Abstract

Sparse Principal Component Analysis (SPCA) is widely used in data processing and dimension reduction; it uses the lasso to produce modified principal components with sparse loadings for better interpretability. However, sparse PCA never considers an additional grouping structure where the loadings share similar coefficients (i.e., feature grouping), besides a special group with all coefficients being zero (i.e., feature selection). In this paper, we propose a novel method called Feature Grouping and Sparse Principal Component Analysis (FGSPCA) which allows the loadings to belong to disjoint homogeneous groups, with sparsity as a special case. The proposed FGSPCA is a subspace learning method designed to simultaneously perform grouping pursuit and feature selection, by imposing a non-convex regularization with naturally adjustable sparsity and grouping effect. To solve the resulting non-convex optimization problem, we propose an alternating algorithm that incorporates the difference-of-convex programming, augmented Lagrange and coordinate descent methods. Additionally, the experimental results on real data sets show that the proposed FGSPCA benefits from the grouping effect compared with methods without grouping effect.

Keywords: SPCA, Dimension Reduction, Feature Grouping, Sparsity, Feature Selection.

1 Introduction

Principal component analysis (PCA) (Jolliffe, 1986) is an important unsupervised technique for feature extraction and dimension reduction, with a wide range of applications in statistics, machine learning such as gene representation and face recognition. PCA finds linear combinations of the original variables/predictors, called principal components (PCs), by projecting the original data onto an orthogonal linear space, such that the derived PCs capture maximal variance along the orthogonal directions. Numerically, PCA can be obtained via the singular value decomposition (SVD) of the data matrix. Denote $X_{n \times p} \in \mathbb{R}^{n \times p}$ a data matrix, consisting of $n$ observations of a random vector $x \in \mathbb{R}^p$ with population covariance matrix $\Sigma \in \mathbb{R}^{p \times p}$, where $n$ and $p$ are the number of observations and the number of variables/predictors, respectively. Without loss of generality, assume that all the predictors are centered with 0 means. Let the SVD of $X$ be $X = U \Sigma V^T$. The principal components (PCs) are $Z = UD$, and the columns of $V$ are the corresponding loadings (or factor coefficients) of the PCs.
Backgrounds The goal of PCA is to recover the top $k$ leading eigenvectors $\mathbf{u}_1, \cdots, \mathbf{u}_k$ of a population covariance matrix $\Sigma$. In high dimensional settings with $p \gg n$, the classical PCA can be inconsistent (Johnstone and Lu, 2009, Nadler, 2008, Paul, 2007). Additional assumptions are needed to avoid such a curse of dimensionality (Wang et al., 2014). Besides, another obvious disadvantage of the classical PCA is that each PC usually involves all the original variables in the linear combination and the loadings (factor coefficients) are typically nonzero, which hinders the interpretability of the derived PCs. In order to deal with the curse of dimensionality and to improve the interpretability of the derived PCs, a sparsity assumption is often imposed on the loadings.

Sparsity in PCA Sparse PCA (SPCA) (Cai et al., 2013, Erichson et al., 2020, Vu et al., 2013, Zou et al., 2006) and its variants have been proposed to encourage sparse and potentially interpretable factors, and to avoid the curse of dimensionality in high dimensional settings where $p \gg n$. In the last decades, significant progress has been made on the methodological development as well as theoretical understanding of sparse PCA. One can turn to Croux et al. (2013), Erichson et al. (2020), Grbovic et al. (2012), Jenatton et al. (2010, 2011), Jin and Sidford (2019), Khan et al. (2015), Tian et al. (2020), Wang et al. (2014), Yi et al. (2017), Zhang and Tong (2019), Zou and Xue (2018), among others, for overviews of the literature. Methods introduced in these articles intend to seek modified principal components for various purposes. For example, SPCA (Erichson et al., 2020, Zou et al., 2006) seeks sparse loadings, and Tian et al. (2020) considers the feature-sparsity (row-sparsity) constrained PCA to perform feature selection and PCA simultaneously.

Structure loadings in PCA One main drawback of the sparse PCA is that, even though it produces modified principal components with sparse loadings for better interpretability, the sparse PCA never considers the structure information among the loadings with similar values or clusters/groups. The row structure is considered in Tian et al. (2020), however it only considers the feature-sparsity (row-sparsity) but no other types of structures among features. Jenatton et al. (2011) proposed a structured variable selection method with sparsity-inducing regularization, capable of encoding more sophisticated prior knowledge about the expected sparsity patterns. However, the method depends heavily on the structured prior which should be given in advance but is usually hard to obtain in real applications. A structured sparse PCA (Jenatton et al., 2010) is proposed as an extension of sparse PCA, based on a structured regularization introduced by Jenatton et al. (2011). Although the factors derived by the structured sparse PCA possess some sparse structure of the data, it suffers from the same issue that the structured sparsity depends on the given structural prior information. Another issue is that the prior knowledge concerning structures of the data may not be correctly specified.

Structure in regression In regression problems, structure is considered between groups of variables known a priori. The fused lasso (Hoefling, 2010, Rinaldo, 2009, Tibshirani et al., 2005) considers ordered coefficient estimation by imposing an $L_1$ penalty on the difference of successive parameters. The group lasso (Friedman et al., 2010, Meier et al., 2008, Yuan and Lin, 2006, Zou and Hastie, 2005) considers feature selection along the group level (the entire group of predictors may be kept or discarded in the model), by imposing non-squared Euclidean norm penalty on grouped predictors with predefined group partition. Check Wang et al. (2019), Yuan et al. (2011), Zhang et al. (2020a) for more variants. There is also some research work considering simultaneous feature clustering/grouping and feature selection in high-dimensional regression problems, referring to Qin et al. (2020), Shen et al. (2012), Yang et al. (2012) for an overview.

Our work This is the first work on principal component analysis that considers simultaneous feature clustering/grouping and feature selection, where the grouping structure is learned from the model rather than from given prior information. We introduce a new method called feature grouping and sparse principal component analysis (FGSPCA) to produce modified principal components with grouping-guided and sparse loadings. Efficient algorithms are proposed to solve our FGSPCA model.

Our contributions We make the following contributions.

• To our knowledge, this is the first paper considering grouping effect among loadings (factor coefficients) as well as the sparsity effect in principal component analysis (PCA).

