RESPONSE-GUIDED PRINCIPAL COMPONENT CLASSIFICATION

by

Duncan Tai Bennett

A Thesis Submitted to the Faculty of the

DEPARTMENT OF MATHEMATICS

In Partial Fulfillment of the Requirements

For the Degree of

MASTER OF SCIENCE

In the Graduate College

THE UNIVERSITY OF ARIZONA

2021

place holder for signature page

Thank you to ...

Contents

List of Abbreviations and Symbols

$\mathbf{X}$ a design matrix, usually with dimensions $N \times p$.

$\mathbf{U}$ of the svd of $\mathbf{X} = \mathbf{UDV}^T$.

$\mathbf{D}$ of the svd of $\mathbf{X} = \mathbf{UDV}^T$.

$\mathbf{V}$ of the svd of $\mathbf{X} = \mathbf{UDV}^T$.

$\mathbf{W}$ a weight matrix.

List of Figures

Abstract

Response-guided principal component regression (RgPCR) is a generalization of ridge regression. This method improves upon principal component regression (PCR) by taking the response values into account during variable selection. In this paper, we will modify RgPCR for binary classification problems using ideas from logistic regression. This technique is called *response-guided principal component classification (RgPCC)*.

1 Introduction

Principal component regression (PCR) was introduced (by Jeffers, 1967) to deal with multicollinearity. This method can achieve dimension reduction and improve prediction performance compared to ordinary least squares. However, its downfall in regression is that the principal components depend soley on the design $\mathbf{X}$ and in this sense the variable selection is "blind", as it does not take the response into account. In early 2020 Lang and Zou [2] introduced Response-guided Principal Component Regression (RgPCR) to remedy the "blind" selection of PCR. This is done by replacing the hard-thresholding of PCR with soft-thresholding via a penalty function. The result is that both the variance of the predictors and the association with the response of principal components is taken into account during thresholding.

In this paper, we will combine RgPCR with logistic regression for binary classification. To do this we optimized a penalized log likelihood function by quadratically approximating and taking advantage of the principal components of “psuedo data" in the resulting expression. The result is a principal component classification algorithm that takes the response into account during variable selection.

In section 2 we will give our motivation and cover the background knowledge necessary. In section 3 we will derive the RgPCC algorithm. In sections 4 and 5 we will compare the performance of RgPCC against other methods on simulated data and then on realworld data. Lastly, in section 6 and 7 we will propose further topics of study and summarize our results.

2 Literature Review

Here we describe two supervised learning methods that have motivated RgPCC. First, we summarized RgPCR, a method developed by Lang and Zou [2]. Then we summarized logistic regression for binary classification.

2.1 Principal Component Analysis (PCA)

2.2 Response-guided Principal Component Regression (RgPCR)

RgPCR is a generalization of ridge regression which we will briefly summarize. Let $\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^T$ be the singular value decomposition of an $N \times p$ design matrix

$\mathbf{X}$. Then with response y we can write the ridge regression solution as

$$\widehat{\boldsymbol{\beta}}^{\text{ridge}} = \arg\min_{\boldsymbol{\beta}} ||\mathbf{y} - \mathbf{X}\boldsymbol{\beta}||_2^2 + \lambda \sum_{j=1}^{p} \beta_j^2. \tag{1}$$

We may rewrite this as

$$\widehat{\boldsymbol{\gamma}}^{\text{ridge}} = \arg\min_{\boldsymbol{\gamma}} ||\mathbf{y} - \mathbf{U}\boldsymbol{\gamma}||_2^2 + \lambda \sum_{j=1}^{p} \frac{\gamma_j^2}{d_j^2}. \tag{2}$$

where $\boldsymbol{\gamma} = \mathbf{D}\mathbf{V}^T\boldsymbol{\beta}$ and d_j is the j^{th} diagonal entry of $\mathbf{D}$. Hence, ridge regression can be viewed as a weighted L_2 penalized regression in the space of principal components. The RgPCR generalization comes from replacing the L_2 penalization with an arbitrary non-decreasing function $p_\lambda(\cdot)$. Some examples of these are LASSO, SCAD and MCP. In general, we write this RgPCR solution as

$$\widehat{\boldsymbol{\gamma}} = \arg\min_{\boldsymbol{\gamma}} ||\mathbf{y} - \mathbf{U}\boldsymbol{\gamma}||_2^2 + \sum_{j=1}^{p} p_\lambda\left(\frac{\gamma_j}{d_j}\right), \tag{3}$$

There are three main advantages to (3). First, the regularization helps prevent overfitting. Secondly, the use of PCA and the orthogonality of U allows for this minimizer to be calculated component-wise. Lastly, the penalty allows the variable selection to be determined by large variance in the predictors and the association with the response of principal components (we can see this by the presence of $\widehat{\gamma}_j^{\text{ols}}$ in the following).

