MAIN AND INTERACTION EFFECTS SELECTION FOR QUADRATIC DISCRIMINANT ANALYSIS VIA PENALIZED LINEAR REGRESSION

BY DEQIANG ZHENG†,§, Jinzhu JIA§,† and Xiangzhong Fang§

and Xiuhua Guo‡,¶

School of Public Health, Capital Medical University‡
School of Mathematical Sciences, Peking University§
Beijing Municipal Key Laboratory of Clinical Epidemiology¶

Discriminant analysis is a useful classification method. Variable selection for discriminant analysis is becoming more and more important in a high-dimensional setting. This paper is concerned with the binary-class problems of main and interaction effects selection for the quadratic discriminant analysis. We propose a new penalized quadratic discriminant analysis (QDA) for variable selection in binary classification. Under sparsity assumption on the relevant variables, we conduct a penalized linear regression to derive sparse QDA by plugging the main and interaction effects in the model. Then the QDA problem is converted to a penalized sparse ordinary least squares optimization by using the composite absolute penalties (CAP). Coordinate descent algorithm is introduced to solve the convex penalized least squares. The penalized linear regression can simultaneously select the main and interaction effects, and also conduct classification. Compared with the existing methods of variable selection in QDA, the extensive simulation studies and two real data analyses demonstrate that our proposed method works well and is robust in the performance of variable selection and classification.

1. Introduction. Nowadays supervised classification has been an important problem in various medical fields such as genomic, disease diagnosis and brain imaging. Many classification methods have been developed, including linear and quadratic discriminant analysis (LDA and QDA) (Anderson, 1984), k-nearest-neighbors (Fix and Hodges, 1951), logistic regression (Cox, 1958), classification tree (Breiman et al., 1984) and SVM (Boser et al., 1992). The referred methods above are introduced and summarized in the book

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†Correspondence to: jzjia@math.pku.edu.cn.

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Among many classification methods, discriminant analysis is widely used in many applications due to simplicity, interpretability, and effectiveness. In many cases, it is believed that only a subset of the available variables (also be called features or predictors) may be contained in the classification structure (or model). When irrelevant predictors are added into the model, they may bring in extra noise, and the classification performance may be degraded due to the unstable and inaccurate estimations of the parameters. Therefore, conducting variable selection before fitting the model is advisable. Variable selection can identify fewer discriminative variables and provide a more accurate classification model to describe the future data. Model selection methods are usually used to carry out the variable selection in a probabilistic framework.

A BIC-type criterion for variable selection on quadratic discriminant analysis has been recently studied by Zhang and Wang (2011) and Murphy et al. (2010). The BIC-type model assumes that the relevant variables and irrelevant variables jointly follow a multivariate normal distribution. The relevant variables have different means or covariances in different classes, and irrelevant variables are conditionally independent of the class label. It means that the irrelevant variables can be completely modeled by a multivariate normal distribution conditionally on the relevant variables. The BIC criteria are based on the full likelihood of mixtures of multivariate normal distributions. Zhang and Wang (2011) proposed a standard backward algorithm to find the set of relevant variables, and Murphy et al. (2010) used a forward-backward algorithm for the variable selection. Zhang and Wang (2011) also showed the BIC’s selection consistency under the normal assumption. However, performance may be compromised when this normal assumption does not hold. Moreover, LDA and QDA are inapplicable for the high-dimensional cases when the model dimensionality $p$ exceeds the sample size $n$, since the sample covariance matrices are consequently singular.

Lasso-type regularization methods (Tibshirani, 1996; Zhao and Yu, 2006) are popular in the literature for high-dimensional variable selection. The Lasso-type regularization procedures impose constraints represented by a penalty function, among which $L_1$-norm and $L_2$-norm penalties have been previously explored for variable selection. Fan and Lv (2010) provided a good review on variable selection and penalty functions. In the high-dimensional classification literature, the Lasso-type regularization methods have been frequently used for variable selection. Among them, Cai and Liu (2011) proposed a direct approach to sparse LDA by estimating the product of precision matrix and the mean vector of two classes, and Mai et al. (2012) also introduced a direct approach to transform the LDA problem to a penalized
linear regression. Fan et al. (2015) proposed a two-step procedure to sparse QDA (IIS-SQDA), where an innovated interaction screening approach was explored based on the innovated transform of the precision matrices of two classes in the first step and a sparse quadratic discriminant analysis was presented for further selecting important interactions and main effects and conducting classification simultaneously in the second step. Fan et al. (2015) also proved the consistency of the estimated coefficient vector of QDA, and further showed that the classification error of IIS-SQDA could be infinitely close to the oracle classification error. However, IIS-SQDA is based on the assumption that the variables follow a Gaussian mixture distribution with conditional independence. If the relevant predictors do not follow the normal assumption, many irrelevant predictors can be selected. Even if the relevant predictors and irrelevant predictors are discriminated correctly, the performance of classification may be much compromised.

In this work we consider binary classification problem with possibly unequal means or covariance matrices. Under some sparsity assumption on the relevant variables, we suggest using the penalized linear regression to derive sparse QDA by plugging the main and interaction effects in the model. Motivated by the sparse LDA approach explored by the method of sparse LDA in Mai et al. (2012), we transform the QDA problem to a penalized sparse ordinary least squares optimization. We intuitively suppose that an interaction effect should be added to the regression model only after the corresponding main effects. Therefore, we propose using the composite absolute penalties (CAP) which was introduced by Zhao et al. (2009). Coordinate descent algorithm is presented to solve the convex penalized least squares. The penalized linear regression can simultaneously select the main and interaction effects, and also conduct classification. Extensive simulation studies and real data analysis demonstrate that our proposed method works well and is more robust than the existing methods in both the performance of variable selection and classification error.