• The proposed FGSPCA performs feature grouping and feature selection simultaneously by imposing a non-convex regularization term with naturally adjustable sparsity and grouping
effect, where the grouping structure is learned from the model rather than from given prior information. Thus it does not need any prior knowledge to construct the regularization term.

• We propose an efficient alternating algorithm to solve the non-convex FGSPCA problem which incorporates the difference-of-convex programming (DC), augmented Lagrange (AL) and coordinate descent methods (CD).

• We conduct experiments on real-world data to evaluate the new method. The experimental results demonstrate the promising performance of the newly proposed algorithms.

The rest of the paper is organized as follows. In Section 2, the SPCA is revisited. In Section 3, we introduce the proposed FGSPCA and the alternating algorithm to solve the FGSPCA problem, which is equivalent to \( k \) independent feature-grouping-and-sparsity constrained (FGS) regression problems. Section 4 is the algorithm for the FGS problem. Experiments to show the performance of FGSPCA and comparisons with other dimension reduction methods are presented in Section 5. A discussion on the extension of FGSPCA to the settings with non-negative loadings falls into Section 6. We conclude the paper in Section 7.

2 Sparse Principal Component Analysis revisited

Regression representation of PCA The regression representation of PCA works as follows: originally, each PC is a linear combination of all the \( p \) variables; thus its loadings can be recovered by regressing the PC on the \( p \) original variables. Lemma 1 (Theorem 1 in Zou et al. (2006)) gives the regression representation of PCA, which reveals the connection between PCA and regression method.

Lemma 1 Denote the SVD of \( X \) by \( X = UDV^T \). Let \( Z_j = U_j D_{jj} \) be the \( j \)-th PC. Consider \( \lambda > 0 \) and the ridge estimates \( \hat{\beta}_{\text{ridge}} \) given by

\[
\hat{\beta}_{\text{ridge}} = \arg\min_\beta \|Z_j - X\beta\|_2^2 + \lambda \|\beta\|_2^2, \tag{2.1}
\]

Let \( \hat{v} = \frac{\hat{\beta}_{\text{ridge}}}{\|\hat{\beta}_{\text{ridge}}\|_2}, \) then \( \hat{v} = \hat{V}_j \).

Since ordinary PCA always gives a unique solution, the ridge penalty \( (\lambda \|\beta\|_2^2) \) is used to guarantee the reconstruction of the principal components (Zou et al., 2006). By adding an \( L_1 \) penalty to (2.1), we consider the following optimization problem,

\[
\hat{\beta} = \arg\min_\beta \|Z_j - X\beta\|_2^2 + \lambda \|\beta\|_2^2 + \lambda_1 \|\beta\|_1, \tag{2.2}
\]

where \( \|\beta\|_1 = \sum_{i=1}^n |\beta_i| \) is the \( L_1 \)-norm of \( \beta \). \( \hat{V}_j = \frac{\hat{\beta}}{\|\hat{\beta}\|_2} \) is an approximation of \( V_j \), and \( X\hat{V}_j \) is the \( j \)-th approximated principal component. Obviously, a large enough value of \( \lambda_1 \) gives a sparse \( \hat{\beta} \).

However, the above optimization problem (2.2) as well as Lemma 1 depend on the results of ordinary PCA. Thus, in order to find the sparse approximations, a two-stage method needs to be implemented: first perform PCA, then use (2.2) to find suitable sparse loadings. Therefore, there is a great need for an integrated “self-contained” regression-type procedure to derive all sequences of PCs. The following Lemma 2 (Theorem 3 in Zou et al. (2006)) provides this requirement (see Appendix A).

Lemma 2 Consider the first \( k \) principal components. Let \( x_i \) be the \( i \)-th row of data matrix \( X \). Denote \( A_{p \times k} = [\alpha_1, \cdots, \alpha_k] \), \( B_{p \times k} = [\beta_1, \cdots, \beta_k] \). For any \( \lambda > 0 \), let

\[
(\hat{A}, \hat{B}) = \arg\min_{A, B} \sum_{i=1}^n \|x_i - AB^T x_i\|_2^2 + \lambda \sum_{j=1}^k \|\beta_j\|_2^2, \quad \text{s.t.} \quad A^T A = I_{k \times k}. \tag{2.3}
\]

Then \( \hat{\beta}_j \propto V_j \) for \( j = 1, \cdots, k \).

The PCA problem is transformed into a regression-type optimization problem with orthonormal constraints on \( A \), and all the sequences of principal components can be derived through Lemma 2. With the restriction \( B = A \), the objective function becomes
\[ \sum_{i=1}^{n} \| \mathbf{x}_i - \mathbf{A} \mathbf{B}^T \mathbf{x}_i \|_2^2 = \sum_{i=1}^{n} \| \mathbf{x}_i - \mathbf{A} \mathbf{A}^T \mathbf{x}_i \|_2^2, \] whose minimizer under the orthonormal constraint on \( \mathbf{A} \) is exactly the first \( k \) loading vectors of the ordinary PCA. Lemma 2 shows that the exact PCA can still be obtained while relaxing the restriction \( \mathbf{B} = \mathbf{A} \) and adding the ridge penalty term.

Note that
\[ \sum_{i=1}^{n} \| \mathbf{x}_i - \mathbf{A} \mathbf{B}^T \mathbf{x}_i \|_2^2 = \| \mathbf{X} - \mathbf{X} \mathbf{B} \mathbf{A}^T \|_2^2. \]

Since \( \mathbf{A} \) is orthonormal, let \( \mathbf{A} \perp \) be any orthonormal matrix such that \( [\mathbf{A}; \mathbf{A} \perp] \) is \( p \times p \) orthonormal. Then we have
\[ \| \mathbf{X} - \mathbf{X} \mathbf{B} \mathbf{A}^T \|_2^2 = \sum_{j=1}^{k} \| \mathbf{X} \alpha_j - \mathbf{X} \beta_j \|_2^2 + \| \mathbf{X} \mathbf{A} \perp \|_2^2. \]
Suppose that \( \mathbf{A} \) is given, the optimal \( \mathbf{B} \) should be obtained by minimizing
\[ \sum_{j=1}^{k} \| \mathbf{X} \alpha_j - \mathbf{X} \beta_j \|_2^2 + \lambda \sum_{j=1}^{k} \| \beta_j \|_2^2 + \lambda \sum_{j=1}^{k} \| \beta_j \|_1, \] s.t. \( \mathbf{A}^T \mathbf{A} = \mathbf{I}_{k \times k}. \) (3.1)

