Sparse principal component regression for 
generalized linear models

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Abstract

Principal component regression (PCR) is a widely-used two-stage procedure: we 
first perform principal component analysis (PCA) and next consider a regression 
model in which selected principal components are regarded as new explanatory 
variables. We should remark that PCA is based only on the explanatory variables, 
so the principal components are not selected using the information on the response 
variable. In this paper, we propose a one-stage procedure for PCR in the framework 
of generalized linear models. The basic loss function is based on a combination of 
the regression loss and PCA loss. The estimate of the regression parameter is ob-
tained as the minimizer of the basic loss function with sparse penalty. The proposed 
method is called the sparse principal component regression for generalized linear 
models (SPCR-glm). SPCR-glm enables us to obtain sparse principal component 
loadings that are related to a response variable, because the two loss functions are 
simultaneously taken into consideration. A combination of loss functions may cause
the identifiability problem on parameters, but it is overcome by virtue of sparse penalty. The sparse penalty plays two roles in this method. The parameter estimation procedure is proposed using various update algorithms with the coordinate descent algorithm. We apply SPCR-glm to two real datasets, Doctor visit data and mouse consomic strain data. SPCR-glm provides easier interpretable PC scores and clearer classification on PC plots than the usual PCA.

**Key Words and Phrases:** Coordinate descent, Generalized linear models, Principal component regression, Sparse regularization, Variable selection.

## 1 Introduction

Principal component regression (PCR) (Massy, 1965; Jolliffe, 1982) is a widely-used two-stage procedure: we first perform principal component analysis (PCA) (Pearson, 1901; Jolliffe, 2002) and next consider a regression model in which selected principal components are regarded as new explanatory variables. There are many extensions of PCR (Hartnett et al., 1998; Rosital et al., 2001; Reiss and Ogden, 2007; Wang and Abbott, 2008). However, we should remark that the PCA is based only on the explanatory variables, so the principal components are not selected using the information on the response variable. If the response variable has a close relation to the principal components with small eigenvalues, PCR cannot present enough prediction accuracy.

To overcome this problem, Kawano et al. (2015) proposed a one-stage procedure for PCR. The basic loss function is based on a combination of the regression squared loss and PCA loss (Zou et al., 2006). The estimate of the regression parameter is obtained as the minimizer of the basic loss function with sparse penalty. The proposed method was called the sparse principal component regression (SPCR). SPCR enables us to obtain sparse principal component loadings that are related to a response variable, because the two loss functions are simultaneously taken into consideration. A combination of loss functions may cause the identifiability problem on parameters, but it is overcome by virtue of sparse penalty. The sparse penalty plays two roles in this method. The parameter estimation procedure was proposed using various iterative algorithms with the coordinate descent algorithm. However, the response variable is restricted to a continuous variable.
In this paper, we propose a one-stage procedure for PCR in the framework of generalized linear models (McCullagh and Nelder, 1989). The regression loss is replaced by the negative log-likelihood function. The proposed method is called the sparse principal component regression (SPCR-glm). The most different point in SPCR-glm from the SPCR is the parameter estimation procedure, because the negative log-likelihood function in the generalized linear models is more difficult than the regression squared loss. To obtain the parameter estimate, we propose a novel update algorithm combining various ideas with coordinate descent algorithm (Friedman et al., 2007; Wu and Lange, 2008).

We apply SPCR-glm to two real datasets, Doctor visit data and mouse consomic strain data, with Poisson regression model and multi-class logistic model, respectively. SPCR-glm provides easier interpretable PC scores and clearer classification on PC plots than the usual PCA. For the doctor visit data, we can also obtain clearer interpretable PC scores. For the consomic strain mouse data, we can also pick up some characteristic mouse consomic strains with smaller within-variance.

This paper is organized as follows. In Section 2 we review the sparse principal component analysis (SPCA) and SPCR. In Section 3 we propose SPCR-glm and introduce some special cases of SPCR-glm. In Section 4 we provide a parameter estimation procedure for SPCR-glm and discuss the selection of tuning parameters in SPCR-glm. Monte Carlo simulations and real data analyses are illustrated in Sections 5, 6 and 7. Concluding remarks are given in Section 8. The R language software package spcr, which implements SPCR-glm, is available on the Comprehensive R Archive Network (R Core Team, 2016). Supplementary materials can be found in https://sites.google.com/site/shuichikawanoen/research/suppl_spcr-glm.pdf

2 Preliminaries

2.1 Sparse principal component analysis

Let \( X = (x_1, \ldots, x_n)^T \) be an \( n \times p \) data matrix with \( n \) observations and \( p \) variables. Without loss of generality, the columns of the matrix \( X \) are assumed to be centered.
Principal component analysis (PCA) is formulated by the following least squares problem (e.g., Hastie et al., 2009);

$$\min_B \sum_{i=1}^{n} || x_i - BB^T x_i ||_2^2 \quad \text{subject to} \quad B^T B = I_k,$$

(1)

where $B = (\beta_1, \ldots, \beta_k)$ is a $p \times k$ principal component loading matrix, $k$ denotes the number of principal components, $I_k$ is the $k \times k$ identity matrix, and $|| \cdot ||_2$ is the $L_2$ norm defined by $||z||_2 = \sqrt{z^T z}$ for an arbitrary finite vector $z$. Let $X = UDV^T$, where $U$ is an $n \times p$ matrix with $U^T U = I_p$, $V = (v_1, \ldots, v_p)$ is a $p \times p$ orthogonal matrix, and $D = \text{diag}(d_1, \ldots, d_p)$ is a $p \times p$ matrix with $d_1 \geq \cdots \geq d_p \geq 0$. Then, the estimate of $B$ is given by $V_k Q^T$, where $V_k = (v_1, \ldots, v_k)$ and $Q$ is an arbitrary $k \times k$ orthogonal matrix.

To easily interpret the principal component loading matrix $B$, Zou et al. (2006) proposed the sparse principal component analysis (SPCA) given by

$$\min_{A,B} \left\{ \sum_{i=1}^{n} || x_i - A B^T x_i ||_2^2 + \lambda \sum_{j=1}^{k} || \beta_j ||_2^2 + \lambda_1 \sum_{j=1}^{k} || \beta_j ||_1 \right\} \quad \text{subject to} \quad A^T A = I_k,$$

(2)

where $A = (\alpha_1, \ldots, \alpha_k)$ is a $p \times k$ matrix, $\lambda$ and $\lambda_1$'s ($j = 1, \ldots, k$) are non-negative regularization parameters, and $|| \cdot ||_1$ is the $L_1$ norm defined by $||z||_1 = \sum_{j=1}^{p} |z_j|$ for an arbitrary finite vector $z = (z_1, \ldots, z_p)^T$. After simple calculation, SPCA is represented by

$$\min_{A,B} \sum_{j=1}^{k} \left\{ || X \alpha_j - X \beta_j ||_2^2 + \lambda || \beta_j ||_2^2 + \lambda_1 || \beta_j ||_1 \right\} \quad \text{subject to} \quad A^T A = I_k.$$

Given a fixed $B$, the minimizer $A$ is obtained by solving the reduced rank Procrustes rotation, which is introduced in Zou et al. (2006). Given a fixed $A$, the minimization problem for $B$ is consistent with that in the elastic net (Zou and Hastie, 2005), so it can be solved using the LARS algorithm (Efron et al., 2004) or the coordinate descent algorithm (Friedman et al., 2007; Wu and Lange, 2008). The parameter estimation procedure can be proposed via an alternate update algorithm of $A$ and $B$.  