The rest of the paper is organized as follows. Section 2 introduces the discriminant analysis and existing variable selection methods. Section 3 proposes the penalized linear regression of sparse quadratic discriminant analysis. The penalized linear regression is established, where the composite absolute penalty is used to carry out variable selection. The coordinate descent algorithm is presented to solve the penalized least squares optimization. Extensive simulation studies and applications to two real data examples are presented in Section 4 and Section 5, respectively. Section 6 concludes with a discussion.
2. Discriminant analysis and existing variable selection methods. We consider a binary classification problem. Let $X \in \mathbb{R}^p$ be a vector of $p$ continuous predictor variables and $G \in \{1, 2\}$ represents the class label. The quadratic discriminate analysis assumes that $P(G = k) = \pi_k > 0$ for $k = 1, 2$ and $X|G = k$ follows a multivariate normal distribution $N(\mu_k, \Sigma_k), k = 1, 2$. Here $\mu_k = (\mu_{k1}, \mu_{k2}, \cdots, \mu_{kp})^T \in \mathbb{R}^p$ and $\Sigma_k \in \mathbb{R}^{p \times p}$ denote the mean vector and covariance matrix for the predictors $X$ in the $k$-th class, respectively. Then the quadratic discriminant function is

$$
\delta_k(x|\pi_k, \mu_k, \Sigma_k) = -\frac{1}{2} \log \det(\Sigma_k) - \frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1}(x - \mu_k) + \log \pi_k, k = 1, 2
$$

where $x \in \mathbb{R}^p$ is the column vector of the predictors for one observation. Let $\hat{\pi}_k, \hat{\mu}_k$ and $\hat{\Sigma}_k$ be the estimates of $\pi_k, \mu_k$ and $\Sigma_k$. Then the optimal Bayes rule minimizing is to predict the new subject as the class with the maximal discriminant function value,

$$
\hat{G} = \arg \max_k \delta_k(x|\hat{\pi}_k, \hat{\mu}_k, \hat{\Sigma}_k), k = 1, 2.
$$

Recently Murphy et al. (2010) and Zhang and Wang (2011) have proposed almost the same variable selection methods based on the BIC criterion for the quadratic discriminant analysis. Let $S = \{j_1, \cdots, j_m\}$ denote a candidate model that contains the $X_{j_1}, \cdots, X_{j_m}$ as the relevant predictors, and $S^c = S_F \setminus S$, where $S_F = \{1, 2, \cdots, p\}$ is the set of all the candidate predictors. The BIC-type criteria are based on the same assumptions:

1. The reverent predictors $X_S$ are the smallest set of the candidate predictors which are sufficient for predicting the class label. The assumption can be described by the following equality

$$
(2.1) \quad P(G = k|X_S, X_{(S^c)}) = P(G = k|X_S),
$$

where $X_S$ and $X_{(S^c)}$ denote the subvector of the predictors corresponding to the set $S$ and $S^c$.

It can be verified that (2.1) is equivalent to saying that the irrelevant predictors are conditionally independent with $G$ given the relevant predictors $X_S$, i.e.,

$$
P(X_{(S^c)}|G, X_S) = P(X_{(S^c)}|X_S).
$$

(2) All of the relevant and irrelevant predictors follow a jointly multivariate normal distribution given the class label. The conditional distribution of the relevant predictors given the class label is

$$
X_S|G = k \sim N(\mu_{k(S)}, \Sigma_{k(S)}),
$$
where $\mu_{k(S)} \in \mathbb{R}^{|S|}$, $\Sigma_{k(S)} \in \mathbb{R}^{(|S|) \times (|S|)}$ is a positive matrix, and $|S|$ is the size of the set $S$. The conditional distribution of the irrelevant predictors given the relevant predictors is

$$X_{i(S^c)}|X_{i(S)} \sim N\left(\mu_{(S)} + B_{(S)}^T X_{S}, \Sigma_{\epsilon(S)} \right),$$

where $\mu_{(S)} \in \mathbb{R}^{p-|S|}$, $B_{(S)} \in \mathbb{R}^{(p-|S|) \times |S|}$, and $\Sigma_{\epsilon(S)} \in \mathbb{R}^{(p-|S|) \times (p-|S|)}$ is a positive definite matrix.

Denote $\theta_{(S)} = \{\mu_{(S)}, B_{(S)}, \Sigma_{\epsilon(S)}, \mu_{k(S)}, \Sigma_{k(S)}, \pi_k, k = 1, 2\}$. Let $(x_i^T, g_i)^T \in \mathbb{R}^{p+1}, i = 1, 2, \ldots, n$ denote the $n$ independent observations, where $x_i = (x_{i1}, x_{i2}, \ldots, x_{ip})^T$ is the associated $p$-dimensional predictors collected from the $i$th subject. If $S$ is the smallest set of the relevant predictors, the full likelihood function $\ell(\theta_{(S)}|x_i, g_i, i = 1, \ldots, n)$ can be written as

$$\ell(\theta_{(S)}|x_i, g_i, i = 1, \ldots, n) = \prod_{i=1}^n P(x_i, g_i|\theta_{(S)})$$

$$= \prod_{i=1}^n P(x_{i(S)}, g_{i(S)}|\mu_{(S)}, B_{(S)}, \Sigma_{\epsilon(S)}) P(x_{i(S)}|g_{i(S)}, \mu_{k(S)}, \Sigma_{k(S)}) P(g_i|\pi_k),$$

where $X_{i(S)}$ and $X_{i(S^c)}$ denote the subvector of the predictors collected from the $i$th subject corresponding to the set $S$ and $S^c$.

Let $\hat{\theta}_{(S)}$ be the maximum likelihood estimators. The BIC proposed by Zhang and Wang (2011) and Murphy et al. (2010) based on the full likelihood is defined as

$$\text{BIC}(S) = -2 \log \ell(\hat{\theta}_{(S)}) + \text{df}(S) \log n,$$

where \text{df}(S) is the number of parameters needed for the model with selected predictors $X_{(S)}$.