Sparse PCA criterion  
By adding the Lasso penalty into the optimization problem of (2.3), the Sparse PCA by Zou et al. (2006) solves the following regularized optimization problem,
\[ (\hat{\mathbf{A}}, \hat{\mathbf{B}}) = \arg \min_{\mathbf{A,B}} \sum_{i=1}^{n} \| \mathbf{x}_i - \mathbf{A} \mathbf{B}^T \mathbf{x}_i \|_2^2 + \lambda \sum_{j=1}^{k} \| \beta_j \|_2^2 + \lambda_1 \sum_{j=1}^{k} \| \beta_j \|_1, \text{ s.t. } \mathbf{A}^T \mathbf{A} = \mathbf{I}_{k \times k}. \] (2.4)

Figure 1: Comparison of different penalty functions, the \( L_1 \)-function (red line), the truncated \( L_1 \)-function (blue line), and the \( L_0 \)-function (green line), and their corresponding solutions. The truncated \( L_1 \)-function \( \min \{ \frac{|x|}{\tau}, 1 \} \) approximates the \( L_0 \)-function \( I(x \neq 0) \) as \( \tau \to 0 \), and it is closer to the \( L_0 \) penalty than the \( L_1 \) penalty. The solution functions show that, compared to the \( L_1 \) penalty, the solution with truncated \( L_1 \) penalty penalizes more aggressively with small coefficients preferred, and it has no bias with large coefficients.

3 The proposed FGSPCA method
To obtain modified PCs with Feature-Grouping-and-Sparsity constrained loadings, we can extend the optimization problem of (2.3) into a more general criterion formula by imposing feature grouping and feature selection penalties simultaneously. We call (3.1) the FGSPCA criterion,
\[ \min_{\mathbf{A,B}} \sum_{i=1}^{n} \| \mathbf{x}_i - \mathbf{A} \mathbf{B}^T \mathbf{x}_i \|_2^2 + \lambda \sum_{j=1}^{k} \| \beta_j \|_2^2 + \lambda_1 \sum_{j=1}^{k} p_1(\beta_j) + \lambda_2 \sum_{j=1}^{k} p_2(\beta_j), \text{ s.t. } \mathbf{A}^T \mathbf{A} = \mathbf{I}_{k \times k}, \] (3.1)
where \( p(\beta) \) and \( p_2(\beta) \) are regularization functions, which take the following penalty form,

\[
p_1(\beta_j) = \sum_{l=1}^{p} \min \left\{ \frac{|\beta_{l}(j)|}{\tau} , 1 \right\}, \quad p_2(\beta_j) = \sum_{l<l'}(l,l') \in \mathcal{E} \min \left\{ \frac{|\beta_{l}(j) - \beta_{l'}(j)|}{\tau} , 1 \right\}.
\]

Here \( \mathcal{E} \subset \{1, \cdots, p\}^2 \) denotes a set of edges on a fully connected and undirected graph (complete graph), with \( l \sim l' \) indicating an edge directly connecting two distinct nodes \( l \neq l' \). \( p_1(\beta) \) and \( p_2(\beta) \) are regularization terms controlling feature selection and feature grouping, respectively. \( \lambda_1(\lambda_2 > 0) \) are the corresponding tuning parameters, and \( \tau > 0 \) is a thresholding parameter which determines when a small regression coefficient or a small difference between two coefficients will be penalized. \( \hat{\beta}_{l}(j) \) is the \( l \)-th element of the vector \( \hat{\beta}_j \). And \( p_1(\beta_j) \) is a truncated \( L_1 \) penalty imposed on \( \beta_j \), which can be viewed as a non-convex surrogate of \( L_0 \) penalty. Figure 1 gives a comparison of different penalty functions and their solutions. Note that based on the FGSPCA criterion, the optimization problem in (2.4) is a special case of (3.1), with non-truncated \( L_1 \) penalty function and parameter \( \lambda_2 = 0 \). Check Appendix B for more structured sparsity regularization functions.

**Remark** 1. A). As shown in Shen et al. (2012), the truncated \( L_1 \)-function \( \min \frac{|\beta_{l}(j)|}{\tau} , 1 \) can be regarded as a non-convex and non-smooth surrogate of \( L_0 \)-function \( 1(\beta_{l} \neq 0) \) when \( \tau \to 0 \). Besides, the selection consistency can be achieved by the \( L_0 \)-penalty and its surrogate—the truncated \( L_1 \)-penalty (Dai et al., 2021, Shen et al., 2013). B). The key point of the FGSPCA with \( p_1(\cdot) \) and \( p_2(\cdot) \) penalty functions can be viewed as performing feature selection and feature grouping simultaneously, while the sparse PCA model with \( L_1 \) penalty cannot keep this selection consistency. C). One might use the \( L_1 \)-function \( |\beta_j| \) as a smooth approximation of \( L_0 \)-function. However, the shrinkage bias tends to be larger as parameter size gets larger (Wu et al., 2018, Yun et al., 2019) as the \( L_1 \) penalty is proportional to the size of parameters. The smooth approximation \( L_1 \)-function has the drawback that it produces biased estimates for large coefficients and lacks oracle selection property (Fan and Li, 2001, Zhang and Huang, 2008). D). Compared to the \( L_1 \) penalty, the truncated \( L_1 \) penalty is closer to the \( L_0 \) penalty and penalizes more aggressively with small coefficients preferred.

### 4 The algorithms

#### 4.1 Alternating algorithm of FGSPCA

**To calculate \( \mathbf{B} \)** If \( \mathbf{A} \) is given, for each \( j \), denote \( \mathbf{Y}_j = \mathbf{X} \alpha_j \). To estimate \( \hat{\mathbf{B}} = [\hat{\beta}_1, \cdots, \hat{\beta}_k] \), the FGSPCA criterion is equivalent to \( k \) independent feature-grouping-and-sparsity constrained regression problems (FGS) defined in the following

\[
\min_{\beta} S(\beta) = ||\mathbf{Y}_j - \mathbf{X} \beta||_2^2 + \lambda ||\beta||_2^2 + \lambda_1 p_1(\beta) + \lambda_2 p_2(\beta).
\]  

(4.1)

Each \( \hat{\beta}_j = \arg \min_{\beta} S(\beta) \) is the solution of the FGS problem, and it can be obtained by Algorithm 2.