The orthogonality of $\mathbf{U}$ allows us to solve (3) component-wise. In particular,

$$\widehat{\gamma}_j = \arg\min_{\gamma_j} \left(\widehat{\gamma}_j^{\text{ols}} - \gamma_j\right)^2 + p_\lambda\left(\frac{\gamma_j}{d_j}\right). \tag{4}$$

where $\widehat{\gamma}_j^{\text{ols}} = \mathbf{y}^T U_j$ (equation (4) follows from the orthogonality of $\mathbf{U}$ and a calculation can be found in [2]). When $p_\lambda(t) = |t|$, the LASSO penalty, then we can find a closed form of (4),

$$\widehat{\gamma}_j^{\text{lasso}} = \left(|\gamma_j^{\text{ols}}| - \frac{\lambda}{2d_j}\right)^+ \cdot \operatorname{sgn}\left(\widehat{\gamma}_j^{\text{ols}}\right). \tag{5}$$

We can recover the solution in the original coordinates by

$$\widehat{\boldsymbol{\beta}} = \sum_{j=1}^{p} \widetilde{V}_j \frac{\widehat{\gamma}_j}{d_j} \tag{6}$$

2.3 Logistic Regression

Logistic regression is a common technique for classification. For now we consider binary classification. Let $\mathbf{X}$ be an $N \times p$ design matrix with $\mathbf{y}$ the $N \times 1$ classifications. Then if we assume that

$$\log\left(\frac{Pr(G=1|X=x)}{Pr(G=0|X=x)}\right) = \boldsymbol{\beta}^T x \tag{7}$$

the log-odds are linear, then we may calculate the conditional probability

$$Pr(G=1|X=x) = \frac{\exp(\boldsymbol{\beta}^T x)}{1+\exp(\boldsymbol{\beta}^T x)}. \tag{8}$$

Note that we may compute all probabilities for the data simultaneously by

$$\mathbf{p} = \frac{\exp(\mathbf{X}\boldsymbol{\beta})}{1+\exp(\mathbf{X}\boldsymbol{\beta})}. \tag{9}$$

where p_i is the probability that x_i is in class 1.

To fit such a line for the log-odds (7), we fit by maximizing the log-likelihood,

$$\ell(\mathbf{X}, \beta) = \sum_{i=1}^{N} \left[y_i \log(p(x_i;\boldsymbol{\beta})) + (1-y_i)\log(1-p(x_i;\boldsymbol{\beta}))\right] \tag{10}$$

This maximization can be found in [1] and has a convenient interpretation. When maximizing by the Newton-Ralphson method, each iteration can be interpreted as solving a weighted least squares problem. That is

$$\begin{aligned}\boldsymbol{\beta}^{\text{new}} &= \boldsymbol{\beta}^{\text{old}} + (\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{y}-\mathbf{p}) && (11)\\ &= (\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{W}\mathbf{z} && (12)\end{aligned}$$

where

$$\mathbf{p} = \frac{\exp(\mathbf{X}\boldsymbol{\beta})}{1+\exp(\mathbf{X}\boldsymbol{\beta})} \tag{13}$$

$$\mathbf{W} = \mathrm{diag}[p_i(1-p_i)] \tag{14}$$

$$\mathbf{z} = \mathbf{X}\boldsymbol{\beta} + \mathbf{W}^{-1}(\mathbf{y}-\mathbf{p}). \tag{15}$$

In particular, $\boldsymbol{\beta}^{\text{new}}$ is the solution to a weighted least squares problem with response $\mathbf{z}$, design $\mathbf{X}$ and weights $\mathbf{W}$.

For our purposes, it will be more convenient to state this as the following equivalent problem, $\boldsymbol{\beta}^{\text{new}}$ estimates the minimizer of

$$\boldsymbol{\beta}^{\text{new}} = \arg\min_{\boldsymbol{\beta}} ||\mathbf{W}^{1/2}(\mathbf{z}-\mathbf{X}\boldsymbol{\beta})||^2 \tag{16}$$

3 Response-guided Principal Component Classification

First, a note on notation. We let p denote the number of predictors in our data, p_λ to a non-decreasing penalty function and p_i to be the i^{th} component of a vector of probabilities $\mathbf{p}$.

Suppose we have a classification problem with design $\mathbf{X}$ and classes $\mathbf{y}$. In logistic regression we fit by maximizing the log-likelihood, we take the opposite of this and penalize the coefficients as such,

$$\boldsymbol{\beta}^{\text{RgPCC}} = \arg\min_{\boldsymbol{\beta}} -\ell(\mathbf{X},\boldsymbol{\beta}) + \sum_{j=1}^{p} p_\lambda(\beta_j) \tag{17}$$

3.1 Method

To solve (17), we can approximate the log-likelihood $\ell(\mathbf{X},\boldsymbol{\beta})$ with a quadratic approximation centered at $\boldsymbol{\beta}^*$ (the minimizer of $-\ell(\mathbf{X},\boldsymbol{\beta})$). This quadratic approximation can be interpreted as the least squares error

$$-\ell(\mathbf{X},\boldsymbol{\beta}) \approx ||\mathbf{W}^{1/2}(\mathbf{z}-\mathbf{X}\boldsymbol{\beta})||^2 = ||\widetilde{\mathbf{y}} - \widetilde{\mathbf{X}}\boldsymbol{\beta}||^2 \tag{18}$$

where $\mathbf{W}$, and $\mathbf{z}$ are as in (26 - 28) with (26) evaluated at $\boldsymbol{\beta} = \boldsymbol{\beta}^*$ and $\mathbf{W}^{1/2}\mathbf{X} = \widetilde{\mathbf{X}}$, $\widetilde{\mathbf{y}} = \mathbf{W}^{1/2}\mathbf{z}$. The derivation of this approximation can be found in [3]. Note that, we may often refer to $\widetilde{\mathbf{X}}$ and $\widetilde{\mathbf{y}}$ as the *pseudo data* and *pseudo response* respectively.