4
2.2 Sparse principal component regression for continuous response

Principal component regression (PCR) is a widely-used two-stage procedure: we first perform principal component analysis (PCA) and next consider a regression model in which selected principal components are regarded as new explanatory variables. We should remark that the PCA is based only on the explanatory variables, so the principal components are not selected using the information on the response variable. If the response variable has a close relation to the principal components with small eigenvalues, the PCR cannot present enough prediction accuracy. To overcome this problem, Kawano et al. (2015) proposed a one-stage procedure for PCR. The proposed method was called the sparse principal component regression (SPCR).

Suppose that we have the continuous response variables $y_1, \ldots, y_n$ and explanatory variables $x_1, \ldots, x_n$. SPCR is formulated by

$$\min_{A, B, \gamma_0, \gamma} \left\{ \sum_{i=1}^{n} (y_i - \gamma_0 - \gamma^T B^T x_i)^2 + w \sum_{i=1}^{n} ||x_i - AB^T x_i||_2^2 ight. \left. + \lambda_\beta \xi \sum_{j=1}^{k} ||\beta_j||_2^2 + \lambda_\gamma (1 - \xi) \sum_{j=1}^{k} ||\beta_j||_1 + \lambda_\gamma ||\gamma||_1 \right\}$$

subject to $A^T A = I_k$,

where $\gamma_0$ is an intercept, $\gamma = (\gamma_1, \ldots, \gamma_k)^T$ is a coefficient vector, $\lambda_\beta$ and $\lambda_\gamma$ are non-negative regularization parameters, $w$ is a positive tuning parameter, and $\xi$ is a tuning parameter on $[0, 1)$. In Formula (3), the first term is the squared loss function of a linear regression model that employs the principal components $B^T x$ as explanatory variables, and the second term is the loss function of PCA, which is used in SPCA. Sparse regularizations in SPCR have two roles: the first is to estimate some parameters to be zero and the second is to overcome an identification problem on the parameters (for details, see Kawano et al., 2015).

The minimization problem (3) is a quadratic programming problem with respect to each parameter $\{B, \gamma_0, \gamma\}$, so that it is easy to construct the parameter estimation procedure, which was proposed using the coordinate descent algorithm by Kawano et al.
In SPCR, the response variable is restricted to a continuous variable. In Section 3, the SPCR is extended to the framework of generalized linear models (McCullagh and Nelder, 1989) to deal with various types of data, including the binary, count and multiclass data.

## 3 Sparse principal component regression for generalized linear models

We assume that the response variable given the explanatory variables is generated from the exponential family

\[
f(y_i | x_i; \theta(x_i), \phi) = \exp \left\{ \frac{y_i \theta(x_i) - u(\theta(x_i))}{\phi} + v(y_i, \phi) \right\},
\]

where \(\theta(x_i)\) is a canonical parameter, \(\phi\) is a nuisance parameter, and \(u(\cdot)\) and \(v(\cdot, \cdot)\) are known specific functions. The mean \(E(Y_i) = \mu_i\) and variance \(\text{Var}(Y_i)\) in the distribution (4) are given by \(u'(\theta(x_i))\) and \(\phi u''(\theta(x_i))\), respectively. Let \(\kappa_i\) be the linear predictor in the framework of generalized linear models with \(\kappa_i = h(u'(\theta(x_i)))\), where \(h(\cdot)\) is a link function (McCullagh and Nelder, 1989). From this relationship, (4) is reformulated by

\[
f(y_i | x_i; \theta(x_i), \phi) = \exp \left\{ \frac{y_i r(\kappa_i) - s(\kappa_i)}{\phi} + v(y_i, \phi) \right\},
\]

where \(r(\cdot) = u^{-1} \circ h^{-1}(\cdot)\) and \(s(\cdot) = u \circ u^{-1} \circ h^{-1}(\cdot)\). The link function \(h(\cdot)\) is often canonical with \(h(\cdot) = u^{-1}(\cdot)\). Then we have \(r(\kappa_i) = \kappa_i\).

Suppose that

\[
\kappa_i(x_i; \gamma_0, \gamma, B) = \gamma_0 + \gamma^T B^T x_i,
\]

where \(\gamma_0\) is an intercept, \(\gamma = (\gamma_1, \ldots, \gamma_k)^T\) is a coefficient vector, \(B = (\beta_1, \ldots, \beta_k)\) is a \(p \times k\) loading matrix. The PC score \(B^T x_i\) is regarded as a new explanatory variable. Here we consider the minimization problem

\[
\min_{A, B, \gamma_0, \gamma} \left[ L_{\text{reg}}(\gamma_0, \gamma, B) + w L_{\text{PCA}}(A, B) + P_1(B; \lambda_\beta, \xi) + P_2(\gamma; \lambda_\gamma) \right]
\]

subject to \(A^T A = I_k\).
where

\[
L_{\text{reg}}(\gamma_0, \gamma, B) = - \sum_{i=1}^{n} \log f(y_i|x_i; \kappa_i(x_i; \gamma_0, \gamma, B), \phi),
\]

\[
L_{\text{PCA}}(A, B) = \sum_{i=1}^{n} ||x_i - AB^T x_i||_2^2,
\]

\[
P_1(B; \lambda_\beta, \xi) = \lambda_\beta \xi \sum_{j=1}^{k} ||\beta_j||_2^2 + \lambda_\beta (1 - \xi) \sum_{j=1}^{k} ||\beta_j||_1,
\]

\[
P_2(\gamma; \lambda_\gamma) = \lambda_\gamma ||\gamma||_1,
\]

\(w\) is a positive tuning parameter, \(A\) is a \(p \times k\) matrix, \(\lambda_\beta\) and \(\lambda_\gamma\) are non-negative regularization parameters, and \(\xi\) is a tuning parameter whose values are between zero and one. The loss function \(L_{\text{reg}}\) is the negative log-likelihood, \(L_{\text{PCA}}\) is another loss function on PCA (Zou et al., 2006), \(P_1(B; \lambda_\beta, \xi)\) is the elastic net regularization on the loading matrix \(B\), and \(P_2(\gamma; \lambda_\gamma)\) is the sparse regularization penalty on \(\gamma\), which implies an automatic selection of principal components. We do not adopt the elastic net regularization on \(\gamma\), because the new explanatory variables based on \(B^T x\) are expected to be weakly correlated by virtue of the PCA loss. The tuning parameter \(w\) plays a role in the weight of the PCA loss; we obtain a better prediction accuracy as \(w\) is smaller, while we obtain a better formulation of principal component loadings as \(w\) is larger. The tuning parameter \(\xi\) controls the trade-off between the \(L_1\) and \(L_2\) penalties for \(B\) (Zou and Hastie, 2005). The minimization problem (6) enables us to perform the regression analysis and PCA, simultaneously. We call this procedure the sparse principal component regression for generalized linear models (SPCR-glm).

In the minimization problem (6), there exists an identification problem for the parameters \(B\) and \(\gamma\): for an arbitrary orthogonal matrix \(P\), we see \(\gamma^T B^T = \gamma^* T B^* T\), where \(\gamma^* = P \gamma\) and \(B^* = B P^T\). As discussed in Tibshirani (1996), Jennrich (2006), Choi et al. (2011), and Hirose and Yamamoto (2015), this problem is overcome by the sparse regularization for \(B\) or \(\gamma\). The sparse regularizations on \(B\) and \(\gamma\) in Formula (6), therefore, have two roles on sparse estimation and identification of parameters.