**Lemma 3** The proposed Algorithm 2 converges. That is

\[
S(\beta^{(m)}) \to c, \text{ as } m \to \infty,
\]

where \( c \) is a non-negative constant value of the objective function, and \( m \) is the number of steps of the DC-AL-CD algorithm for the inner FGS problem.

**Lemma 3** above gives a theoretical convergence guarantee for Algorithm 2 (see Appendix C.1). When solving the problem (4.1), the proposed Algorithm 2 could potentially lead to a local optimum, as the objective function in (4.1) is non-convex. Thus it is crucial to pick a suitable initial value \( \beta^{(0)} \). Since (4.1) is a regression problem, possible candidate initial values are those estimated by any regression solver, such as glmnet in R and sklearn in python.

**To calculate \( \mathbf{A} \)** If \( \mathbf{B} \) is given, ignore the penalty term in (3.1).

\[
\min_{\mathbf{A}} ||\mathbf{X} - \mathbf{X} \mathbf{B}^T \mathbf{A}^T||_2^2 \quad \text{s.t.} \quad \mathbf{A}^T \mathbf{A} = \mathbf{I}_{k \times k}.
\]

(4.2)

This is the orthogonal Procrustes Rotation Problem (see Appendix C.2). The solution can be obtained through a reduced rank form of the Procrustes Rotation, given in Lemma 4 (Theorem 4 in Zou et al. (2006)). The SVD of \( (\mathbf{X}^T \mathbf{X}) \mathbf{B} = \mathbf{U} \mathbf{D}^T \), then \( \hat{\mathbf{A}} = \mathbf{U} \mathbf{V}^T \).
Lemma 4 Reduced Rank Procrustes Rotation. \(M_{n \times p}\) and \(N_{n \times k}\) denote two matrices. Consider the constrained minimization problem

\[
\hat{A} = \arg \min_A \|M - NA^T\|_2^2 \quad \text{s.t.} \quad A^T A = I_{k \times k}.
\]  
(4.3)

Suppose the SVD of \(M^T N\) is \(UDV^T\), then \(\hat{A} = UV^T\).

An alternating algorithm is proposed to minimize the FGSPCA criterion (3.1).

Algorithm 1: The alternating algorithm of FGSPCA

Step 1: Initialization. Let \(A\) start with \(V[, 1 : k]\), the loadings of the first \(k\) ordinary principal components;

Step 2: For a fixed \(A = [\alpha_1, \cdots, \alpha_k]\), let \(Y_j = X\alpha_j\). \(B = [\beta_1, \cdots, \beta_k]\), each \(\beta_j\) is obtained by solving the FGS problem (4.1) using Algorithm 2, for \(j = 1, \cdots, k\);

Step 3: For a fixed \(B = [\beta_1, \cdots, \beta_k]\), compute the SVD of \((X^T X)B = UDV^T\). Then update \(A = UV^T\);

Step 4: Repeat Step 2—3 until convergence;

Step 5: Normalization. Let \(\hat{V}_j = \frac{\hat{\beta}_j}{\|\hat{\beta}_j\|_2}\), for \(j = 1, \cdots, k\).

Remark 2 The initialization of \(A, V[, 1 : k]\), can be loadings of any kind of PCA methods. For simplicity, let \(V[, 1 : k]\) be the loadings of the first \(k\) ordinary principal components. Obviously, \(V[, 1 : k]\) can be the loadings of the first \(k\) PCs of sparse PCA. The convergence criterion in Step 4 can be that the difference between two adjacent iterations of \(B\) is small.

Adjusted total variance Denote \(\hat{Z} = [\hat{Z}_1, \cdots, \hat{Z}_k]\) the modified PCs. Due to the grouping and sparsity constraints, \(\hat{Z}_i\) is correlated with \(\hat{Z}_i, i = 1, \cdots, k - 1\), thus we should remove from \(\hat{Z}_k\) the correlation effect of \(\hat{Z}_i, i = 1, \cdots, k - 1\) using regression projection. In light of Zou et al. (2006), we compute the adjusted total variance by the QR decomposition. Suppose \(\hat{Z} = QR\), where \(Q\) is orthonormal and \(R\) is upper triangular. The explained total variance is equal to \(\sum_{j=1}^{k} R_{jj}^2\).

4.2 Algorithm of the FGS problem

The proposed FGSPCA model is equivalent to \(k\) independent feature-grouping-and-sparsity-constrained regression problems (FGS). Thus this section gives an algorithm for the FGS problem, which is a core part of Algorithm 1. The general form of the FGS problem is stated as follows,

\[
\min_{\beta} S(\beta) = \sum_{i=1}^{n} (y_i - x_i^T \beta)^2 + \lambda \sum_{l=1}^{p} \beta_l^2 + \lambda_1 \sum_{l=1}^{p} \min \left( \frac{|\beta_l|}{\tau}, 1 \right) + \lambda_2 \sum_{l<l', (l,l') \in E} \min \left( \frac{|\beta_l - \beta_{l'}|}{\tau}, 1 \right).
\]  
(4.4)

To solve the above non-convex optimization problem (4.4), we propose an integrated DC-AL-CD algorithm (Algorithm 2) that incorporates the difference-of-convex algorithm (DC), augmented Lagrange (AL) and coordinate descent methods (CD).

The procedure to solve the FGS problem consists of three steps. First, the non-convex objective function is decomposed into a difference of two convex functions. Then a sequence of approximations of the trailing convex function is constructed with its affine minorization (through linearizing). Second, a quadratic problem with equality constraints is converted to an unconstrained version with slack variables, which is subsequently reconstructed by the augmented Lagrange method. Third, the unconstrained optimization problem is solved with coordinate descent.

