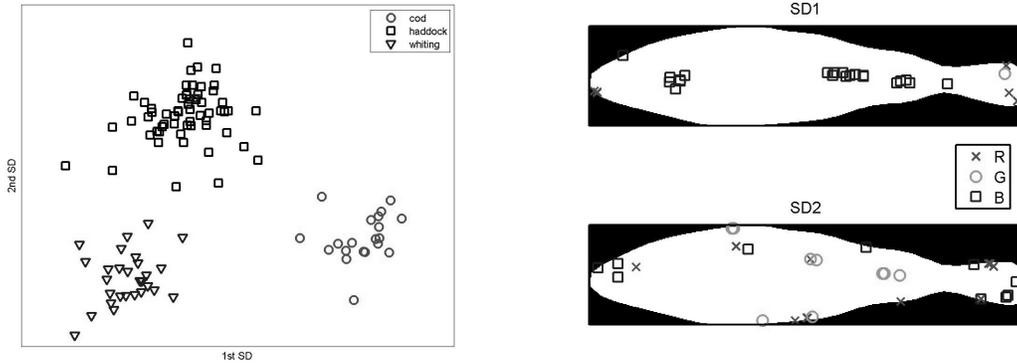


Figure 4: On the left, the projection of the fish data onto the first and second SDA discriminant vectors. On the right, the selected texture features are displayed on the fish mask. The first SDA discriminant vector is mainly dominated by blue intensities whereas the second SDA discriminant vector consists of both red, green, and blue intensities. Only texture features were selected by SDA.

more than one prototype is required in order to properly model each class, or if the number of features is large relative to the number of observations. In this paper, we addressed the latter setting. We proposed an approach for extending LDA to the high-dimensional setting in such a way that the resulting discriminant vectors involve only a subset of the features. Our proposal is based upon the simple optimal scoring framework, which recasts LDA as a regression problem. We are consequently able to make use of existing techniques for performing sparse regression when the number of features is very large relative to the number of observations. Furthermore, our proposal is easily extended to more complex settings, such as the case where the observations from each class are drawn from a mixture of Gaussian distributions.

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