In numerical studies, we encountered the problem that SPCR-glm sometimes failed to give many sparse estimates of the loading matrix \(B\). To obtain many sparse estimates of \(B\), we propose to assign different regularization parameters for the components of \(B\): the
term $\lambda \beta (1 - \xi) \sum_{j=1}^{k} ||\beta_j||_1$ is replaced by $(1 - \xi) \sum_{j=1}^{k} \sum_{l=1}^{p} \lambda_{\beta,l} j |\beta_{lj}|$, where $\lambda_{\beta,lj}$ is a non-negative regularization parameter. We call this procedure the adaptive sparse principal component regression for generalized linear models (aSPCR-glm). In numerical studies, we utilized $\lambda_{\beta,lj} = \lambda_{\beta} / |\hat{\beta}_{lj}^\dagger|$ with $q \geq 0$, where $\hat{\beta}_{lj}^\dagger$ is an estimate of $\beta_{lj}$ derived from SPCR-glm. This idea is based on the adaptive lasso by Zou (2006).

3.1 Sparse principal component logistic regression

Suppose that we have a binary response variable $y_i \in \{0, 1\}$. The logistic regression model is given when $\phi = 1$, $u(\kappa_i) = \log\{1 + \exp(\kappa_i)\}$, and $v(y_i, \phi) = 0$. The regression loss function is

$$L_{reg} = - \sum_{i=1}^{n} \left[ y_i (\gamma_0 + \gamma^T B^T x_i) - \log\{1 + \exp(\gamma_0 + \gamma^T B^T x_i)\} \right].$$

3.2 Sparse principal component Poisson regression

Suppose that we have a count response variable $y_i \in \{0, 1, 2, \ldots\}$. The Poisson regression model is given when $\phi = 1$, $u(\kappa_i) = \exp(\kappa_i)$, and $v(y_i, \phi) = - \log y_i!$. The regression loss function is

$$L_{reg} = - \sum_{i=1}^{n} \left\{ y_i (\gamma_0 + \gamma^T B^T x_i) - \exp(\gamma_0 + \gamma^T B^T x_i) - \log y_i! \right\}.$$

3.3 Sparse principal component multiclass-logistic regression

We assume that the categorical values with $G$ levels are observed for response variable $C$. The multiclass-logistic regression model is given by

$$\Pr(C = g|x) = \frac{\exp(\gamma_{0g} + \gamma_g^T B^T x)}{\sum_{g=1}^{G} \exp(\gamma_{0g} + \gamma_g^T B^T x)}, \quad (g = 1, \ldots, G),$$

where $\gamma_{0g}$’s $(g = 1, \ldots, G)$ are intercepts, $\gamma_g = (\gamma_{1g}, \ldots, \gamma_{pg})^T$’s $(g = 1, \ldots, G)$ are the coefficient vectors. This is not a traditional model. This symmetric modeling procedure was used by Zhu and Hastie (2004), because it enables us to make an easier parameter estimation algorithm than the traditional model. Denote by $Y = (y_1, \ldots, y_G)$ the $n \times G$ indicator response matrix with elements $y_{ig} = I(c_i = g)$. The regression loss function is
given by
\[ L_{\text{reg}} = -\sum_{g=1}^{G} \sum_{i=1}^{n} [y_{ig}(\gamma_{0g} + \gamma_{g}^{T}B^{T}x_{i}) - \log\{1 + \exp(\gamma_{0g} + \gamma_{g}^{T}B^{T}x_{i})\}]. \]

We note that, by slightly modifying the density (4) with the response vectors, the minimization problem for the multiclass-logistic regression is a special case of SPCR-glm.

There is an identifiability problem in the symmetric modeling. The probabilities with \(\{\gamma_{0g}, \gamma_{g}\}\) are identical to these with \(\{\gamma_{0g} - \gamma_{0}^*, \gamma_{g} - \gamma^*\}\). This is not overcome if any constraints are not imposed. This crucial problem was discussed in Friedman et al. (2010). According to Friedman et al. (2010), \(\gamma_{j}^{*} (j = 1, \ldots, p)\) is provided by a median of \(\{\gamma_{j1}, \ldots, \gamma_{jG}\}\), and then \(\gamma_{0}^*\) is determined by mean centering of \(\{\gamma_{01}, \ldots, \gamma_{0G}\}\) by means of regularization. For details, see Theorem 1 in Friedman et al. (2010).

### 3.4 Related work

As a related work, we refer to PLS generalized linear regression (PLS-GLR) proposed by Bastien et al. (2005). PLS-GLR can perform the partial least squares (Wold, 1975; Frank and Friedman, 1993) under the situation that the response variable belongs to the exponential family or is censored. Although PLS-GLR is similar to our proposed method SPCR-glm, PLS-GLR does not integrate the two loss functions for generalized linear models and PCA with the \(L_1\) type regularization. In addition, PLS-GLR is a two-stage procedure, but SPCR-glm is a one-stage procedure. In Sections 5 and 7, we will compare the two methods through numerical studies.

### 4 Implementation

#### 4.1 Computational algorithm

Since SPCR-glm is a special case of aSPCR-glm, we focus on an estimation algorithm for aSPCR-glm. We estimate the parameters \(\{B, \gamma_0, \gamma\}\) in aSPCR-glm by the coordinate descent algorithm (Friedman et al., 2007; Wu and Lange, 2008), because the minimization problem includes \(L_1\) type regularizations. The parameter \(A\) is estimated according to Zou et al. (2007).
In SPCR, it is easy to implement the coordinate descent algorithm, because the optimization is a quadratic programming problem. But, in aSPCR-glm, the optimization is not a quadratic programming problem, because the log-likelihood function \( (4) \) is a nonlinear convex function in general. Therefore, for the current estimates of the parameters \( \{ \tilde{B}, \tilde{\gamma}_0, \tilde{\gamma} \} \), we employ a second-order Taylor expansion to the negative log-likelihood function around current estimates. The Taylor expansion leads to the approximated minimization problem given by

\[
\min_{A,B,\gamma_0,\gamma} \left[ -\sum_{i=1}^{n} \eta_i(z_i - \gamma_0 - \gamma^T \tilde{B}^T x_i)^2 + w \sum_{i=1}^{n} ||x_i - \tilde{A}B^T x_i||^2_2 \\
+ \lambda_\beta \xi \sum_{j=1}^{k} ||\beta_j||^2_2 + (1 - \xi) \sum_{j=1}^{k} \sum_{l=1}^{p} \lambda_{\beta,jl} |\beta_{jl}| + \lambda_\gamma ||\gamma||_1 \right]
\]

subject to \( A^T A = I_k \),

where

\[
\eta_i = -\frac{u''(\tilde{\gamma}_0 + \tilde{\gamma}^T \tilde{B}^T x_i)}{2\phi},
\]

\[
z_i = \tilde{\gamma}_0 + \tilde{\gamma}^T \tilde{B}^T x_i - \frac{y_i - u'(\tilde{\gamma}_0 + \tilde{\gamma}^T \tilde{B}^T x_i)}{u''(\tilde{\gamma}_0 + \tilde{\gamma}^T \tilde{B}^T x_i)}.
\]

This approximation leads to the updated equations given as follows.