Even though the BIC criterion was proved to be consistent, it is not applicable when the sample size $n_k$ is less than the dimension $p$ of the predictors for any class $k = 1, 2$, and is clearly ill-posed if $n_k < p$. When the sample size $n_k$ is less than the dimension $p$, Fan et al. (2015) proposed a two-step procedure for sparse QDA (IIS-SQDA). For the two-class mixture Gaussian
classification, the Bayes rule is an equivalent decision rule of the following form,

\[
Q(x) = \frac{1}{2} x^T (\Sigma_2^{-1} - \Sigma_1^{-1}) x + x^T (\Sigma_1^{-1} \mu_1 - \Sigma_2^{-1} \mu_2) + \zeta,
\]

where \(\zeta\) is some constant depending only on \(\pi_k, \mu_k, \Sigma_k, k = 1, 2\). A new observation \(x\) is predicted as the class 1 if and only if \(Q(x) > 0\). The first step in IIS-SQDA is to sparsify the support \(\Omega = \Sigma_2^{-1} - \Sigma_1^{-1}\) for interaction screening. Two transformations based on the precision matrices are used to find the interaction variables. One regularization method was proposed for further selecting important interactions and main effects in the second step of IIS-SQDA. Although IIS-SQDA is proved to enjoy the sure screening property in selecting the interactions and is close to the oracle classification in the performance of the misclassification, it depends on the Gaussian mixture assumption and is not robust.

3. Regularization methods and coordinate descent algorithm.

The approach to selecting variable proposed in this work is motivated by the Bayes decision function (2.2) for the binary-class QDA. Suppose we numerically code the class labels \(g = 1\) and \(g = 2\), respectively, as \(y = 1\) and \(y = -1\). We use the linear regression model where the predictors are the main and interaction effects of the variables. The coefficients of the linear regression model are estimated by the following least squares

\[
(\hat{\beta}_0^{\text{ols}}, \hat{\beta}_\odot^{\text{ols}}, \hat{\beta}_\otimes^{\text{ols}}) = \arg \min_{\beta_0, \beta_\odot, \beta_\otimes} \sum_{i=1}^{n} (y_i - \beta_0 - x_i^T \beta_\odot - \tilde{x}_i^T \beta_\otimes)^2,
\]

where \(\beta_0 \in \mathbb{R}, \beta_\odot \in \mathbb{R}^p, \beta_\otimes \in \mathbb{R}^{\frac{p(p+1)}{2}}\), and \(\tilde{x}_i\) denotes the vector of all interaction effects with the following form

\[
\tilde{x}_i = (x_{i1}^2, x_{i1}x_{i2}, \cdots, x_{i1}x_{ip}, x_{i2}^2, x_{i2}x_{i3}, \cdots, x_{ip}^2)^T.
\]

Denote \(\hat{\beta} = (\hat{\beta}_0^T, \hat{\beta}_\odot^T, \hat{\beta}_\otimes^T)^T\). For the linear regression model in the variable selection problem, the classical regularized estimates of the parameters \(\beta\) are given by a penalized least squares

\[
\hat{\beta}(\lambda) = \arg \min_{\beta_0, \beta_\odot, \beta_\otimes} \sum_{i=1}^{n} (y_i - \beta_0 - x_i^T \beta_\odot - \tilde{x}_i^T \beta_\otimes)^2 + P_\lambda(\beta),
\]

where \(\lambda\) is a tuning parameter(s) and controls the amount of regularization, and \(P_\lambda(\beta)\) denotes a generic penalty function.
Some well-known regularization methods are lasso (Tibshirani, 1996), SCAD (Fan and Li, 2001), elastic net (Zou and Hastie, 2005), fused lasso (Tibshirani, 2005), grouped lasso (Yuan and Lin, 2006), adaptive lasso (Zou, 2006), MCP (Zhang, 2010), SICA (Lv and Fan, 2009) and CAP (Zhao et al., 2009), among others. To apply the group selection for the overlapping patterns of the groups, we propose to use the composite absolute penalty (CAP) (Zhao et al., 2009), which allows overlapping patterns of the groups and different norms to be combined in the penalty. Therefore, we named our proposed resulting classifier the CAP-SQDA. Let $\beta \odot = (\beta_1, \beta_2, \cdots, \beta_p)^T$ and $\beta \otimes = (\beta_{1,1}, \beta_{1,2}, \cdots, \beta_{1,p}, \beta_{2,2}, \beta_{2,3}, \cdots, \beta_{p,p})^T$. For the linear regression model, the form of the CAP is

$$P_\lambda(\beta) = \lambda \sum_{k=1}^{p} \sum_{l=k}^{p} \left[ \alpha_{1,k,l} |\beta_{k,l}| + \alpha_{2,k,l} \|v(\beta_k, \beta_l, \beta_{k,l})\|_{\gamma_{k,l}} \right],$$

where $\lambda$ is the tuning parameter, $\alpha_{1,k,l} > 0$ and $\alpha_{2,k,l} > 0$ are the weighted factors, $\| \cdot \|_{\gamma}$ denotes the $L_{\gamma}$ norm, and $v(\beta_k, \beta_l, \beta_{k,l})$ denotes the vector consisting of $\beta_k, \beta_l, \beta_{k,l}$ with the following form:

$$v(\beta_k, \beta_l, \beta_{k,l}) = \begin{cases} (\beta_k, \beta_l, \beta_{k,l})^T, & k < l, \\ (\beta_k, \beta_{k,k})^T, & k = l. \end{cases}$$

In our application, we keep the uniform weights $\alpha_{1,k,l} = \alpha_1$, $\alpha_{2,k,l} = \alpha_2$, and uniform norms $\gamma_{k,l} = 2$. The penalty function in our proposed method is expressed as follows

$$P_{\lambda_1, \lambda_2}(\beta) = \sum_{k=1}^{p} \sum_{l=k}^{p} \left[ \lambda_1 |\beta_{k,l}| + \lambda_2 \|v(\beta_k, \beta_l, \beta_{k,l})\|_2 \right],$$

where $\lambda_1$ and $\lambda_2$ are tuning parameters.

We suppose that an interaction effect should be added to the regression model only after the corresponding main effects. It means that the penalty for the interactions should be larger than that for the main effects. Thus we make the constraint $\lambda_1 / \lambda_2 > p$ for the two tuning parameters in the penalty function. The constraint for the tuning parameters is also identical to the IIS-SQDA (Fan et al., 2015). Hence CAP-SQDA proposed in this work is able to adaptively and automatically choose between sparse QDA and sparse LDA by using the penalized linear regression.