The difference-of-convex algorithm (DC) Using \(\min(a, b) = a - (a - b)_+\), we decompose the non-convex objective function \(S(\beta)\) into a difference of two convex functions, \(S(\beta) = S_1(\beta) - S_2(\beta)\), where the two convex functions \(S_1(\beta)\) and \(S_2(\beta)\) are given respectively by

\[
S_1(\beta) = \sum_{i=1}^{n} (y_i - x_i^T \beta)^2 + \lambda \sum_{l=1}^{p} \beta_l^2 + \lambda_1 \sum_{l=1}^{p} \left( \frac{|\beta_l|}{\tau} - 1 \right)_+ + \lambda_2 \sum_{l<l', (l,l') \in E} \left( \frac{|\beta_l - \beta_{l'}|}{\tau} - 1 \right)_+.
\]  

\[S_2(\beta) = \lambda_1 \sum_{l=1}^{p} \left( \frac{|\beta_l|}{\tau} - 1 \right)_+ + \lambda_2 \sum_{l<l', (l,l') \in E} \left( \frac{|\beta_l - \beta_{l'}|}{\tau} - 1 \right)_+.
\]
Algorithm 2: The integrated DC-AL-CD algorithm for the FGS problem

**Data:** Design matrix $X \in \mathbb{R}^{n \times p}$, response vector $y \in \mathbb{R}^n$.

**Input:** Model parameters $\tau, \lambda, \lambda_1, \lambda_2$; algorithm convergence parameters $\rho (= 1.05), \nu (= 1), \delta^* (= 10^{-5})$.

**Output:** $\hat{\beta}^{(m)}$.

Initialization: $\hat{\beta}^{(0)}$, $m = 0$;

/* The Outer Loop. */

while $S(\hat{\beta}^{(m)}) - S(\hat{\beta}^{(m+1)}) > 0$ do

$m \leftarrow m + 1$;

Update $F^{(m)}, E^{(m)}$ according to (4.6);

/* The Inner Loop. */

Initialization: $\hat{\beta}^{(m,0)} = \hat{\beta}^{(m-1)}$, $\tau^{0} = 0$, $\nu = 0, k = 0$;

while $\|\hat{\beta}^{(m,k)} - \hat{\beta}^{(m,k-1)}\|_\infty \geq \delta^*$ do

$k \leftarrow k + 1$;

Update $\tau^{k}$ and $\nu$ according to (4.9);

Update $\hat{\beta}^{(m,k)}$ according to (4.10);

Update $\hat{\beta}^{(m,k)}$ according to (4.11);

end

end

We then construct a sequence of approximations of $S_2(\beta)$ iteratively. At the $m$-th iteration, we replace $S_2(\beta)$ with its affine minorization at the $(m - 1)$-th iteration.

$$S_2^{(m)}(\beta) \approx S_2(\hat{\beta}^{(m-1)}) + \langle \beta - \hat{\beta}^{(m-1)}, \partial S_2(\beta) \rangle_{\beta = \hat{\beta}^{(m-1)}}$$

$$\propto S_2(\hat{\beta}^{(m-1)}) + \frac{\lambda_1}{\tau} \sum_{l=1}^{p} I\{|\hat{\beta}_l^{(m-1)}| < \tau\} \cdot |\beta_l| + \frac{\lambda_2}{\tau} \sum_{l<l', l', l' \in \mathcal{E}} I\{|\hat{\beta}_l^{(m-1)} - \hat{\beta}_{l'}^{(m-1)}| < \tau\} \cdot |\beta_l - \beta_{l'}|.$$ (4.5)

Finally, a sequence of approximations of $S(\beta)$ is constructed iteratively. For the $m$-th approximation, an upper convex approximating function to $S(\beta)$ can be obtained by $S^{(m)}(\beta) = S_1(\beta) - S_2^{(m)}(\beta)$, which formulates the following subproblem.

$$\min_{\beta} S^{(m)}(\beta) = \sum_{i=1}^{n} (y_i - x_i^T \beta)^2 + \lambda \sum_{l=1}^{p} \beta_l^2 + \frac{\lambda_1}{\tau} \sum_{l \in F^{(m-1)}} |\beta_l| + \frac{\lambda_2}{\tau} \sum_{l < l', (l,l') \in \mathcal{E}} |\beta_l - \beta_{l'}|,$$ (4.6)

where

$$F^{(m-1)} = \{l : |\hat{\beta}_l^{(m-1)}| < \tau\},$$

$$\mathcal{E}^{(m-1)} = \{(l,l') \in \mathcal{E} : |\hat{\beta}_l^{(m-1)} - \hat{\beta}_{l'}^{(m-1)}| < \tau\}.$$ (4.6)

**Augmented Lagrange method (AL)** Denote $\beta_{l'} = \beta_l - \beta_{l'}$ and define $\xi = (\beta_1, \ldots, \beta_p, \beta_{12}, \ldots, \beta_{1p}, \ldots, \beta_{(p-1)p})$. The $m$-th subproblem (4.5) can be reformulated as an equality-constrained convex optimization problem,

$$\min_{\xi} \sum_{i=1}^{n} (y_i - x_i^T \beta)^2 + \lambda \sum_{l=1}^{p} \beta_l^2 + \frac{\lambda_1}{\tau} \sum_{l \in F^{(m-1)}} |\beta_l| + \frac{\lambda_2}{\tau} \sum_{l < l', (l,l') \in \mathcal{E}} |\beta_{l'}|,$$ (4.7)

subject to $\beta_{l'} = \beta_l - \beta_{l'}$, $\forall l < l' : (l,l') \in \mathcal{E}^{(m-1)}$. 

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The augmented Lagrangian for (4.7) is
\[
L_{\nu}^{(m)}(\xi, \tau) = \sum_{i=1}^{n} (y_i - x_i^T \beta)^2 + \lambda \sum_{l=1}^{p} \beta_l^2 + \frac{\lambda_1}{\tau} \sum_{l \in E^{(m-1)}} |\beta_l| + \frac{\lambda_2}{\tau} \sum_{l < l' \in (1, p)} |\beta_{ll'}| \\
+ \frac{\nu}{2} \sum_{l < l' \in (1, p)} (\beta_{ll'} - \beta_{l'l'})^2.
\]
(4.8)
Here \(\tau_{ll'}\) and \(\nu\) are the Lagrangian multipliers for the linear constraints and for the computational acceleration. Update \(\tau_{ll'}\) and \(\nu\)
\[
\tau_{ll'}^{k+1} = \tau_{ll'}^k + \nu \lambda (\beta_{ll'}^{(m,k)} - \beta_{l'l'}^{(m,k)} - \beta_{l'l'}^{(m,k)}), \quad \nu^{k+1} = \rho \nu^k.
\]
(4.9)
Here \(\rho\) controls the convergence speed of the algorithm, which is chosen to be larger than 1 (e.g. \(\rho = 1.05\)) for acceleration of the convergence.