**\( \beta_{ij} \) given \( \gamma_0, \gamma_j \) and \( A \):** The coordinate-wise update for \( \beta_{ij} \) has the form:

\[
\hat{\beta}_{l'j'} \leftarrow \frac{S \left( \sum_{i=1}^{n} x_{il'} \{ \eta_i Z_i \gamma_{j'} + 2w Y_{j'i}^* \} , (1 - \xi) \lambda_{\beta,l'j'} \right)}{\gamma_{j'}^2 \sum_{i=1}^{n} \eta_i x_{il'}^2 + 2w \sum_{i=1}^{n} x_{il'}^2 + 2\lambda_{\beta} \xi},
\]

\((l' = 1, \ldots, p; j' = 1, \ldots, k)\),

where

\[
Z_i = z_i - \gamma_0 - \sum_{j=1}^{k} \sum_{l \neq l'} \gamma_j \beta_{ij} x_{il} - \sum_{j \neq j'} \gamma_{j'} \beta_{lj'} x_{il'},
\]

\[
Y_{j'i}^* = y_{j'i}^* - \sum_{l \neq l'} \beta_{lj'} x_{il},
\]

and \( S(z, \eta) \) is the soft-thresholding operator with

\[
\text{sign}(z)(|z| - \eta)_+ = \begin{cases} 
  z - \eta, & (z > 0 \text{ and } \eta < |z|), \\
  z + \eta, & (z < 0 \text{ and } \eta < |z|), \\
  0, & (\eta \geq |z|).
\end{cases}
\]

Here \( y_{j'}^* = X \alpha_j \).
\( \gamma_j \) given \( \gamma_0, \beta_{lj} \) and \( A \): The update expression for \( \gamma_j \) is given by
\[
\hat{\gamma}_j' \leftarrow \frac{S \left( \sum_{i=1}^{n} \eta_i z_i^{**} x_{ij}', \lambda_{\gamma} \right)}{\sum_{i=1}^{n} \eta_i x_{ij}^{*2}}, \quad (j' = 1, \ldots, k),
\] (8)
where
\[
x_{ij}^* = \beta_j^T x_i,
\]
\[
y_{i}^{**} = z_i - \gamma_0 - \sum_{j \neq j'} \hat{\gamma}_j x_{ij}'.
\]

\( A \) given \( \gamma_0, \beta_{lj} \) and \( \gamma_j \): The estimate of \( A \) is obtained by
\[
\hat{A} = U V^T,
\]
where \((X^T X)B = U D V^T\).

\( \gamma_0 \) given \( \beta_{lj}, \gamma_j \) and \( A \): The estimate of \( \gamma_0 \) is derived from
\[
\hat{\gamma}_0 = \frac{1}{\sum_{i=1}^{n} \eta_i} \sum_{i=1}^{n} \eta_i \left\{ z_i - \sum_{j=1}^{k} \hat{\gamma}_j \left( \sum_{l=1}^{p} \hat{\beta}_{lj} x_{il} \right) \right\}.
\]
The update procedure can be directly implemented for the logistic model and Poisson regression model. The multiclass-logistic regression model has a special structure, as described in Section 3.3, so we need a slight modification, which is given in the supplementary material Appendix A.

The updates described earlier lead us to the parameter estimation procedure, which is summarized in the following steps:

**Step 1** Set the values of the tuning parameters \( \{w, \xi\} \) and the regularization parameters \( \{\lambda_{\beta}, \lambda_{\beta, lj}, \lambda_{\gamma}\} \).

**Step 2** Initialize the parameters \( \{A, B, \gamma_0, \gamma\} \).

**Step 3** Update the objective \( \eta_i \) \((i = 1, \ldots, n)\).

**Step 4** Update the estimates of the parameters.

**Step 5** Repeat Step 3 and Step 4 until convergence.
4.2 Selection of tuning parameters

We have four tuning parameters. To reduce the computational cost, the two tuning parameters $w$ and $\xi$ are fixed in advance. The tuning parameter $w$ is set to be a small value, because the regression loss is more important than the PCA loss. The tuning parameter $\xi$ is set to be a small value, because the sparse regularization is more important than the ridge regularization. The latter idea is often used in the elastic net. The remaining parameters $\lambda_\beta$ and $\lambda_\gamma$ are automatically selected by the cross-validation.

Let us divide the original dataset into $K$ datasets $(y^{(1)}, X^{(1)}), \ldots, (y^{(K)}, X^{(K)})$. The $K$-fold cross-validation criterion for aSPCR-glm is given by

$$CV_{glm} = -\frac{1}{K} \sum_{k=1}^{K} \sum_{i \in C_k} \left\{ y_i (\hat{\gamma}_0^{(-k)} + \hat{\gamma}^{(-k)T} \hat{B}^{(-k)T} x_i) - u(\hat{\gamma}_0^{(-k)} + \hat{\gamma}^{(-k)T} \hat{B}^{(-k)T} x_i) + v(y_i, \hat{\phi}^{(-k)}) \right\},$$

where $C_k \; (k = 1, \ldots, K)$ is the set of indexes for the divided dataset $(y^{(k)}, X^{(k)})$, and $\hat{\gamma}_0^{(-k)}, \hat{B}^{(-k)}$, $\hat{\gamma}^{(-k)}, \hat{\phi}^{(-k)}$ are the estimates computed with the data removing the $k$-th part. The $K$-fold cross-validation criterion for the multiclass-logistic model is given by

$$CV_{multi} = -\frac{1}{K} \sum_{k=1}^{K} \sum_{g=1}^{G} \sum_{i \in C_k} \left\{ y_{ig} (\hat{\gamma}_{0g}^{(-k)} + \hat{\gamma}_g^{(-k)T} \hat{B}^{(-k)T} x_i) - \log \{1 + \exp(\hat{\gamma}_{0g}^{(-k)} + \hat{\gamma}_g^{(-k)T} \hat{B}^{(-k)T} x_i)\} \right\},$$

where $\hat{\gamma}_{0g}^{(-k)}, \hat{B}^{(-k)}, \hat{\gamma}_g^{(-k)}$ are the estimates computed with the data removing the $k$-th part.

We employed $K = 5$ in our simulation. The candidates of the regularization parameters $\lambda_\beta$ and $\lambda_\gamma$ were determined according to the function glmnet in R.

5 Illustrative example

We generated a dataset $\{(y_i, x_i); i = 1, \ldots, 200\}$ for a binary response variable and 10-dimensional explanatory variables. The explanatory variables were given by $x_i = P(u_i^T, v_i^T)^T$, where

$$u_i \sim \frac{1}{4} \sum_{j=1}^{4} N_2(a_j, 0.5^2 I_2), \quad v_i \sim N_8(0, \Sigma), \quad P = \text{blockdiag}(Q^T, I_8).$$

Here, $a_1 = (2, 2)^T, a_2 = (-2, 2)^T, a_3 = (-2, -2)^T, a_4 = (2, -2)^T$, $(\Sigma)_{ij} = 0.8|^{i-j}|$, and $Q$ is a $2 \times 2$ matrix whose $i$-th column is the eigenvector corresponding to the $i$-th largest
eigenvalue of $\text{Var}(\mathbf{u})$. Note that $\mathbf{u}_i$ presents four clusters which have four centers at $\mathbf{a}_j$’s. We can easily show that $\mathbf{\nu}_1 = (0, 1, 0, \ldots, 0)^T$ and $\mathbf{\nu}_2 = (1, 0, \ldots, 0)^T$ are the eigenvectors of $\text{Var}(P\mathbf{u})$ and the third and fourth eigenvalues of $\text{Var}(\mathbf{x})$, respectively. We also see $(\mathbf{\nu}_2^T \mathbf{x}_i, \mathbf{\nu}_1^T \mathbf{x}_i)^T = \mathbf{u}_i$. The response variable $y_i$ was distributed according to the Bernoulli distribution with probability $\theta_i$ that satisfies $\log\{\theta_i/(1-\theta_i)\} = \mathbf{x}_i^T \mathbf{\nu}_1 + \mathbf{x}_i^T \mathbf{\nu}_2$. This setting implies that the response is related to the principal components corresponding to the third and fourth eigenvalues of $\text{Var}(\mathbf{x})$.