Equation (17) can be rewritten as an approximate RgPCR problem

$$\arg\min_{\boldsymbol{\beta}} ||\widetilde{\mathbf{y}} - \widetilde{\mathbf{X}}\boldsymbol{\beta}||^2 + \sum_{j=1}^{p} p_\lambda(\beta_j) \tag{19}$$

For particular choices of p_λ, this may be solved using techniques from [2]. That is, by viewing the above in terms of principal components we may solve the equivalent problem

$$\arg\min_{\boldsymbol{\gamma}} ||\widetilde{\mathbf{y}} - \widetilde{\mathbf{U}}\boldsymbol{\gamma}||^2 + \sum_{j=1}^{p} p_\lambda\left(\frac{\gamma_j}{d_j}\right) \tag{20}$$

where $\widetilde{\mathbf{X}} = \widetilde{\mathbf{U}}\widetilde{\mathbf{D}}\widetilde{\mathbf{V}}^T$ is the SVD decomposition of $\widetilde{\mathbf{X}}$ and $\boldsymbol{\gamma} = \widetilde{\mathbf{D}}\widetilde{\mathbf{V}}^T\boldsymbol{\beta}$. The matrices $\widetilde{\mathbf{U}}$ and $\widetilde{\mathbf{V}}$ are orthogonal matrices and are $N \times p$ and $p \times p$ matrices respectively. Let d_j denotes the diagonal entries of $\widetilde{\mathbf{D}}$ for $1 \leq j \leq p$. For our description here, we assume that $\widetilde{\mathbf{X}}$ has full rank, but the following still holds with a thin SVD decomposition.

As with RgPCR, we may take advantage of the orthogonality of $\widetilde{\mathbf{U}}$ and optimize componentwise. That is, with $\widehat{\gamma}_j^{\text{ols}} = \mathbf{y}^T\widetilde{U}_j$,

$$\arg\min_{\gamma_j} (\widehat{\gamma}_j^{\text{ols}} - \gamma_j)^2 + p_\lambda\left(\frac{\gamma_j}{d_j}\right). \tag{21}$$

From [2], when $p_\lambda(t) = |t|$ is the LASSO penalty, we have the closed form solution of (21)

$$\widehat{\gamma}_j = \left(|\widehat{\gamma}_j^{\text{ols}}| - \frac{\lambda}{d_j}\right)^+ \cdot \operatorname{sgn}\left(\widehat{\gamma}_j^{\text{ols}}\right), \tag{22}$$

where a^+ denotes the positive real part of a real number a. We can then rewrite this in the original coordinates using

$$\widehat{\boldsymbol{\beta}} = \sum_{j=1}^{p} \widetilde{V}_j \frac{\widehat{\gamma}_j}{d_j}. \tag{23}$$

3.2 Iterative Approximations

In practice, a single quadratic approximation of $-\ell(\mathbf{X}, \boldsymbol{\beta})$ may not produce a minimum close to the true minimum. Just as in logistic regression, we take the quadratic approximations iteratively to improve our approximation of the minimum. That is, for some approximate minimizer $\boldsymbol{\beta}^{(n)}$, we solve

$$\arg\min_{\boldsymbol{\beta}} -\ell(\mathbf{X}, \boldsymbol{\beta}) + \sum_{j=1}^{p} p_\lambda(\beta_j) \tag{24}$$

which can be approximated by

$$-\ell(\mathbf{X}, \boldsymbol{\beta}) \approx ||\widetilde{\mathbf{y}}^{(n)} - \widetilde{\mathbf{X}}^{(n)}\boldsymbol{\beta}||^2 \tag{25}$$

where

$$\mathbf{p}^{(n)} = \frac{\exp(\mathbf{X}\boldsymbol{\beta}^{(n)})}{1 + \exp(\mathbf{X}\boldsymbol{\beta}^{(n)})} \tag{26}$$

$$\mathbf{W}^{(n)} = \mathrm{diag}[p_i^{(n)}(1 - p_i^{(n)})] \tag{27}$$

$$\mathbf{z}^{(n)} = \mathbf{X}\boldsymbol{\beta}^{(n)} + (\mathbf{W}^{(n)})^{-1}(\mathbf{y} - \mathbf{p}^{(n)}). \tag{28}$$

$$\widetilde{\mathbf{X}}^{(n)} = (\mathbf{W}^{(n)})^{1/2}\mathbf{X} \tag{29}$$

$$\widetilde{\mathbf{y}}^{(n)} = (\mathbf{W}^{(n)})^{1/2}\mathbf{z}^{(n)} \tag{30}$$