**Coordinate Descent methods (CD)** We use the coordinate descent methods to compute \(\hat{\xi}^{(m, k+1)}\) in (4.8). For each component of \(\xi\), we fix the other components at their current values. Set an initial value \(\hat{\xi}^{(m,0)} = \hat{\xi}^{(m-1)}\), where \(\hat{\xi}^{(m-1)}\) is the solution of the subproblem (4.5) for the \((m-1)\)-th approximation. Then update \(\hat{\xi}^{(m, k)}\) by the following formulas, for \(k = 1, 2, \cdots\)

- Given \(\hat{\beta}^{(m, k-1)}\), update \(\hat{\beta}^{(m, k)}(l = 1, 2, \cdots, p)\) by
  \[
  \hat{\beta}_{l}^{(m, k)} = \alpha^{-1} \gamma,
  \]
  (4.10)
  where \(\alpha = 2\lambda + 2 \sum_{i=1}^{n} x_{il}^2 + \nu \lambda |l' : (l, l') \in E^{(m-1)}|\). And \(\gamma = \gamma^*\) if \(|\hat{\beta}_{l}^{(m-1)}| \geq \tau\); otherwise, \(\gamma = \text{ST}(\gamma^*, \frac{\lambda}{\tau})\). Here \(\text{ST}(x, \delta) = \text{sign}(x)(|x| - \delta)_+\) is the soft threshold function, and

  \[
  \gamma^* = 2 \sum_{i=1}^{n} x_{il} b_{il}^{(m, k)} - \sum_{(l, l') \in E^{(m-1)}} \tau_{ll'}^k + \nu \lambda \sum_{(l, l') \in E^{(m-1)}} \left( \hat{\beta}_{ll'}^{(m, k)} + \hat{\beta}_{l'l'}^{(m, k)} \right),
  \]

  where \(b_{il}^{(m, k)} = y_i - x_i^T \hat{\beta}_{il}^{(m, k)}\); \(x_i(l)\) is the vector \(x_i\) without the \(l\)-th component.

- Given \(\hat{\beta}^{(m, k-1)}_{ll'}\), update \(\hat{\beta}^{(m, k)}_{ll'}(1 \leq l < l' \leq p)\) (with \(\hat{\beta}^{(m, k)}_{l} \) already updated and fixed).
  Then

  \[
  \hat{\beta}_{ll'}^{(m, k)} = \begin{cases} \frac{1}{\nu} \text{ST} \left( \tau_{ll'}^k + \nu \lambda (\hat{\beta}_{ll'}^{(m, k)} - \hat{\beta}_{l'l'}^{(m, k)}), \frac{\lambda}{\tau} \right), & \text{if } (l, l') \in E^{(m-1)} \\
  \hat{\beta}_{ll'}^{(m, k-1)}, & \text{if } (l, l') \notin E^{(m-1)}\end{cases}
  \]

(4.11)
The process of coordinate descent iterates until convergence, satisfies the termination condition \(\|\hat{\beta}^{(m, k)} - \hat{\beta}^{(m, k-1)}\|_\infty \leq \delta^*\) (e.g. \(\delta^* = 10^{-5}\)). Hence, \(\hat{\beta}^{(m)} = \hat{\beta}^{(m, t^*)}\) where \(t^*\) denotes the iteration at termination.

## 5 Experiments

### 5.1 Pitprops data

The pitprops data is a classic data set widely used for PCA analysis, as it is usually difficult to show the interpretability of principal components. It is used in ScoTLASS (Jolliffe et al., 2003) and in SPCA (Zou et al., 2006). As a demonstration of the performance of the new FGSPCA method, especially the grouping effect and sparsity effect, we also employ the pitprops data set and consider the first six principal components.

Table 1 shows the sparse loadings and the corresponding variance obtained by SPCA (Zou et al., 2006) (the left column) and FGSPCA (the right column). From Table 1, it can be seen that SPCA has a strong sparsity effect with respect to the number of zero loadings but a weak grouping effect. On the
The great improvement on the total variance by FGSPCA contributes to the grouping effect, as the “No. of Groups” shows the number of groups of loadings where a small number indicates strong grouping effect with similar loadings collapsing into groups. The “No. of Nonzeroes” is the number of non-zero loadings which indicates the sparsity, the smaller the more sparse.

Table 1: Pitprops Data: Loadings of the first six principal components by SPCA and FGSPCA.

| Variable | SPCA PC1 | SPCA PC2 | SPCA PC3 | SPCA PC4 | SPCA PC5 | SPCA PC6 | FGSPCA PC1 | FGSPCA PC2 | FGSPCA PC3 | FGSPCA PC4 | FGSPCA PC5 | FGSPCA PC6 |
|----------|----------|----------|----------|----------|----------|----------|------------|------------|------------|------------|------------|------------|
| topdiam  | 0.477    | 0        | 0        | 0        | 0        | 0        | -0.373     | 0          | 0          | 0          | 0          | 0          |
| length   | -0.476   | 0        | 0        | 0        | 0        | 0        | -0.373     | 0          | 0          | 0          | 0          | 0          |
| moist    | 0.785    | 0        | 0        | 0        | 0        | 0        | 0          | 0.704      | 0          | 0          | 0          | 0          |
| testg    | 0.619    | 0        | 0        | 0        | 0        | 0        | 0          | 0.710      | 0          | 0          | 0          | 0          |
| overg    | 0.177    | 0.641    | 0        | 0        | 0        | 0        | 0          | 0          | 0          | 0          | 0          | 0          |
| ringtop  | 0        | 0.589    | 0        | 0        | 0        | 0        | -0.373     | -0.368     | 0          | 0          | 0          | 0          |
| bowmax   | -0.344   | -0.021   | 0        | 0        | 0        | 0        | -0.373     | 0          | 0          | 0.479      | 0          | 0          |
| bowdist  | -0.416   | -0.373   | 0        | 0        | 0        | 0        | 0.293      | 0          | 0          | 0          | 0          | 0          |
| whors    | -0.400   | 0        | 0        | 0        | 0        | 0        | 0          | 0.418      | 0          | 0          | 0          | 0          |
| clear    | 0        | 0        | 0        | 0        | -1       | 0        | 0          | 0          | 0          | 0          | -0.908     | 0          |
| knots    | 0.013    | 0        | 0        | 0        | -1       | 0        | 0          | 0          | 0          | 0          | -0.788     | 0          |
| diaknot  | 0        | 0        | -0.016   | 0        | 0        | 1        | 0          | 0.293      | 0          | 0          | 0          | 0          |
| No. of Groups | 6 | 4 | 4 | 1 | 1 | 1 | 2 | 3 | 1 | 2 | 3 | 1 |
| No. of Nonzeroes | 7 | 4 | 4 | 1 | 1 | 1 | 9 | 7 | 2 | 2 | 3 | 1 |
| Variance (%) | 28.0 | 14.4 | 15.0 | 7.7 | 7.7 | 7.7 | 30.9 | 13.7 | 14.5 | 9.5 | 9.6 | 7.7 |
| Adjusted Variance (%) | 28.0 | 14.0 | 13.3 | 7.4 | 6.8 | 6.2 | 31.0 | 13.7 | 13.9 | 8.1 | 7.7 | 4.5 |
| Cum. Adj. Variance (%) | 28.0 | 42.0 | 55.3 | 62.7 | 69.5 | 75.8 | 31.0 | 44.7 | 58.6 | 66.7 | 74.4 | 78.9 |