Figure 1: Scatter plots of principal and PLS components. (a) The true structure of the principal components. (b) PCA. (c) PLS-GLR. (d) SPCR-glm.
We applied SPCR-glm with $k = 3$ into the dataset, and then conducted PCA and PLS-GLR described in Section 3.4. The tuning parameters in SPCR-glm were set to $w = 0.01, \xi = 0.001, \lambda_\beta = 3, \text{ and } \lambda_\gamma = 0.1$. Figure 1 shows the true scatter plot of $(\nu_2^T x_i, \nu_1^T x_i)^T = u_i$'s in (a) and the scatter PC plots for PCA in (b), for PLS-GLR in (c), and for our proposed method in (d). We observe that (b) and (c) fail to capture the true structure, while (d) succeeds to find the true structure by the second and third principal components.

6 Simulation studies

To investigate the performances of our proposed method, Monte Carlo simulations were conducted. We used four models in this study: two for binary data and two for count data.

In the first model, we considered the 20-dimensional covariate vector $x = (x_1, \ldots, x_{20})^T$ according to a multivariate normal distribution $N(0_{20}, \Sigma_2)$, and generated the response $y$ by

$$y_i \sim B(1, p_i), \quad \log \left( \frac{p_i}{1 - p_i} \right) = 4x_i^T \xi^*, \quad i = 1, \ldots, n.$$ 

We used $\Sigma_2 = \text{blockdiag}(\Sigma_2^*, I_{11})$ and $\xi^* = (\nu_1^*, 0, \ldots, 0)^T$, where $(\Sigma_2^*)_{ij} = 0.9^{\lvert i - j \rvert} (i, j = 1, \ldots, 9)$ and $\nu_1^* = (-1, 0, 1, 1, 0, -1, -1, 0, 1)$ is a sparse approximation of the fourth eigenvector of $\Sigma_2^*$.

In the second model, we considered the 30-dimensional covariate vector $x = (x_1, \ldots, x_{30})^T$ according to a multivariate normal distribution $N(0_{30}, \Sigma_3)$, and generated the response $y$ by

$$y_i \sim B(1, p_i), \quad \log \left( \frac{p_i}{1 - p_i} \right) = 2x_i^T \xi_1^* + 2x_i^T \xi_2^*, \quad i = 1, \ldots, n.$$ 

We used $\Sigma_3 = \text{blockdiag}(\Sigma_2^*, \Sigma_3^*, I_{15})$ with $(\Sigma_3^*)_{ij} = 0.9^{\lvert i - j \rvert} (i, j = 1, \ldots, 6)$, $\xi_1^* = (\nu_1^*, 0, \ldots, 0)^T$, and $\xi_2^* = (0, \ldots, 0, \nu_2^*, 0, \ldots, 0)^T$, where $\nu_2^* = (1, 0, -1, -1, 0, 1)$ is a sparse approximation of the third eigenvector of $\Sigma_3^*$.

In the third model, we considered the 20-dimensional covariate vector $x = (x_1, \ldots, x_{20})^T$ according to a multivariate normal distribution $N(0_{20}, \Sigma_2)$, and generated the response $y$
Table 1: Mean (standard deviation) values of the EL for Cases 1 and 2. The bold values correspond to the smallest means.

| Case | n   | k   | aSPCR-Log(0.1) | aSPCR-Log(0.5) | aSPCR-Log(1) | SPCR-Log | PCR    | PLS    |
|------|-----|-----|----------------|----------------|--------------|----------|--------|--------|
| 1    | 200 | 1   |                | 0.328          | 0.421        | 0.347    | 0.697  | 0.666  |
|      |     |     | (0.100)        | (0.092)        | (0.184)      | (0.098)  | (0.005) | (0.035) |
| 5    | 0.354|     | 0.316          | 0.688          | 0.365        | 0.701    | 0.366  |        |
|      | (0.119)|    | (0.067)        | (0.038)        | (0.127)      | (0.009)  | (0.048) |        |
| 400  | 1   | 0.301|                | 0.287          | 0.285        | 0.299    | 0.695  | 0.633  |
|      |     |     | (0.071)        | (0.043)        | (0.043)      | (0.059)  | (0.002) | (0.046) |
| 5    | 0.375|     | 0.287          | 0.678          | 0.388        | 0.696    | 0.301  |        |
|      | (0.165)|    | (0.043)        | (0.066)        | (0.172)      | (0.004)  | (0.025) |        |
| 2    | 200 | 2   |                | 0.449          | 0.692        | 0.460    | 0.698  | 0.675  |
|      |     |     | (0.046)        | (0.041)        | (0.021)      | (0.047)  | (0.008) | (0.040) |
| 5    | 0.455|     | 0.468          | 0.695          | 0.457        | 0.703    | 0.509  |        |
|      | (0.050)|    | (0.081)        | (0.003)        | (0.046)      | (0.011)  | (0.074) |        |
| 400  | 2   | 0.411|                | 0.401          | 0.691        | 0.410    | 0.693  | 0.614  |
|      |     |     | (0.035)        | (0.019)        | (0.027)      | (0.020)  | (0.005) | (0.034) |
| 5    | 0.413|     | 0.401          | 0.693          | 0.415        | 0.695    | 0.427  |        |
|      | (0.043)|    | (0.018)        | (0.003)        | (0.043)      | (0.006)  | (0.028) |        |

by

\[ y_i \sim Pois(\lambda_i), \quad \log(\lambda_i) = 0.8 x_i^T \xi^*, \quad i = 1, \ldots, n. \]

In the fourth model, we considered the 30-dimensional covariate vector \( x = (x_1, \ldots, x_{30})^T \) according to a multivariate normal distribution \( N(0_{30}, \Sigma_3) \), and generated the response \( y \) by

\[ y_i \sim Pois(\lambda_i), \quad \log(\lambda_i) = 0.5 x_i^T \xi_1^* + 0.5 x_i^T \xi_2^*, \quad i = 1, \ldots, n. \]

The sample size was set to \( n = 200, 400 \). For Cases 1 and 2, we used SPCR-glm for binary data (SPCR-Log) and aSPCR-glm for binary data with \( q = 0.1, 0.5, 1 \) (aSPCR-Log(\( q \))). For Cases 3 and 4, we used SPCR-glm for count data (SPCR-Poi) and aSPCR-glm for count data with \( q = 0.1, 0.5, 1 \) (aSPCR-Poi(\( q \))). The proposed methods were
Table 2: Mean (standard deviation) values of the EL for Cases 3 and 4. The bold values correspond to the smallest means.

| Case | n   | k | aSPCR-Poi(0.1) | aSPCR-Poi(0.5) | aSPCR-Poi(1) | SPCR-Poi | PCR   | PLS   |
|------|-----|---|----------------|----------------|--------------|----------|-------|-------|
| 3    | 200 | 1 | 1.386          | 1.378          | **1.375**    | 1.395    | 1.915 | 1.875 |
|      |     |   | (0.060)        | (0.079)        | (0.082)      | (0.079)  | (0.071)| (0.092)|
| 5    | 1.382 | **1.368** | 1.382          | 1.389          | 1.932       | 1.392   |
|      | (0.042)|   | (0.042)        | (0.075)        | (0.071)      | (0.075)  |       | (0.039)|
| 4    | 200 | 2 | 1.403          | **1.394**      | 1.510        | 1.406    | 1.658 | 1.625 |
|      |     |   | (0.045)        | (0.046)        | (0.113)      | (0.045)  | (0.043)| (0.055)|
| 5    | 1.404 | **1.399** | 1.552          | 1.407          | 1.665       | 1.423   |
|      | (0.050)|   | (0.052)        | (0.115)        | (0.049)      | (0.045)  |       | (0.040)|
| 4    | 400 | 2 | 1.360          | **1.357**      | 1.439        | 1.361    | 1.655 | 1.566 |
|      |     |   | (0.039)        | (0.037)        | (0.099)      | (0.039)  | (0.047)| (0.053)|
| 5    | 1.360 | **1.359** | 1.477          | 1.362          | 1.659       | 1.368   |
|      | (0.036)|   | (0.036)        | (0.122)        | (0.037)      | (0.047)  |       | (0.033)|
Table 3: Mean (standard deviation) values of TPR and TNR for Cases 1 and 2. The bold values correspond to the largest means.