In optimizing the penalized linear regression, we always center each predictor variable. When we center all variables (including all predictors $x_i$ and $\tilde{x}_i$ and all codes $y_i$ for $i = 1, 2, \cdots, n$), the optimum value of $\beta_0$ is 0 for all
values $\lambda_1$ and $\lambda_2$. Then the optimization for CAP-SQDA can be expressed in the more explicit form as

\[
(\hat{\beta}_\odot, \hat{\beta}_\odot) = \arg \min_{\beta_\odot, \beta_\odot} \sum_{i=1}^{n} (y_i - x_i^T \beta_\odot - \tilde{x}_i^T \beta_\odot)^2 \\
+ \sum_{k=1}^{p} \sum_{l=k}^{p} [\lambda_1 |\beta_{k,l}| + \lambda_2 \|v(\beta_k, \beta_l, \beta_{k,l})\|_2].
\]

Zhao et al. (2009) proposed using the BLASSO algorithm to compute CAP estimates in general. However, the BLASSO algorithm is tries to solve the whole solution path and so is only applicable for one tuning parameter. There are two tuning parameters in our proposed optimization problem (3.2). Therefore BLASSO is not appropriate for the optimization (3.2). Cyclical coordinate descent methods are natural approaches for solving convex problems $\ell_1$ and $\ell_2$ constraints. These methods have been widely proposed for the lasso-type regularization problems, including the classical sparse group lasso (Friedman et al., 2008), and the glmnet (Friedman et al., 2010). We also use the coordinate descent method to solve the penalized least squares problem (3.2).

The coordinate descent algorithm for solving the optimization (3.2) can be converted to a general one-dimensional optimization

\[
\arg \min_{\theta \in \mathbb{R}} a\theta^2 + b\theta + c|\theta| + d \sum_{j=1}^{s} \sqrt{\theta^2 + e_j},
\]

where $a \geq 0, c \geq 0, d \geq 0, e_j > 0$ and $s \in \{0, 1, 2, \ldots, p\}$.

If $|b| \leq c$, the minimizer is easily seen to be $\hat{\theta} = 0$. If $|b| > c$, the one-dimensional optimization (3.3) can be solved by Newton’s type method or the optimize function in the R packages, which is a combination of golden section search and successive parabolic interpolation. Specially, if $b > c$, the minimizer $\hat{\theta}$ lies in the interval $(\frac{c-b}{2a}, 0)$; otherwise if $b < -c$, the minimizer $\hat{\theta} \in (0, \frac{c-b}{2a})$.

To apply the one-dimensional optimization (3.3) in the CAP-SQDA, de-
note the following matrices

\[
H = \left( \sum_{i=1}^{n} x_{i1}^2, \sum_{i=1}^{n} x_{i2}^2, \ldots, \sum_{i=1}^{n} x_{ip}^2 \right)^T,
\]

\[
\tilde{H} = \left( \sum_{i=1}^{n} \tilde{x}_{i1}^2, \sum_{i=1}^{n} \tilde{x}_{i2}^2, \ldots, \sum_{i=1}^{n} \tilde{x}_{ip}^2 \right)^T,
\]

\[
X = (x_1, x_2, \ldots, x_n)^T \in \mathbb{R}^{n \times p},
\]

\[
\tilde{X} = (\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_n)^T \in \mathbb{R}^{n \times \tilde{p}},
\]

\[
Y = (y_1, y_2, \ldots, y_n)^T.
\]

where \( \tilde{p} = p(p + 1)/2 \). We also need to compute the following products in the coordinate descent algorithm

\[
C = X^T Y, \quad \tilde{C} = \tilde{X}^T Y,
\]

\[
G = X^T X, \quad \tilde{G} = \tilde{X}^T \tilde{X}, \quad B = X^T \tilde{X}.
\]

For the update of the main effect parameters \( \beta_k \), the parameters in Equation (3.2) \( a, b, c, d, e_j \) can be calculated as

\[
a = H, \quad L = \{ l \neq k : I(\beta_l^2 + \beta_{k,l}^2 > 0) \} \cup \{ k : \beta_{k,k}^2 > 0 \},
\]

\[
s = |L|, \quad c = (p - s)\lambda_2, \quad d = \lambda_2, \quad e_j = I(L(j) \neq k)\beta_{L(j)}^2 + \beta_{k,L(j)}^2,
\]

\[
b = 2 \left( \beta_{\odot \setminus k}^T G_{k \setminus k} + \beta_{\odot}^T B_k - C_k \right),
\]

where \( I(\cdot) \) denotes the indicator function, \( \beta_{\odot \setminus k} \) the subvector of \( \beta_{\odot} \) removing the kth element, \( G_{k \setminus k} \) the kth row of \( G \) with the kth element removed, \( B_k \) the kth row of \( B \), and \( C_k \) the kth element of \( C \).

For the update of the interaction effect parameter \( \beta_{k,l} \), the parameters in Equation (3.3) \( a, b, c, d, e_j \) can be calculated as

\[
m = (k - 1)p - (k - 1)(k - 2)/2 + (l - k + 1), a = \tilde{H},
\]

\[
s = I(k \neq l)I(\beta_k^2 + \beta_l^2 > 0) + I(k = l)I(\beta_k^2 > 0),
\]

\[
e_1 = I(k \neq l)(\beta_k^2 + \beta_{k,l}^2 > 0) + I(k = l)(\beta_k^2 > 0),
\]

\[
c = \lambda_1 + \lambda_2I(s = 0), d = \lambda_2I(s = 1),
\]

\[
d = 2(\beta_{\odot}^T B^m + \beta_{\odot \setminus m}^T \tilde{G}_{m \setminus m} - \tilde{C}_m),
\]

where \( B^m \) denotes the mth column of \( B \). This leads to the following algorithm:

**Step 1:** Start with \((\hat{\beta}_{\odot}, \hat{\beta}_{\odot})^T = (\beta_{\odot}^{(0)}, \beta_{\odot}^{(0)})\).
Step 2: For the updated estimate of $\beta_k$ in the $t$th loop, fix $\beta_l, l \neq k$ and $\beta_{k,l}$, and calculate $a, b, c, d, e_j$; if $|b| < c$, set $\beta_k^{(t+1)} = 0$; otherwise minimize the optimization (3.3) and obtain the update $\hat{\beta}_k^{(t+1)}$ of $\beta_k$. Update all the parameters $\beta_k, 1 \leq k \leq p$ and $\beta_{k,l}, 1 \leq k \leq l \leq p$ in order.