As with the first iteration, we can solve

$$\arg\min_{\boldsymbol{\beta}} ||\widetilde{\mathbf{y}}^{(n)} - \widetilde{\mathbf{X}}^{(n)}\boldsymbol{\beta}||^2 + \sum_{j=1}^{p} p_\lambda(\beta_j) \tag{31}$$

to estimate the solution to (25). Then, as with the first iteration, we can express the above using principal components

$$\arg\min_{\boldsymbol{\gamma}} ||\widetilde{\mathbf{y}}^{(n)} - \widetilde{\mathbf{U}}^{(n)}\boldsymbol{\gamma}||^2 + \sum_{j=1}^{p} p_\lambda\left(\frac{\gamma_j}{d_j^{(n)}}\right) \tag{32}$$

and take advantage of the orthogonality of $\widetilde{\mathbf{U}}$ so solve componentwise

$$\arg\min_{\gamma_j} (\widehat{\gamma}_j^{\mathrm{ols},(n)} - \gamma_j)^2 + p_\lambda\left(\frac{\gamma_j}{d_j^{(n)}}\right). \tag{33}$$

3.3 Algorithm for LASSO penalty

Here, we will briefly describe the algorithm used to approximate a solution to (17) when we use the LASSO penalty. This will generalize to any penalty that has an RgPCR closed form solution.

(Step 1) Guess an initial $\widehat{\beta}^{(0)}$

(Step 2) With $\widehat{\beta}^{(0)}$ calculate the following

$$\begin{aligned}\mathbf{p}^{(0)} &= \frac{\exp(\mathbf{X}\boldsymbol{\beta}^{(0)})}{1+\exp(\mathbf{X}\boldsymbol{\beta}^{(0)})} = \frac{\exp(\mathbf{U}\boldsymbol{\gamma}^{(0)})}{1+\exp(\mathbf{U}\boldsymbol{\gamma}^{(0)})}\\ \mathbf{W}^{(0)} &= \operatorname{diag}[p_i^{(0)}(1-p_i^{(0)})]\\ \mathbf{z}^{(0)} &= \mathbf{X}\boldsymbol{\beta}^{(0)} + (\mathbf{W}^{(0)})^{-1}(\mathbf{y}-\mathbf{p}^{(0)}).\end{aligned}$$

(Step 3) Compute the solution to the RgPCR problem

$$\arg\min_{\boldsymbol{\gamma}} ||\widetilde{\mathbf{y}}^{(0)} - \widetilde{\mathbf{U}}^{(0)}\boldsymbol{\gamma}||^2 + \lambda \sum_{j=1}^{p} \left|\frac{\gamma_j}{d_j^{(0)}}\right| \tag{34}$$

using the closed form solution

$$\widehat{\gamma}_j^{(1)} = \left(|\widehat{\gamma}_j^{\text{ols}}| - \frac{\lambda}{d_j}\right)^{+} \cdot \operatorname{sgn}\left(\widehat{\gamma}_j^{\text{ols}}\right), \tag{35}$$

where $\widehat{\gamma}_j^{\text{ols}} = \widetilde{y}^{(0)}\widetilde{U}_j^{(0)}$

(Step 4) repeat steps 2 and 3 using $\widehat{\boldsymbol{\gamma}}^{(1)}$ and similarly using $\widehat{\boldsymbol{\gamma}}^{(k)}$ until $\varepsilon^{(k)} = \frac{||\boldsymbol{\beta}^{(k)}-\boldsymbol{\beta}^{(k+1)}||}{||\boldsymbol{\beta}^{(k)}||} < \varepsilon$ for some desired tolerance ε.

(Step 5) Recover the solution in the original coordinates with

$$\widehat{\boldsymbol{\beta}}^{(n)} = \sum_{j=1}^{p} \widetilde{V}_j^{(n)} \frac{\widehat{\gamma}_j^{(n)}}{d_j^{(n)}}.$$

4 Numerical Studies

In this section we compare RgPCC with LASSO penalty to conventional logistic regression. We first summarize how our simulated data was created and then discuss the results of the methods mentioned previously. We will consider a variety of sample sizes, dimensions and sparsities in $\boldsymbol{\gamma}$ and compare error rates in $\mathbf{p}, \boldsymbol{\beta}, \boldsymbol{\gamma}$ and classification. We will also vary which components of $\boldsymbol{\gamma}$ are nonzero. Again, please note that p is the number of predictors while $\mathbf{p}$ is a vector of probabilities.

p	N	$\boldsymbol{\gamma}$ sparsity
12	100, 200	1, 3, 5
50	100, 200	1, 3
80	100, 200	1

Figure 1: Parameters of data creation.

The convergence of our algorithm is based on the tolerance of $\varepsilon = 0.1$, which means we will terminate our Newton-Ralphson method when

$$\varepsilon^{(k)} = \frac{||\boldsymbol{\beta}^{(k)} - \boldsymbol{\beta}^{(k+1)}||}{||\boldsymbol{\beta}^{(k)}||} < 0.1.$$

4.1 Creation of Simulated Data

Let $\mathbf{X}$ be our design matrix where each row of $\mathbf{X}$ is independently generated from $N(0, \Sigma)$ where $\Sigma_{ij} = \rho^{|i-j|}$ with $\rho = 0.8$.