| Case | n   | k | aSPCR-Log(0.1) | aSPCR-Log(0.5) | aSPCR-Log(1) | SPCR-Log |
|------|-----|---|----------------|----------------|--------------|----------|
| 1    | 200 | 1 | TPR            | 0.930          | 0.956        | 0.736    | 0.933    |
|      |     |   |                | (0.256)        | (0.176)      | (0.394)  | (0.246)  |
|      |     |   | TNR            | 0.267          | 0.580        | 0.920    | 0.190    |
|      |     |   |                | (0.228)        | (0.201)      | (0.086)  | (0.240)  |
| 5    |     |   | TPR            | 0.928          | 0.980        | 0.048    | 0.915    |
|      |     |   |                | (0.210)        | (0.114)      | (0.123)  | (0.232)  |
|      |     |   | TNR            | 0.349          | 0.585        | 1        | 0.270    |
| 400  |     |   | TPR            | 0.973          | 0.993        | 0.991    | 0.983    |
|      |     |   |                | (0.154)        | (0.066)      | (0.083)  | (0.119)  |
|      |     |   | TNR            | 0.349          | 0.585        | 1        | 0.270    |
| 5    |     |   | TPR            | 0.876          | 0.991        | 0.088    | 0.863    |
|      |     |   |                | (0.236)        | (0.083)      | (0.184)  | (0.244)  |
|      |     |   | TNR            | 0.349          | 0.585        | 1        | 0.270    |
| 2    | 200 | 2 | TPR            | 0.980          | 0.991        | 0.018    | 0.982    |
|      |     |   |                | (0.112)        | (0.032)      | (0.103)  | (0.112)  |
|      |     |   | TNR            | 0.278          | 0.474        | 1        | 0.190    |
|      |     |   |                | (0.167)        | (0.154)      | (0)      | (0.154)  |
|      |     |   | TPR            | 0.977          | 0.906        | 0.003    | 0.984    |
|      |     |   |                | (0.107)        | (0.243)      | (0.017)  | (0.095)  |
|      |     |   | TNR            | 0.300          | 0.519        | 1        | 0.197    |
|      |     |   |                | (0.178)        | (0.221)      | (0)      | (0.155)  |
| 400  |     | 2 | TPR            | 0.990          | 1            | 0.012    | 1        |
|      |     |   |                | (0.100)        | (0)          | (0.100)  | (0)      |
|      |     |   | TNR            | 0.300          | 0.519        | 1        | 0.197    |
|      |     |   |                | (0.178)        | (0.221)      | (0)      | (0.157)  |
| 5    |     |   | TPR            | 0.987          | 1            | 0.004    | 0.982    |
|      |     |   |                | (0.093)        | (0)          | (0.019)  | (0.127)  |
|      |     |   | TNR            | 0.331          | 0.612        | 1        | 0.218    |
|      |     |   |                | (0.149)        | (0.133)      | (0)      | (0.143)  |
Table 4: Mean (standard deviation) values of TPR and TNR for Cases 3 and 4. The bold values correspond to the largest means.

| Case | n   | k | aSPCR-Poi(0.1) | aSPCR-Poi(0.5) | aSPCR-Poi(1) | aSPCR-Poi |
|------|-----|---|----------------|----------------|--------------|------------|
| 3    | 200 | 1 | TPR            |                |              |            |
|      |     |   | **0.993**      | 0.981          | 0.973        | 0.980      |
|      |     |   | (0.066)        | (0.118)        | (0.143)      | (0.140)    |
|      |     |   | TNR            |                |              |            |
|      |     |   | 0.247          | 0.607          | **0.921**    | 0.150      |
|      |     |   | (0.160)        | (0.198)        | (0.115)      | (0.161)    |
| 5    | 200 | 1 | TPR            |                |              |            |
|      |     |   | **0.996**      | 0.995          | 0.980        | 0.990      |
|      |     |   | (0.033)        | (0.037)        | (0.106)      | (0.100)    |
|      |     |   | TNR            |                |              |            |
|      |     |   | 0.250          | 0.659          | **0.964**    | 0.165      |
|      |     |   | (0.152)        | (0.183)        | (0.068)      | (0.140)    |
| 4    | 200 | 1 | TPR            |                |              |            |
|      |     |   | **0.980**      | 0.980          | 0.980        | 0.980      |
|      |     |   | (0.140)        | (0.140)        | (0.140)      | (0.140)    |
|      |     |   | TNR            |                |              |            |
|      |     |   | 0.287          | 0.737          | **0.987**    | 0.182      |
|      |     |   | (0.183)        | (0.183)        | (0.055)      | (0.165)    |
| 5    | 200 | 1 | TPR            |                |              |            |
|      |     |   | 0.999          |                | **0.996**    | 0.990      |
|      |     |   | (0.100)        | (0.033)        | (0.100)      | (0.100)    |
|      |     |   | TNR            |                |              |            |
|      |     |   | 0.305          | 0.800          | **0.994**    | 0.180      |
|      |     |   | (0.175)        | (0.166)        | (0.021)      | (0.144)    |
| 4    | 200 | 2 | TPR            |                |              |            |
|      |     |   | 0.971          | 0.953          | 0.526        | **0.976**  |
|      |     |   | (0.143)        | (0.145)        | (0.396)      | (0.142)    |
|      |     |   | TNR            |                |              |            |
|      |     |   | 0.270          | 0.659          | **0.974**    | 0.172      |
|      |     |   | (0.151)        | (0.150)        | (0.050)      | (0.149)    |
| 5    | 200 | 2 | TPR            |                |              |            |
|      |     |   | 0.964          | 0.938          | 0.366        | **0.969**  |
|      |     |   | (0.156)        | (0.159)        | (0.397)      | (0.150)    |
|      |     |   | TNR            |                |              |            |
|      |     |   | 0.296          | 0.691          | **0.982**    | 0.189      |
|      |     |   | (0.161)        | (0.151)        | (0.042)      | (0.170)    |
| 4    | 400 | 2 | TPR            |                |              |            |
|      |     |   | **0.990**      | 0.986          | 0.766        | 0.990      |
|      |     |   | (0.100)        | (0.073)        | (0.336)      | (0.100)    |
|      |     |   | TNR            |                |              |            |
|      |     |   | 0.291          | 0.749          | **0.992**    | 0.183      |
|      |     |   | (0.145)        | (0.147)        | (0.019)      | (0.129)    |
| 5    | 400 | 2 | TPR            |                |              |            |
|      |     |   | **0.993**      | 0.987          | 0.635        | 0.992      |
|      |     |   | (0.070)        | (0.082)        | (0.411)      | (0.080)    |
|      |     |   | TNR            |                |              |            |
|      |     |   | 0.304          | 0.754          | **0.992**    | 0.192      |
|      |     |   | (0.149)        | (0.157)        | (0.022)      | (0.135)    |
fitted to the simulated data with one or five components \((k = 1, 5)\) for Cases 1 and 3, and two or five components \((k = 2, 5)\) for Cases 2 and 4. The regularization parameters \(\lambda_\beta\) and \(\lambda_\gamma\) were selected by five-fold cross-validation in Section 4.2. The tuning parameters \(w\) and \(\zeta\) were set to 0.01 and 0.001, respectively. Our proposed methods were compared with PLS-GLR and PCR. The performance was evaluated by the value of the negative expected log-likelihood function \(-E[\log f(y|x; \hat{\theta})]\) (EL). The simulation was conducted 100 times. EL was estimated by 1,000 random samples.