Step 3: Iterate the entire step (2) over $t = 1, 2, \cdots$ until convergence.

Let $\lambda = (\lambda_1, \lambda_2)$, and denote $\hat{\beta}_0, \hat{\beta}_\circ(\lambda), \hat{\beta}_\otimes(\lambda)$ as the estimates of the parameters $\beta_0, \beta_\circ, \beta_\otimes$ respectively by solving the penalized linear regression problem. Then the classification rule is to assign a new observation $z \in \mathcal{R}^p$ to class 1 if and only if $\hat{\beta}_0 + z^T \hat{\beta}_\circ(\lambda) + \tilde{z}^T \hat{\beta}_\otimes(\lambda) > 0$ where $\tilde{z}$ is the corresponding interaction effects to $z$. In practice, we need to select a good tuning parameter such that the misclassification error is as small as possible. Five cross-validation (CV) is a popular method for tuning, and hence we use it here. Note that there are two tuning parameters in the CAP-SQDA, so the detail of CV can be referred to as the elastic net (Zou and Hastie, 2005). The Lasso-type estimates are generally biased. Therefore, we suggest that OLS is used in the CAP-QDA if the dimension of the active main and interaction effects in the penalized linear regression is smaller than the sample size.

The active sets for the main and interaction effects are

$$S_1 = \{k : \hat{\beta}_k(\lambda) \neq 0\},$$

$$S_2 = \{(k-1)p - (k-1)(k-2)/2 + (l-k+1) : \hat{\beta}_{k,l}(\lambda) \neq 0\}.$$

If $|S_1| + |S_2| < n$, the OLS estimates of $\beta_\circ S_1$ and $\beta_\otimes S_2$ have the following form

$$(\hat{\beta}_{\circ S_1}^{\text{ols}}, \hat{\beta}_{\otimes S_2}^{\text{ols}}) = \left[(x_{S_1}, \tilde{x}_{S_2})^T (x_{S_1}, \tilde{x}_{S_2})\right]^{-1} (x_{S_1}, \tilde{x}_{S_2})^T y.$$

Then if the dimension of the selected effects is smaller than the sample size, the sparse QDA classifier is defined as follows: assigning the new observation $z$ and the corresponding interactions $\tilde{z}$ to class 1 if

$$\hat{\beta}_0 + z^T \hat{\beta}_{\circ S_1}^{\text{ols}} + \tilde{z}^T \hat{\beta}_{\otimes S_2}^{\text{ols}} > 0.$$

4. Simulation studies. In this section, a number of simulations are conducted to compare the performance of the proposed methods with the two methods based on the full likelihood BIC: the backward procedure presented in Zhang and Wang (2011), denoted by BIC$_b$ method, and the forward-backward procedure proposed in Murphy et al. (2010), denoted by BIC$_{fb}$ method. Five simulation experiments are considered. In the first three experiments named Model 1 - Model 3, the predictors are generated from the multivariate normal distributions, and the predictors in the other two experiments named Model 4 and Model 5 are not multivariate normally
distributed random variables. In each simulation experiment, we consider low-dimensional settings with \( p = 20 \) and high-dimensional settings with \( p = 100, 200 \).

For each simulation experiment setting, 50 observations for each class generated from the true model are served as the training data while 5000 extra independent observations for each class are served as the testing data. For comparison, we consider five performance measures including misclassification rate (MR), the numbers of irrelevant main effects (FP.main) and irrelevant interaction effects (FP.inter) falsely included in the classification rule, and the numbers of relevant main effects (FN.main) and interaction effects (FN.inter) falsely excluded in the classification rule. The five performance measures are the same as the classification and variable selection performances employed in Fan et al. (2015).

1. Model 1: The relevant predictors are \( X_S = \{X_1, X_2\} \). For the first class, the mean vector and covariance matrix are \( \mu_{1,S} = (2.5, -1)^T \) and \( \Sigma_{1,S} = [1, 0; 0, 1] \in \mathbb{R}^2 \), respectively; for the second class, they are \( \mu_{2,S} = (-0.5, 0)^T \) and \( \Sigma_{2,S} = [3, 1; 1, 3] \in \mathbb{R}^2 \), respectively. The remaining \( p - 2 \) variables are independently and independently generated as \( N(u, 1) \), where \( u \) is generated from \( U[0, 1] \).

This model is borrowed from Zhang and Wang (2011). There are two main effects and three interaction terms in the Bayes rules for Model 1. There is small difference between the two covariance matrices of the predictors for two classes. It means that the interaction effects are weak in Model 1.