other hand, FGSPCA has a strong grouping effect with respect to the number of groups of loadings. In detail, for the first PC obtained by FGSPCA, the loadings belong to two groups with nonzero values, and a sparse-group with zero values. And these groups are learned automatically from the model rather than from prior knowledge. The grouping effect among loadings further improves the interpretability.

It can be seen from Figure 2 that, compared with the modified principal components of SCoTLASS and SPCA, PCs obtained by FGSPCA account for a larger amount of variance (78.9%-FGSPCA vs. 75.8%-SCoTLASS vs. 69.3%-SCoTLASS) with a much stronger grouping structure on the loadings. The great improvement on the total variance by FGSPCA contributes to the grouping effect, as fewer parameters need to be estimated due to the grouping effect. Compared with SPCA, FGSPCA estimated a smaller number of parameters (12 vs. 18) due to the grouping effect of the loading structures. The number of parameters that need to be estimated is equal to the number of non-zero loadings in SPCA, and equal to the number of groups of loadings in FGSPCA.

5.2 Synthetic examples

**Synthetic examples with hidden factors** We adopt the same synthetic example settings as Zou et al. (2006). In order to be self-contained, we introduce the generating mechanism of the synthetic example here with three hidden factors

\[
V_1 \sim N(0, 290), \quad V_2 \sim N(0, 300), \quad V_3 \sim N(0, 1), \quad \epsilon \sim N(0, 1),
\]

(5.1)

and \(V_1, V_2, \epsilon\) are independent. We construct 10 variables which are defined as follows,

\[
X_j = V_1 + \epsilon_j^1, \quad \epsilon_j^1 \sim N(0, 1), \quad j = 1, 2, 3, 4,
\]

\[
X_j = V_2 + \epsilon_j^2, \quad \epsilon_j^2 \sim N(0, 1), \quad j = 5, 6, 7, 8,
\]

\[
X_j = V_3 + \epsilon_j^3, \quad \epsilon_j^3 \sim N(0, 1), \quad j = 9, 10,
\]

\(\{\epsilon_j^k\}\) are independent, \(k = 1, 2, 3\) \(j = 1, \ldots, 10\).

Since we know the data generating mechanism, we can easily calculate the exact covariance matrix of \(\{X_1, \ldots, X_{10}\}\) which is used to perform the ordinary PCA, SPCA, simple thresholding and FGSPCA.

Note that the variance of the three hidden factors is 290, 300, and 282.7875 respectively. From Table 2, the first two principal components account for 100% of the total explained variance by
Figure 2: Comparison of PEV, Cumulative Variance of Different Dimension Reduction Methods (PCA, SCoTLASS, SPCA, and FGSPCA) on the pitprops data set. PCA: ordinary PCA based on SVD (Jolliffe, 1986), SCoTLASS: modified PCA (Jolliffe et al., 2003), SPCA: sparse PCA (Zou et al., 2006), and FGSPCA: our new method of feature grouping and sparse PCA.

Table 2: Synthetic example with three hidden factors: Loadings of the first three/two principal components by PCA, SPCA, Simple Thresholding and FGSPCA, as well as the number of groups, the number of nonzeros and variance.

| Variable | PCA | SPCA | Simple Thresholding | FGSPCA |
|----------|-----|------|---------------------|--------|
| X1       | 0.116 0.479 0.062 | 0 0.5 | 0 -0.5 | 0 0.5 |
| X2       | 0.116 0.479 0.059 | 0 0.5 | 0 -0.5 | 0 0.5 |
| X3       | 0.116 0.479 0.114 | 0 0.5 | 0 -0.5 | 0 0.5 |
| X4       | 0.116 0.479 0.114 | 0 0.5 | 0 -0.5 | 0 0.5 |
| X5       | -0.395 0.145 -0.269 | -0.5 0 | 0 0 | -0.415 0 |
| X6       | -0.395 0.145 -0.269 | -0.5 0 | 0 0 | -0.415 0 |
| X7       | -0.395 0.145 -0.269 | -0.5 0 | 0 0 | -0.415 0 |
| X8       | -0.395 0.145 -0.269 | -0.5 0 | 0 0 | -0.415 0 |
| X9       | -0.401 -0.010 0.582 | 0 0 | -0.503 0 | -0.395 0 |
| X10      | -0.401 -0.010 0.582 | 0 0 | -0.503 0 | -0.395 0 |
| No. of Groups | 2 3 4 | 1 1 1 | 1 1 | 2 1 |
| No. of Nonzeros | 10 8 10 | 4 4 4 | 4 4 | 6 4 |
| Variance (%) | 60.23 39.77 0 | 41.02 39.65 38.88 39.65 | 59.17 39.65 |
| Adjusted Variance (%) | 60.23 39.77 0 | 41.02 39.65 38.88 38.73 | 59.11 39.28 |
| Cum. Adj. Var. (%) | 60.23 100 100 | 41.02 80.67 38.88 77.61 | 59.11 98.39 |

the ordinary PCA, which suggests considering only the first two derived variables by other dimension reduction methods. Ideally, the first derived variable should recover the factor $V$ using $X_5, X_6, X_7, X_8, X_9, X_{10}$ with larger absolute weights on $X_5, X_6, X_7, X_8$ than that on $X_9, X_{10}$. Meanwhile the weights on $X_5, X_6, X_7, X_8$ should be the same, and the weights on $X_9, X_{10}$ should be identical as well. The second derived variable should recover the factor $V$ only using $X_1, X_2, X_3, X_4$ with same weight coefficients.