To generate our response data, let $\mu = \mathbf{X}\boldsymbol{\beta}^* = \mathbf{U}\boldsymbol{\gamma}^*$ where $\boldsymbol{\gamma}^* = \mathbf{D}\mathbf{V}^T\boldsymbol{\beta}^*$. Then the classes $\mathbf{y}$ come from a Bernoulli distribution with parameter $\mathbf{p} = \frac{\exp(\mathbf{U}\boldsymbol{\gamma}^*)}{1+\exp(\mathbf{U}\boldsymbol{\gamma}^*)} = \frac{\exp(\mu)}{1+\exp(\mu)}$. Therefore the response data is dependent on $\boldsymbol{\gamma}^*$ and the data $\mathbf{X}$. We make a variety of choices for $\boldsymbol{\gamma}^*$ (denoted just as $\boldsymbol{\gamma}$ below) which have varying amounts of sparsity and created varying levels of linear separability.

4.2 Performance of RgPCC on Simulated Data

Here we fit RgPCC, logistic regression and PC logistic regression to our simulated data. To test the quality of the fit, we see how well our models predict the true probability vector $\mathbf{p}$ (the parameter of the Bernoulli distribution above) over a test set of size $5N$. We measure the accuracy of our predicted $\widehat{\mathbf{p}}$ using the 1-norm, 2-norm and EGKL. These are defined as follows:

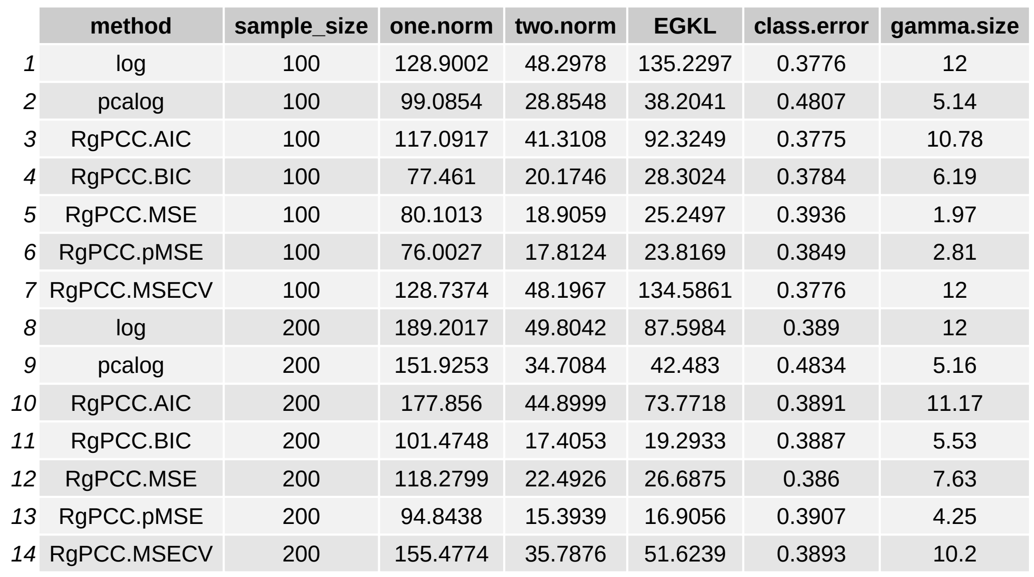
$$||v||_1 =$$
$$||v||_2 =$$
$$EGKL(v) =$$

We fit the models using samples of size N for dimension p from Figure 1. We also vary the nonzero components of the true $\boldsymbol{\gamma}$. We neglect the case where $N < p$, although there are no theoretical issues in this case and will be covered in further research.

We use the following values for the true $\boldsymbol{\gamma}$:

$$\begin{aligned}
\boldsymbol{\gamma}_1 &= (25, 0, \dots, 0) \\
\boldsymbol{\gamma}_2 &= (20, 10, 10, 0, \dots, 0) \\
\boldsymbol{\gamma}_3 &= (15, 10, 5, 5, 3, 0, \dots, 0) \\
\boldsymbol{\gamma}'_1 &= (0, 0, 0, 0, 0, 25, 0, \dots, 0) \\
\boldsymbol{\gamma}'_2 &= (0, 0, 0, 0, 0, 20, 10, 10, 0, \dots, 0) \\
\boldsymbol{\gamma}'_3 &= (0, 0, 0, 0, 0, 15, 10, 5, 5, 3, 0, \dots, 0)
\end{aligned}$$

Below we show only a few cases of all the tests. The rest of the results are present in the last section but have the same conclusion as the one presented here.