Table 1 presents the variable selection and classification results for Model 1. It can be seen from the table that different methods exhibit similar performance in MR. CAP-SQDA has the best classification performance in all settings \( p = 20, 100 \) and 200 although the methods BIC and IIS-SQDA are consistent with the assumptions of Model 1. BIC has the smallest values of FP.main whereas IIS-SQDA has the smallest values of FN.main in the main effect selection under all settings. CAP-SQDA gives smaller FN.mains than BIC. CAP-SQDA has the smallest values of FP.inter in the situations \( p = 100, 200 \) whereas BIC has the smallest values of FN.inter across all settings in terms of interaction selection. Both of IIS-SQDA and CAP-SQDA have poor interaction selection performances which can be shown that the values of FP.inter are approximately equal to 3. The reason is that model 1 is similar to a LDA model. BIC criterion is a method for variable selection rather than effect selection essentially, therefore, presents the best performance in terms of FN.inter. The results in Table 1 demonstrate that our proposed method CAP-SQDA can effectively select important effects and conduct classification simultaneously for Model 1 under all dimensional
| $p$ | Method     | MR(%)  | FP.main | FP.inter | FN.main | FN.inter |
|-----|------------|--------|---------|----------|---------|----------|
| 20  | BIC        | 6.68(0.57) | 0.06(0.23) | 0.14(0.56) | 0.77(0.42) | 1.54(0.84) |
|     | BIC        | 6.67(0.58) | 0.06(0.28) | 0.14(0.56) | 0.75(0.43) | 1.50(0.87) |
|     | IIS-SQDA   | 6.92(1.69) | 0.95(2.55) | 0.84(0.63) | 0.11(0.39) | 2.98(0.14) |
|     | CAP-SQDA   | 6.54(0.48) | 1.04(2.73) | 0.48(1.46) | 0.52(0.50) | 2.65(0.55) |
|     | OLS-SQDA   | 6.91(1.05) | 1.04(2.73) | 0.48(1.46) | 0.52(0.50) | 2.65(0.55) |
|     | ORACLE     | 6.44(0.25) | 0(0)     | 0(0)     | 0(0)     | 0(0)     |
| 100 | BIC        | 7.05(0.99) | 0.36(0.52) | 0.81(1.22) | 0.68(0.46) | 1.36(0.93) |
|     | IIS-SQDA   | 7.00(2.21) | 1.31(4.94) | 0.95(0.88) | 0.06(0.23) | 2.98(0.14) |
|     | CAP-SQDA   | 6.54(0.49) | 2.06(3.82) | 0.50(1.23) | 0.46(0.50) | 2.93(0.26) |
|     | OLS-SQDA   | 6.76(0.74) | 2.06(3.82) | 0.50(1.23) | 0.46(0.50) | 2.93(0.26) |
|     | ORACLE     | 6.40(0.24) | 0(0)     | 0(0)     | 0(0)     | 0(0)     |
| 200 | BIC        | 7.13(0.97) | 0.49(0.65) | 1.11(1.57) | 0.74(0.44) | 1.48(0.88) |
|     | IIS-SQDA   | 7.07(2.48) | 1.05(3.15) | 0.87(0.33) | 0.18(0.38) | 2.99(0.10) |
|     | CAP-SQDA   | 6.55(0.47) | 0.65(1.44) | 0.51(1.28) | 0.60(0.49) | 2.67(0.47) |
|     | OLS-SQDA   | 7.13(1.15) | 0.65(1.44) | 0.51(1.28) | 0.60(0.49) | 2.67(0.47) |
|     | ORACLE     | 6.38(0.23) | 0(0)     | 0(0)     | 0(0)     | 0(0)     |
settings.

(2) Model 2: The mean vectors of all variables are \( \mu_1 = (0, 0, \cdots)^T \) and \( \mu_2 = (0.6, 0.8, 0, \cdots)^T \) for the two classes. The precision matrix for the first class is \( \Omega_1 = I_{p \times p} \), and \( \Omega_2 = \Omega_1 + \Omega \) for the other class, where \( \Omega \) is a sparse matrix with \( \Omega_{3,3} = \Omega_{4,4} = \Omega_{5,5} = -0.6 \) and \( \Omega_{3,4} = \Omega_{3,5} = \Omega_{4,5} = -0.15 \). The other three nonzero entries in the lower triangle of \( \Omega \) are determined by symmetry. This model is borrowed from Fan et al. (2015). There are two main effects and six interaction terms in the Bayes rules for Model 2. The relevant predictors are \( X_S = \{X_1, X_2, \cdots, X_5\} \).

| \( p \) | Method | MR(%) | FP.main | FP.inter | FN.main | FN.inter |
|-------|-------|-------|---------|----------|---------|----------|
| 20    | BIC   | 26.73(2.38) | 2.06(0.62) | 1.49(1.74) | 1.53(0.52) | 2.78(1.49) |
|       | BIC_0 | 26.45(2.27) | 2.10(0.57) | 1.48(1.69) | 1.52(0.52) | 2.66(1.49) |
|       | IIS-SQDA | 24.30(3.08) | 3.39(4.70) | 0.88(1.83) | 0.18(0.43) | 1.33(1.55) |
|       | CAP-SQDA | 24.91(2.44) | 2.34(4.11) | 0.60(1.04) | 0.67(0.80) | 2.93(0.57) |
|       | OLS-SQDA | 26.39(2.64) | 5.78(7.36) | 2.11(5.65) | 0.54(0.75) | 2.91(0.77) |
|       | ORACLE | 18.63(0.38) | 0(0) | 0(0) | 0(0) | 0(0) |
| 100   | BIC_0 | 26.41(2.45) | 2.11(0.60) | 2.12(1.79) | 1.37(0.56) | 2.83(1.33) |
|       | IIS-SQDA | 27.21(4.65) | 5.54(9.10) | 0.26(0.62) | 0.34(0.55) | 2.48(1.52) |
|       | CAP-SQDA | 26.23(2.89) | 2.59(3.19) | 0.58(1.62) | 0.54(0.67) | 3.37(0.79) |
|       | OLS-SQDA | 28.30(3.34) | 1.93(1.77) | 0.16(0.56) | 0.62(0.74) | 3.23(0.77) |
|       | ORACLE | 18.62(0.42) | 0(0) | 0(0) | 0(0) | 0(0) |
| 200   | BIC_0 | 27.04(3.05) | 2.27(0.71) | 2.34(1.86) | 1.45(0.65) | 2.75(0.72) |
|       | IIS-SQDA | 28.31(4.69) | 6.05(10.80) | 0.37(0.84) | 0.45(0.55) | 2.96(1.37) |
|       | CAP-SQDA | 25.87(2.84) | 1.92(2.76) | 0.53(1.23) | 0.86(0.63) | 2.01(0.69) |
|       | OLS-SQDA | 28.27(3.70) | 1.93(1.77) | 0.16(0.56) | 0.62(0.74) | 3.23(0.77) |
|       | ORACLE | 18.60(0.37) | 0(0) | 0(0) | 0(0) | 0(0) |