Tables 1 and 2 represent the means and standard deviations of ELs for Cases 1 and 2, and these two results show similar tendency. PCR was the worst in all cases. Our proposed methods outperform other methods when \(k = 1, 2\), and were competitive with PLS-GLR when \(k = 5\). The proposed method with \(q = 0.5\) was superior to other methods in almost all cases. The smallest ELs were provided by the proposed method with \(q = 1\) in Case 1 for \(n = 400\) and \(k = 1\) and in Case 3 for \(n = 200\) and \(k = 1\). The performance of aSPCR-Log(0.1) or aSPCR-Poi(0.1) was similar to that of aSPCR-Log or aSPCR-Poi, respectively.

We also computed the true positive rate (TPR) and the true negative rate (TNR) for aSPCR-Log(\(q\)), SPCR-Log, aSPCR-Poi(\(q\)), and SPCR-Poi, which are defined by

\[
\text{TPR} = \frac{1}{100} \sum_{k=1}^{100} \frac{\left| \left\{ j : \hat{\zeta}_j^{(k)} \neq 0 \land \zeta_j^* \neq 0 \right\} \right|}{\left| \left\{ j : \zeta_j^* \neq 0 \right\} \right|},
\]

\[
\text{TNR} = \frac{1}{100} \sum_{k=1}^{100} \frac{\left| \left\{ j : \hat{\zeta}_j^{(k)} = 0 \land \zeta_j^* = 0 \right\} \right|}{\left| \left\{ j : \zeta_j^* = 0 \right\} \right|},
\]

where \(\hat{\zeta}_j^{(k)}\) is the estimated \(j\)-th coefficient for the \(k\)-th simulation, and \(\left| \{ \ast \} \right|\) is the number of elements included in a set \(\{ \ast \}\). Tables 3 and 4 represent the means and standard deviations of TPR and TNR, and present similar results. In Table 3, many methods provide higher ratios of TPRs except for aSPCR-Log(1), while aSPCR-Log(1) provides higher ratios of TNRs. The results for Cases 3 and 4 show that TPRs are higher in almost all situations, but TNRs of aSPCR-Poi(0.1) and aSPCR-Poi are too lower.
7 Applications

In this section, two real data analyses are illustrated. We observe easier interpretable PC scores and clearer classification on PC plots than the usual PCA.

7.1 Doctor visits data

We applied SPCR-glm to the doctor visits data in Cameron and Trivedi (1986). This dataset consists of 5,190 observations originating from the Australian Health Survey that contains information on the number of consultations with a doctor or specialist and on 11 variables: (1) Gender, (2) Age, (3) Income, (4) Illness, (5) Reduced, (6) Health, (7) Private, (8) Freepoor, (9) Freerepeat, (10) Nchronic, and (11) Lchronic. The dataset is available from the package AER in R.

To model a relationship between the number of consultations, which is count data, and the 11 variables, we utilized SPCR-glm with \( k = 5 \). We compared SPCR-glm with PCR and PLS-GLR. The tuning parameters in SPCR-glm were set to \( w = 0.1, \xi = 0.001, \lambda_\gamma = 0, \lambda_\beta = 10 \). The reason why \( \lambda_\gamma = 0 \) is that we do not aim to select the number of principal components automatically.

Figure 2: Scatter plots of principal components given by SPCR-glm for the doctor visits data.
Table 5: The estimates of $B$ for the doctor visits data.

| variable   | PC1   | PC2   | PC3   | PC4   | PC5   |
|------------|-------|-------|-------|-------|-------|
| Gender     | -0.535| -0.011| 0.082 | 0     | 0.535 |
| Age        | -0.451| 0     | -0.322| -0.090| -0.062|
| Income     | 0.497 | 0     | -0.351| 0     | 0     |
| Illness    | -0.047| 0.530 | 0     | -0.226| 0     |
| Reduced    | 0.019 | 0.688 | -0.085| 0     | 0     |
| Health     | 0.061 | 0.416 | 0.212 | -0.002| 0     |
| Private    | 0.084 | 0.008 | -0.195| 0     | 0.710 |
| Freepoor   | 0     | 0     | 0.779 | 0     | 0     |
| Freerepeat | -0.459| 0     | -0.152| 0     | -0.422|
| Nchronic   | -0.034| 0.043 | -0.032| -0.751| 0     |
| Lchronic   | -0.131| 0.259 | -0.089| 0.594 | 0     |

Figure 2 is the scatter PC plots on SPCR-glm. Some clusters are observed by PC3, PC4, and PC5. This may imply that the dataset is divided into several clusters. This finding is not seen in the scatter PC plots on PCR and PLS-GLR (Appendix B). Furthermore, we computed the five-fold cross validation for SPCR-glm, PCR, and PLS-GLR, to compare the prediction performance. The validation values were 0.652, 0.662, and 0.651, respectively.

The estimates $\hat{\gamma}_0$ and $\hat{\gamma}$ for SPCR-glm were given by

$$\hat{\gamma}_0 = -1.484, \quad \hat{\gamma} = (-0.106, 0.433, -0.124, -0.087, 0.065)^T,$$

and the estimate of the loading matrix $B$ is shown in Table 5. We can interpret some of the principal component loadings as follows. PC2 represents an index of health state, because it provides larger values for Illness, Reduced, and Health factors, where the first and second factors are a clinical history in past two weeks and the third factor is a general health index. PC3 shows whether it is easy to visit the hospital, because it provides larger values for Freepoor factor and smaller values for the age factor, where Freepoor means whether the individual has a free government health insurance due to low income or not. PC4 represents an overall index for chronic disease, because it provides
larger values for Lchronic factor and smaller values for Illness and Nchronic factors, where Nchronic is a chronic condition not limiting activity while Lchronic is that limiting activity. Meanwhile, it is difficult to interpret the principal component loadings for PCR and PLS-GLR (Appendix B).

7.2 Mouse consomic strain data

Takada et al. (2008) provided the dataset on mouse inter-subspecific consomic strains. The consomic strain (CS) was made from the standard strain C57BL/6 (B6) by replacing a chromosome by the corresponding chromosome on the MSM/Ms (MSM). The phenotypes of B6 are different from those of MSM. If the several phenotypes of the CS are identical to those of MSM, we can assume that the genetic factor corresponding to the phenotypes depends on the replaced chromosome. There were $G = 30$ strains, including B6, MSM and 28 CSs, with $p = 36$ traits. Each strain had 7-16 animals. Various properties on mice can be seen in Takada et al. (2008) and at the website http://molossinus.lab.nig.ac.jp/phenotype/. This dataset can be downloaded from the web server ftp://molossinus.lab.nig.ac.jp/pub/phenotypedb/CONSOMIC_10W/.

We analyzed the male data in this dataset by the usual PCA and our method SPCR-glm with $k = 3$, $w = 0.01$, $\xi = 0.001$, $\lambda_\beta = 4$, and $\lambda_\gamma = 10$. There were very few missing observations with the ratio 0.39%, which were imputed by the package mice in R. The resulting PC plots are shown in Figure 3 and the PC loadings and regression coefficients by SPCR-glm are given in Tables 6 and 7.