	method	sample_size	one.norm	two.norm	EGKL	class.error	gamma.size
1	log	100	128.9002	48.2978	135.2297	0.3776	12
2	pcalog	100	99.0854	28.8548	38.2041	0.4807	5.14
3	RgPCC.AIC	100	117.0917	41.3108	92.3249	0.3775	10.78
4	RgPCC.BIC	100	77.461	20.1746	28.3024	0.3784	6.19
5	RgPCC.MSE	100	80.1013	18.9059	25.2497	0.3936	1.97
6	RgPCC.pMSE	100	76.0027	17.8124	23.8169	0.3849	2.81
7	RgPCC.MSECV	100	128.7374	48.1967	134.5861	0.3776	12
8	log	200	189.2017	49.8042	87.5984	0.389	12
9	pcalog	200	151.9253	34.7084	42.483	0.4834	5.16
10	RgPCC.AIC	200	177.856	44.8999	73.7718	0.3891	11.17
11	RgPCC.BIC	200	101.4748	17.4053	19.2933	0.3887	5.53
12	RgPCC.MSE	200	118.2799	22.4926	26.6875	0.386	7.63
13	RgPCC.pMSE	200	94.8438	15.3939	16.9056	0.3907	4.25
14	RgPCC.MSECV	200	155.4774	35.7876	51.6239	0.3893	10.2

Figure 2: For $\boldsymbol{\gamma}'_2$ and $p = 12$.

	method	sample_size	one.norm	two.norm	EGKL	class.error	gamma.size
1	log	100	219.7315	119.8399	3337.828	0.4469	50
2	pcalog	100	147.4434	62.2117	241.1183	0.412	16.61
3	RgPCC.AIC	100	168.0875	77.802	288.5035	0.4282	32.88
4	RgPCC.BIC	100	88.2784	25.8719	37.0038	0.4077	5.7
5	RgPCC.MSE	100	86.9706	25.1717	35.639	0.4087	5.55
6	RgPCC.pMSE	100	86.0024	24.6228	34.8048	0.4066	5.33
7	RgPCC.MSECV	100	95.7481	30.1532	46.0895	0.4088	8.06
8	log	200	295.6583	112.8611	392.142	0.4326	50
9	pcalog	200	204.7182	58.4586	107.592	0.4175	18.21
10	RgPCC.AIC	200	148.4187	33.7531	45.4301	0.4129	10.64
11	RgPCC.BIC	200	127.0452	25.9331	31.4919	0.4123	7.18
12	RgPCC.MSE	200	174.8136	44.7253	68.5684	0.4161	19.38
13	RgPCC.pMSE	200	127.0452	25.9331	31.4919	0.4123	7.18
14	RgPCC.MSECV	200	127.0452	25.9331	31.4919	0.4123	7.18

Figure 3: For $\boldsymbol{\gamma}_2'$ and $p = 50$.

Overall, we see that RgPCC provides a slight improvement in the testing classification error compared to logistic regression and PC logistic regression. However, the real improvement in in the accuracy of our prediction of $\mathbf{p}$.

Overall, we can see that RgPCC provides slight improvements in the classification error to logistic regression and principal component logistic regression when the true $\boldsymbol{\gamma}$ is nonzero in the leading principal components. However, when the nonzero components of $\boldsymbol{\gamma}$ are not the leading principal components we see a significant different between principal component logistic regression and our other methods.

We can see that the testing error for $\mathbf{p}$ is improved with RgPCC by at least a factor of 4 in each case. RgPCC avoids overfitting the data as much as logistic regression does. In particular, there is drastic improvement in classification when $\boldsymbol{\gamma}^*$ is very sparse (that is for $\boldsymbol{\gamma}_1$). Similar results occur when $N = 200$ but are left in the table and results section.

We also run a few examples for higher dimensional data. Our method should excel in this via its use of principal components and sparsity in $\boldsymbol{\gamma}$.

where

$$\boldsymbol{\gamma}_1 = (25, 0, 0, 0, 0, 0, \ldots, 0)$$
$$\boldsymbol{\gamma}_2 = (10, 5, 5, 0, 0, 0, \ldots, 0)$$

Here we see similar results as in the low dimensional case. At this point, we know that RgPCC performs better, if no just as well, as logistic regression does. However, there are still many aspect of the method we wish to study.

4.3 Performance of RgPCC on Realworld Data

In this section we apply four real datasets to compare the prediction performance of RgPCC with conventional binary classification methods. We look at the following data sets.

- Divorce Predictors (170 instances, 54 predictors, binary response)
- Cryotherapy (90 instances, 7 predictors, binary response)
- Audit (777 instances, 18 predictors, binary response)
- Ecoli (336 instances, 8 predictors, binary response)

We will compare the methods RgPCC, logistic, PCA logistic and ridge regression. We will tune RgPCC by AIC and BIC. Thus we will compare a total of five different methods.

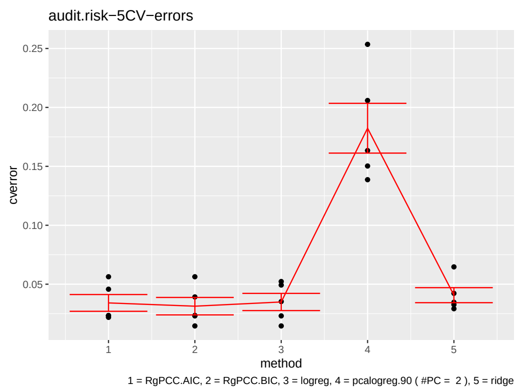
To compare the performance of our binary classification methods based on the error of each fold of 5-fold cross validation. We then perform Tukey's multiple pairwise comparison to test if the methods differ significantly or not.