(3) Model 3: The mean vectors are \( \mu_1 = (0, 0, \cdots)^T \) and \( \mu_2 = (0.6, 0.8, 0.6, 0.8, 0, \cdots)^T \) for the two classes. The precision matrix is \( \Omega_1 = I_{p \times p} \) for the first class, and \( \Omega_2 = \Omega_1 + \Omega \) for the second class, where \( \Omega_{1,1} = \Omega_{2,2} = -0.6 \) and \( \Omega_{1,2} = \Omega_{2,1} = -0.15 \). This model is consistent with the effects assumption in our proposal. There are four main effects and two interaction terms in the Bayes rules. The relevant predictors are \( X_S = \{X_1, X_2, X_3, X_4\} \).
| $p$ | Method | MR(%) | FP.main | FP.inter | FN.main | FN.inter |
|-----|--------|-------|---------|----------|---------|----------|
| 20  | BIC$_b$| 30.67(3.06) | 0.03(0.17) | 1.40(1.44) | 2.05(0.62) | 1.23(1.08) |
|     | BIC$_{fb}$| 30.26(2.85) | 0.02(0.14) | 1.34(1.28) | 2.00(0.56) | 1.12(1.05) |
|     | IIS-SQDA | 27.74(3.24) | 2.50(3.58) | 0.51(1.25) | 1.10(0.84) | 0.73(0.87) |
|     | CAP-SQDA | 28.47(3.20) | 2.43(4.58) | 0.10(0.33) | 1.54(1.26) | 1.33(0.65) |
|     | OLS-SQDA | 29.03(3.37) | 2.43(4.58) | 0.10(0.33) | 1.54(1.26) | 1.33(0.65) |
|     | ORACLE  | 22.68(0.35) | 0(0)      | 0(0)    | 0(0)    | 0(0)    |
| 100 | BIC$_{fb}$| 30.35(3.58) | 0.14(0.37) | 2.07(1.62) | 1.92(0.59) | 1.32(1.01) |
|     | IIS-SQDA | 30.73(4.48) | 6.10(8.74) | 0.50(0.91) | 1.14(0.89) | 1.40(0.95) |
|     | CAP-SQDA | 29.18(2.87) | 3.77(6.95) | 0.03(0.17) | 1.62(0.97) | 1.62(0.78) |
|     | OLS-SQDA | 30.78(3.87) | 3.77(6.95) | 0.03(0.17) | 1.62(0.97) | 1.62(0.78) |
|     | ORACLE  | 22.67(0.45) | 0(0)      | 0(0)    | 0(0)    | 0(0)    |
| 200 | BIC$_{fb}$| 32.01(4.00) | 0.36(0.54) | 2.21(1.72) | 2.11(0.52) | 1.40(0.98) |
|     | IIS-SQDA | 33.82(5.48) | 10.06(16.02) | 0.42(0.72) | 1.43(0.90) | 1.55(0.96) |
|     | CAP-SQDA | 29.90(2.95) | 2.69(3.81) | 0.06(0.31) | 1.89(0.97) | 1.28(0.53) |
|     | OLS-SQDA | 31.02(4.22) | 2.69(3.81) | 0.06(0.31) | 1.89(0.97) | 1.28(0.53) |
|     | ORACLE  | 22.70(0.41) | 0(0)      | 0(0)    | 0(0)    | 0(0)    |
(4) Model 4: Assume that part of the variables is not Gaussianly distributed for each class. Suppose also that the first two variables are relevant. For the first class, $X_1$ and $X_2$ are independently generated from $1 - \chi^2(1)$, where $\chi^2(1)$ is the chi-squared distribution with one degree of freedom. For the second class, $X_1$ and $X_2$ are independently generated from, $1.2 - \sqrt{3} \ast \chi^2(1)$ and $1.6 - \sqrt{3} \ast \chi^2(1)$, respectively. The next three variables are generated from the following rules

$$X_3 = b_{11} + b_{12}X_1 + \chi^2(1),$$
$$X_4 = b_{21} + b_{22}X_2 + \chi^2(1),$$
$$X_5 = b_{31} + b_{32}X_1 + b_{33}X_2 + \chi^2(1),$$

where $b_i$ is $U[-1, 1]$. The next $p/2 - 5$ variables are independently generated from the standard normal distribution. The remaining $p/2$ variables are independently generated from $\chi^2(1)$.

(5) Model 5: The first five variables are generated as in Model 4. The remaining $p - 5$ are irrelevant. The next $p/2 - 5$ variables are independently generated from $N(\tilde{\mu}, 1)$, and the remaining $p/2$ variables are independently generated from Beta distribution $B(\nu, 0.5)$, where $\tilde{\mu}$ and $\nu$ are $U(0, 1)$ and $U(1, 5)$ random variables, respectively.

Table 4 summarizes the classification results for Model 4 and Model 5. We not only give the misclassification rates, but also report the values of MR of CAP-SQDA minus the ones of BIC and IIS-SQDA (MRM). According to Table 4, although the misclassification rates of all methods in models 4 - 5 are obviously larger than those of the ORACLE classifier when the assumption of mixed gaussian distribution for all variables does not hold, CAP-SQDA exhibits the best performance in terms of MR across all settings. In some settings such as $p = 100, 200$ for Model 5, MRs of CAP-SQDA are significantly smaller than the ones of BIC and IIS-SQDA. The results demonstrate that our proposed method is robust for QDA in classification.

5. Application.

5.1. parkinson dataset. We apply the classification methods to the parkinson dataset shared in UCI in 2008 (Little et al., 2007). This dataset is composed of a range of biomedical voice measurements from normal people and Parkinson’s disease (PD) patients. There are $p = 22$ predictors in this dataset. The main aim is to discriminate healthy people from those with PD. There are $n_1 = 147$ for the PD and $n_2 = 48$. We randomly split 195 samples into a training set consisting of 73 samples from PD and 24 samples from the healthy. For each split, we applied five different methods to the
Table 4