The first PC (PC1) by SPCR-glm largely depended on the score

$$1.74 \times \text{PERIPENAL} - 1.27 \times \text{ALP},$$

where PERIPENAL is the fat value around kidney and ALP is the Alkaline Phosphatase value. B6 and MSM presented around zero value of PC1, which implies that PC1 is an index related to CSs. CS11 clearly presented around zero value on PC2 and a lower value on PC1 and was separate from other mice in Figure 3(a). In fact, CS11 had a small PERIPENAL and a large ALP, which showed a small score on PC1. In Figure 3(c), CS11 was not separate from other mice.
Figure 3: Scatter plots of PC scores for the mouse consomic strain data.
Table 6: The estimates of $B$ for the mouse consomic strain data.

| variable                  | PC1  | PC2  | PC3  |
|---------------------------|------|------|------|
| BODY_WEIGHT               | 0    | 0    | 0    |
| BODY_LENGTH               | 0    | -0.223 | 0   |
| TAIL_LENGTH               | 0    | -0.050 | 0   |
| HEAD_BODY_LENGTH          | 0    | 0    | 0    |
| TESTIS_AVERAGE            | -0.148 | 0    | -0.869 |
| SPLEEN                    | 0    | 0    | 0    |
| LIVER                     | 0    | 0    | 0    |
| KIDNEY_AVERAGE            | -0.150 | 0.851 | -0.541 |
| HEART                     | 0    | 0.225 | -0.343 |
| EPIDIDYMAL                | 0    | 0.360 | -0.610 |
| PERIRENAL                 | 1.740 | 0    | 0    |
| MESENTRIC                 | 0    | 0.350 | 0    |
| INGUINAL                  | 0.633 | 0.139 | 0    |
| DORSAL_WHITE_FAT          | 0    | 0    | 0    |
| DORSAL_BROWN_FAT          | 0    | 0    | -0.429 |
| BMI                       | 0    | 0    | 0    |
| VISCERAL                  | 0    | 0    | 0    |
| SUBCUTANEOUS              | 0.468 | 0    | 0    |
| TOTAL_FAT_PAT_WEIGHT      | 0.359 | 0    | 0    |
| LEAN_WEIGHT               | 0    | -2.661 | 0   |
| AI                        | 0    | 0    | 0    |
| IP                        | 0    | 0    | -0.014 |
| HDL                       | 0    | 0    | 0    |
| T_CHOLESTEROL             | 0    | -0.467 | -1.787 |
| NON_HDL                   | 0    | 0    | -0.393 |
| TG                        | -0.066 | 0    | 0.540 |
| AMYL                      | 0    | 0    | -0.005 |
| ALB1                      | 0    | 0    | 0.869 |
| ALP                       | -1.266 | 0    | 0    |
| ALT                       | 0    | 0    | -0.200 |
| TBIL                      | 0.042 | 0    | 0    |
| BUN                       | 0    | 0    | 0.009 |
| CALCIUM                   | 0.340 | 0    | 0    |
| TP                        | 0.153 | 0    | 0.387 |
| GLOB                      | 0    | 0    | -0.046 |
| POTASSIUM                 | 0    | 0    | 0    |
Table 7: The estimates of $\gamma$ for the mouse consomic strain data.

| strain | $\gamma_1$ | $\gamma_2$ | $\gamma_3$ |
|--------|------------|------------|------------|
| B6     | 0          | -0.471     | 0          |
| MSM    | 0          | 1.164      | 0          |
| CS1    | 0          | 0          | 0          |
| CS2C   | -0.282     | 0.149      | -0.142     |
| CS2T   | -0.203     | 0          | 0          |
| CS3    | -0.228     | 0.663      | 0          |
| CS4    | 0          | 0.685      | 0          |
| CS5    | 0          | 0          | 1.151      |
| CS6C   | 0.353      | 0          | 0          |
| CS6T   | 0.304      | 0          | 0          |
| CS7    | 0.040      | 0          | 0          |
| CS7C   | 0.153      | -0.166     | 0.168      |
| CS7T   | -0.177     | 0          | -0.029     |
| CS8    | 0.089      | 0.338      | 0          |
| CS9    | 0          | 0.231      | -1.037     |
| CS11   | -1.054     | 0          | 0          |
| CS12C  | 0          | 0          | 0.115      |
| CS12T  | -0.141     | 0          | 0          |
| CS13C  | -0.260     | 0          | 0          |
| CS13T  | 0          | 0          | 0          |
| CS14   | 0.228      | 0          | -0.317     |
| CS15   | -0.163     | -0.470     | 0          |
| CS16   | 0.026      | 0          | -0.065     |
| CS17   | 0          | 0          | -0.357     |
| CS18   | 0.506      | -0.003     | 0.923      |
| CS19   | 0          | -0.429     | -0.552     |
| CSXC   | 0          | -0.042     | 0          |
| CSXT   | 0          | 0          | 0.350      |
| CSY    | 0          | 0          | 0          |
| mt     | 0.092      | 0          | 0.181      |
The second PC (PC2) by SPCR-glm largely depended on the score

\[ 0.85 \times \text{KIDNEY\_AVERAGE} - 2.66 \times \text{LEAN\_WEIGHT}, \]

where \text{LEAN\_WEIGHT} is the weight after removing the white fat pad and \text{KIDNEY\_AVERAGE} is the mean of two kidney (right and left) weights divided by \text{LEAN\_WEIGHT}. There were many traits related to the weight. Among those, the above two traits were selected. For example, the \text{BODY\_WEIGHT} largely depended on the individuals among the same CS, so that the within-variance was large, but the \text{LEAN\_WEIGHT} did not largely depend on the individuals among the same CS, so that the within-variance was small. This would be why \text{LEAN\_WEIGHT} was more favorable than other traits related to the weight. In Figure 3(a), the PC2 clearly separates the basic strain MSM from other strains. The MSM was a small mouse with a large kidney and the consomic strains had a more similar property to B6 than MSM, because the consomic strains were based on the B6, which is explained from PC2.

The third PC (PC3) by SPCR-glm largely depended on the score

\[-0.87 \times \text{TESTIS\_AVERAGE} - 1.79 \times \text{T\_CHOLESTEROL} + 0.87 \times \text{ALB1},\]

where \text{TESTIS\_AVERAGE} is the mean of two testis weights, \text{T\_CHOLESTEROL} is the cholesterol value, and \text{ALB1} is the albumin value. In Figure 3(b), CS5, CS9 and CS18 were separate from other mice, but not in Figure 3(d). In fact, CS5 and CS18 had a small \text{TESTIS\_AVERAGE} and a small \text{T\_CHOLESTEROL} and CS9 had a very large \text{T\_CHOLESTEROL}. However, we have not yet found a significant property on \text{ALB1}. It may imply that \text{ALB1} has a significant property which has not been found.

CS1, CS13T and CSY had the zero regression coefficient, as seen in Table 7. This implies that they did not have any significant property on the three PCs. In fact, their CSs were known to have no significant property.

8 Conclusion

We presented a one-stage procedure for PCR in the framework of generalized linear models with sparse regularization. We called this procedure SPCR-glm. SPCR-glm enabled us to
treat various types of response variable. The estimation algorithm was obtained based on the coordinate descent algorithm. Through the numerical studies, our proposed method was superior to competing methods in terms of prediction accuracy, TPR, TNR, and interpretable of the principal component loadings.

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