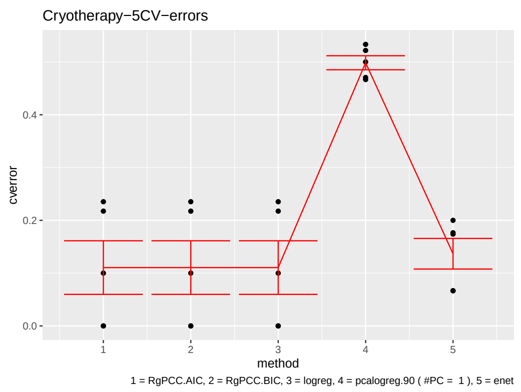
The following is a summary of the error results, more can be found in the section 6.

	RgPCC AIC	RgPCC BIC	Logistic	PC Logistic	Ridge
Divorce	0.023529	0.023529	0.058823	0.035294	0.023529
Cryo	0.12222	0.12222	0.12222	0.5	0.14444
Audit	0.033548	0.030967	0.034838	0.18193	0.04129
Ecoli	0.041666	0.038690	0.041666	0.053571	0.044642

Figure 4: The mean classification errors over each of the 5 folds.

When running the Tukey's multiple pairwise comparisons we noticed that in most cases the difference in the errors was insignificantly different with p-values around $0.99 \geq \alpha = 0.05$. However, there were a few cases in which PC logistic was significantly different than all the other methods (Audit data and Cryotherapy). This data is given below.





Thus, in terms of classification error RgPCC is comparable to logistic and ridge regression in application settings.

5 Conclusions and Further Research

5.1 Conclusions

As we continue work on RgPCC, we plan to investigate and improve a in a few key areas.

5.2 Speed

This method of RgPCC improves upon testing error in binary classification compared to logistic regression. We also believe that this use of principal component analysis should improve the speed of the computation, especially when there is sparsity in the solution with respect to the principal components. We wish to further explore this, especially in higher dimensions and when $p > N$.

5.3 C_p-type Statistic for Parameter Tuning

Using cross-validation for parameter selection is data and time intensive. In Zou and Lang's paper [2], the regularization parameter in RgPCR can be selected using Stein's unbiased risk estimation. In later works, we will also investigate if this method can be generalized to RgPCC.

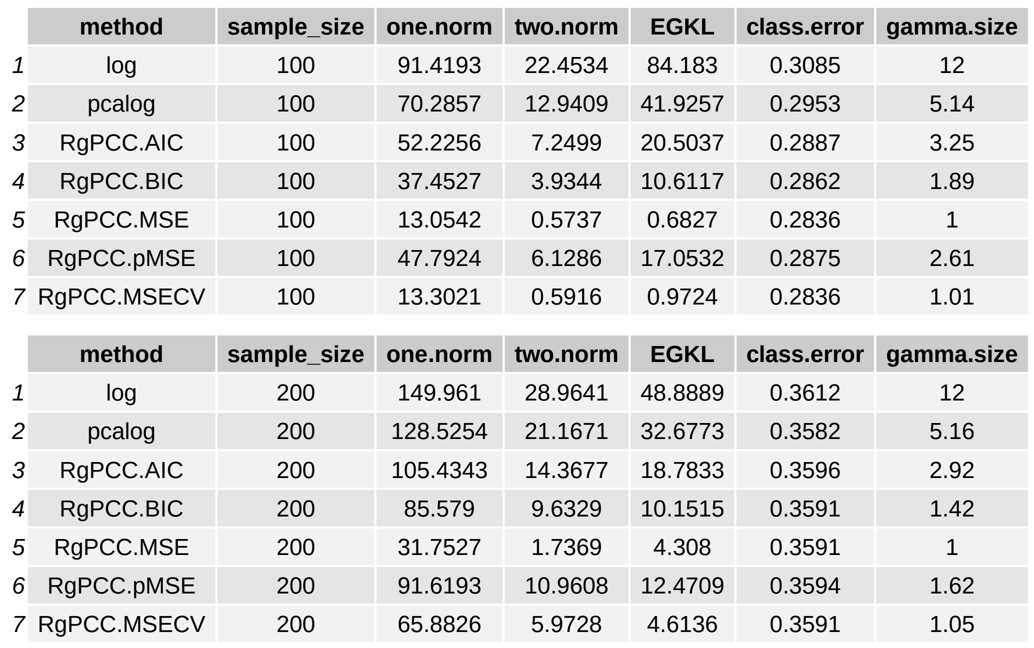
5.4 Further Generalization

In many cases, data is not presented in a manner such that classes are linearly separable. Kernel methods embed data in higher dimensional spaces in a way that makes classes linearly separable, without have to work in the higher dimensional space directly. We would like to be able to apply RgPCC in these nonlinear cases as well.

We would also like to extend this to multiclass classification through ideas from logistic regression for multiclass classification. We can also take the ideas from [3] to generalize this method to other classifiers such as SVM.