*Performance measures of different classification methods for Model 4 and Model 5*

| p  | Method | model 4 | model 5 |
|----|--------|---------|---------|
|    |        | MR(%)   | MRM(%)  | MR(%)   | MRM(%)  |
| 20 | BIC<sub>b</sub> | 24.96(10.26) | 7.76(10.03) | 19.44(8.62) | 4.86(9.01) |
|    | BIC<sub>f</sub> | 24.53(10.35) | 7.33(9.89) | 19.31(8.53) | 4.73(8.82) |
|    | IIS-SQDA  | 23.53(7.30) | 6.32(6.95) | 22.01(7.66) | 7.42(7.76) |
|    | CAP-SQDA  | 17.20(3.32) | –        | 14.58(2.75) | –        |
|    | OLS-SQDA  | 18.78(4.17) | –        | 14.96(3.16) | –        |
|    | ORACLE    | 4.63(0.18) | –        | 4.62(0.18) | –        |
| 100| BIC<sub>b</sub>| 33.30(9.43) | 9.33(10.71) | 23.52(8.64) | 7.82(8.22) |
|    | IIS-SQDA  | 29.79(8.02) | 5.82(8.89) | 27.91(8.54) | 12.21(8.35) |
|    | CAP-SQDA  | 23.96(6.40) | –        | 15.70(2.66) | –        |
|    | OLS-SQDA  | 24.56(6.73) | –        | 16.72(3.24) | –        |
|    | ORACLE    | 4.63(0.18) | –        | 4.63(0.18) | –        |
| 200| BIC<sub>b</sub>| 39.10(8.01) | 12.95(9.06) | 27.31(7.54) | 10.73(7.87) |
|    | IIS-SQDA  | 32.33(9.19) | 6.18(9.36) | 31.22(8.85) | 14.65(8.64) |
|    | CAP-SQDA  | 26.15(6.42) | –        | 16.57(2.86) | –        |
|    | OLS-SQDA  | 27.01(7.26) | –        | 17.36(3.83) | –        |
|    | ORACLE    | 4.63(0.18) | –        | 4.63(0.18) | –        |
training data and then calculated the classification error using the test data. The tuning parameters are selected via the five-fold cross validation. We repeated the random splitting for 100 times. The means and standard errors of classification errors and model sizes for different classification methods are summarized in Table 5.

FULL method has the worst performance in the classification. It means that the variable selection is necessary for the analysis of the parkinson dataset. BIC\(_b\) method and BIC\(_{fb}\) method select on average 10.63 and 7.88 variables, respectively. IIS-SQDA method has the smallest MR, but select 11.20 variables and 20.94 effects. Our proposed method selects the smallest numbers of variables and effects and achieves very close classification accuracy compared with the IIS-SQDA method.

| Method   | MR(%)    | Variable | Main | Interaction | All       |
|----------|----------|----------|------|-------------|-----------|
| FULL     | 22.51(1.92) | –        | –    | –           | –         |
| BIC\(_b\) | 18.01(3.99) | 10.63(1.81) | –    | –           | –         |
| BIC\(_{fb}\) | 21.36(4.33) | 7.88(2.00) | –    | –           | –         |
| IIS-SQDA | 15.78(3.91) | 11.20(4.19) | 9.92(4.33) | 11.02(8.60) | 20.94(10.59) |
| CAP-SQDA | 15.94(2.72) | 4.44(1.70) | 2.86(1.93) | 2.12(0.79) | 4.98(2.14) |
| OLS-SQDA | 16.11(3.04) | 4.44(1.70) | 2.86(1.93) | 2.12(0.79) | 4.98(2.14) |

**NOTE:** FULL represents the QDA without variable selection.

5.2. Breast cancer dataset. The breast cancer dataset consists of the gene expressions from 77 patients, originally studied in Van et al. (2002). The goal is to predict whether a female breast cancer patient relapses from gene expression data. The dataset contains a total of 78 samples, with 44 of them in the good prognosis group and 34 of them in the poor prognosis group. Since there are some missing values with one patient in the poor prognosis group, it was removed in the study Fan et al. (2015). Same as Fan et al. (2015), we use the \( p = 231 \) genes in Van et al. (2002) and randomly split the 77 samples into a training set and a test set. 26 samples from the good prognosis group and 19 samples from the poor prognosis group are randomly selected in the training set randomly. We apply the classification methods and the results are summarized in Table 6.

For the analysis of the breast cancer dataset, BIC\(_b\) method and BIC\(_{fb}\) method select on average 10.63 and 7.88 variables, respectively. IIS-SQDA
method has the lower MR, but select 11.20 variables and 20.94 effects. Our proposed method selects the smallest number of variables and effects and achieves high classification accuracy. \(BIC_{fb}\) selects the smallest variables, but has the largest MR. IIS-SQDA method achieves the lowest MN, but selects the largest number of variables and effects, where both of the numbers of the Main effects and All effects are larger than the sample size of the training set. Our proposal method misclassifies 2.46 clinical outcomes more than IIS-method, whereas it selects nearly half the number of effects fewer than the IIS-method. Both our proposal method and the IIS-method select very fewer interaction effects. It means that a sparse LDA is suitable for the breast cancer dataset. In the study of Fan et al. (2015), the penalized logistic regression analysis with the main effects only also has high classification accuracy with \(MN = 6.95\). It demonstrate that our proposal method can adaptively and automatically choose between the sparse LDA and the sparse QDA.

| Method   | MN       | Main      | Interaction | All       |
|----------|----------|-----------|-------------|-----------|
| BIC\(fb\) | 11.57(2.30) | 7.72(3.26) | –           | –         |
| IIS-SQDA  | 6.39(2.46)  | 47.77(11.60) | 3.03(3.20)  | 50.80(13.10) |
| CAP-SQDA  | 8.85(2.24)  | 21.42(9.07)  | 1.06(1.48)  | 22.48(10.06) |
| OLS-SQDA  | 9.25(2.34)  | 21.42(9.07)  | 1.06(1.48)  | 22.48(10.06) |

**NOTE:** MN represents the misclassification number.

6. Conclusion. In this paper we propose a penalized linear regression, named CAP-SQDA, for quadratic discriminant analysis with two classes, and develop a coordinate descent algorithm to solve the penalized least-squares problem. The proposed procedure first transform the sparse QDA problem to a penalized sparse ordinary least squares optimization by using composite absolute penalty, and apply main effect and interaction selection through regularization. The efficiency and robustness of CAP-SQDA have been demonstrated through simulation studies and real data analysis through comparison it with other methods. For real datasets CAP-SQDA usually selects much few variables while achieves high classification accuracy.

In the future study, it would be interesting to generalize the proposed method to problems for quadratic discriminant analysis of multi-class classification. The key of the variable selection for the multi-class quadratic
discriminant analysis is to propose a new composite penalty. In addition, developing an efficient computing method is the need of CAP-SQDA for ultrahigh-dimensional data analysis.

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