6 Figures

6.1 Tables of Simulated Results



	method	sample_size	one.norm	two.norm	EGKL	class.error	gamma.size
1	log	100	91.4193	22.4534	84.183	0.3085	12
2	pcalog	100	70.2857	12.9409	41.9257	0.2953	5.14
3	RgPCC.AIC	100	52.2256	7.2499	20.5037	0.2887	3.25
4	RgPCC.BIC	100	37.4527	3.9344	10.6117	0.2862	1.89
5	RgPCC.MSE	100	13.0542	0.5737	0.6827	0.2836	1
6	RgPCC.pMSE	100	47.7924	6.1286	17.0532	0.2875	2.61
7	RgPCC.MSECV	100	13.3021	0.5916	0.9724	0.2836	1.01

	method	sample_size	one.norm	two.norm	EGKL	class.error	gamma.size
1	log	200	149.961	28.9641	48.8889	0.3612	12
2	pcalog	200	128.5254	21.1671	32.6773	0.3582	5.16
3	RgPCC.AIC	200	105.4343	14.3677	18.7833	0.3596	2.92
4	RgPCC.BIC	200	85.579	9.6329	10.1515	0.3591	1.42
5	RgPCC.MSE	200	31.7527	1.7369	4.308	0.3591	1
6	RgPCC.pMSE	200	91.6193	10.9608	12.4709	0.3594	1.62
7	RgPCC.MSECV	200	65.8826	5.9728	4.6136	0.3591	1.05

Figure 5: For γ_2' and $p = 12$.

	method	sample_size	one.norm	two.norm	EGKL	class.error	gamma.size
1	log	100	210.0333	111.4804	3043.972	0.4216	50
2	pcalog	100	120.832	42.9534	133.9528	0.3665	16.61
3	RgPCC.AIC	100	80.3707	22.2387	35.1172	0.3609	7.22
4	RgPCC.BIC	100	63.9284	15.7583	19.9299	0.358	3.93
5	RgPCC.MSE	100	58.5378	12.4238	12.4689	0.3586	2.02
6	RgPCC.pMSE	100	62.5865	14.9977	18.4198	0.3569	3.7
7	RgPCC.MSECV	100	58.6641	13.2569	14.5907	0.356	2.85

	method	sample_size	one.norm	two.norm	EGKL	class.error	gamma.size
1	log	200	292.2532	111.7781	327.7571	0.4232	50
2	pcalog	200	195.8345	55.9057	96.0681	0.4022	18.21
3	RgPCC.AIC	200	145.4733	34.351	46.6281	0.394	6.81
4	RgPCC.BIC	200	120.4454	25.6383	31.3403	0.3921	3.52
5	RgPCC.MSE	200	137.4826	31.367	41.0866	0.3929	5.38
6	RgPCC.pMSE	200	107.4107	21.7626	25.4853	0.3941	2.85
7	RgPCC.MSECV	200	107.4107	21.7626	25.4853	0.3941	2.85

Figure 6: For $\boldsymbol{\gamma}_2'$ and $p = 12$.

	method	sample_size	one.norm	two.norm	EGKL	class.error	gamma.size
1	log	200	447.4376	230.4442	6306.2512	0.4565	80
2	pcalog	200	244.6892	86.3616	163.7597	0.4287	27.21
3	RgPCC.AIC	200	174.8162	50.1733	67.5138	0.4228	8.12
4	RgPCC.BIC	200	142.1117	35.8792	44.0206	0.4223	3.91
5	RgPCC.MSE	200	174.8162	50.1733	67.5138	0.4228	8.12
6	RgPCC.pMSE	200	143.7075	36.5861	44.9593	0.4225	4.22
7	RgPCC.MSECV	200	150.7253	39.6019	49.4351	0.422	4.87

	method	sample_size	one.norm	two.norm	EGKL	class.error	gamma.size
1	log	300	452.0082	173.9669	515.7646	0.4522	80
2	pcalog	300	290.4376	79.9708	138.9784	0.438	28.67
3	RgPCC.AIC	300	200.8527	42.5285	58.9005	0.4326	8.19
4	RgPCC.BIC	300	170.7052	32.663	40.9651	0.4326	4.43
5	RgPCC.MSE	300	126.9332	20.117	20.1521	0.4326	2.24
6	RgPCC.pMSE	300	126.9332	20.117	20.1521	0.4326	2.24
7	RgPCC.MSECV	300	182.119	36.2148	47.0899	0.4324	5.34

Figure 7: For $\boldsymbol{\gamma}_2'$ and $p = 12$.

6.2 Graphs of Tuning

References

[1] T. Hastie, R. Tibshirani, and J. Friedman (2009) — *The Elements of Statistical Learning : Data Mining, Inference, and Prediction (second edition)*, New York, NY: Springer.

[2] W. Lang, and H. Zou (2020) — *A simple method to improve principal components regression*, WILEY, https://onlinelibrary.wiley.com/doi/abs/10.1002/sta4.288

[3] H. Wang and C. Leng (2007) — *Unified LASSO Estimation by Least Squares Approximation*, Journal of the American Statistical Association, 102:479, 1039-1048, DOI; 10.1198/016214507000000509, https://doi.org/10.1198/016214507000000509