Results on Table 2 show that all the methods (SPCA, Simple Thresholding, FGSPCA) can perfectly recover the factor $V$ by the second derived variable. However, as for the first derived variable, SPCA recovers the factor $V$ only using $X_5, X_6, X_7, X_8$ without $X_9, X_{10}$, as the weights on $X_9, X_{10}$ are zeroes. Simple Thresholding recovers the factor $V$ using $X_7, X_8, X_9, X_{10}$ which is far from being correct by placing larger absolute weights on $X_9, X_{10}$ than $X_7, X_8$. FGSPCA perfectly recovers the
factor $V_2$ using $X_5, X_6, X_7, X_8, X_9, X_{10}$ with larger absolute weights on $X_5, X_6, X_7, X_8$ than on $X_9, X_{10}$, moreover, the weights on $X_5, X_6, X_7, X_8$ are estimated as the same, and the weights on $X_9, X_{10}$ are the same as well, which is consistent with the ideal results we analyzed in the above.

The results of variance from Table 2 and Figure 3 show that the total variance explained by the first two PCs is 98.39% for FGSPCA and 80.67% for SPCA, which demonstrates a great improvement of 17.72% due to the grouping effect of FGSPCA. On the other hand, compared with the 100% explained total variance of SVD, FGSPCA is only 1.61% less.

![Figure 3: Comparison of PEV, Cumulative Variance of Different Dimension Reduction Methods](image)

(a) PEV (Percentage of Explained Variance)  
(b) Cumulative Variance

Figure 3: Comparison of PEV, Cumulative Variance of Different Dimension Reduction Methods (PCA, SPCA, Simple Thresholding, and FGSPCA) on the synthetic data with three hidden factors. PCA: ordinary PCA based on SVD (Jolliffe, 1986), SPCA: sparse PCA (Zou et al., 2006), and FGSPCA: our new method of feature grouping and sparse PCA.

**Synthetic examples with hidden groups**  We introduce another synthetic example with ten hidden factors which belong to three hidden groups,

$$
V_1^{(g)} \sim N(0, 290), \quad V_2^{(g)} \sim N(0, 300),
V_3^{(g)} = -0.3V_1^{(g)} + 0.925V_2^{(g)} + \epsilon^{(g)}, \quad \epsilon^{(g)} \sim N(0, 1),
\quad g = 1, 2, 3,
$$

and

$$\{V_1^{(g)}, V_2^{(g)}, \epsilon^{(g)}\} \text{ are independent, } \quad g = 1, 2, 3.$$

For the 10-th hidden factor, its covariance with other hidden factors is defined as follows

$$
\text{Cov}(V_{10}, V_1^{(g)}) = 290, \quad \text{Cov}(V_{10}, V_2^{(g)}) = 300, \quad \text{Cov}(V_{10}, V_3^{(g)}) = 282.7875,
\text{Cov}(V_{10}, V_{10}) = 295, \quad g = 1, 2, 3.
$$

The first 90 variables are constructed with the ten hidden factors which are divided into three hidden groups, where the details are as follows,

$$
X_j^{(g)} = V_1^{(g)} + \epsilon_j^{(G_y,1)}, \quad \epsilon_j^{(G_y,1)} \sim N(0, 1), \quad j = 1, 2, 3, 4,
X_j^{(g)} = V_2^{(g)} + \epsilon_j^{(G_y,2)}, \quad \epsilon_j^{(G_y,2)} \sim N(0, 1), \quad j = 5, 6, 7, 8,
X_j^{(g)} = V_3^{(g)} + \epsilon_j^{(G_y,3)}, \quad \epsilon_j^{(G_y,3)} \sim N(0, 1), \quad j = 9, 10,
\{\epsilon_j^{(G_y,k)}\} \text{ are independent, } \quad g = 1, 2, 3, \quad k = 1, 2, 3, \quad j = 1, \ldots, 10.
$$
The last 10 variables are defined as follows,

$$X_j = \sum_{g=1}^{3} \sum_{k=1}^{3} V_k^{(g)} + V_{10} + \epsilon_j, \quad \epsilon_j \sim N(0, 1), \quad j = 91, \cdots, 100.$$  

Here $\{\epsilon_j^{(G_{g,k})}\}$ and $\epsilon_j$ are independent. Since we know the data generating mechanism, we can easily calculate the exact covariance matrix of $\{X_1, \cdots, X_{100}\}$ which is used to perform the ordinary PCA, SPCA and FGSPCA.

Figure 4 clearly demonstrates the comparison results with respect to the PEV and the cumulative variance. Results in Figure 4 show that the first principal component accounts for most of the total variance with respect to the PEV. In terms of the cumulative variance, FGSPCA has an obvious and significant improvement over SPCA.

5.3 Model complexity

Model complexity The model complexity of FGSPCA is the number of groups of loadings, while the model complexity of SPCA is the number of non-zero loadings, which is the number of parameters needed to be estimated in the model.

Figure 5 gives the comparison of the model complexity and the cumulative variance by SPCA and FGSPCA. It can be seen from Figure 5 that, compared with the modified principal components of SPCA, the PCs obtained by FGSPCA explain a larger amount of the total variance, while the model complexity is much lower. Compared with SPCA, the model complexity of FGSPCA is much lower, which shows that, due to the grouping effect of the loading structures, the number of parameters needed to be estimated is small. The great improvement on the total variance by FGSPCA contributes to the grouping effect, as the model becomes less complex and fewer parameters need to be estimated due to the grouping effect.

5.4 Parameter tuning

Parameter tuning The parameters in FGSPCA can be elaborately chosen using the traditional cross-validation method. However, it is worth noting that empirical experiments show that FGSPCA
is quite robust to the parameters $\lambda, \lambda_1, \lambda_2, \tau$, and different combinations of these parameters may give the same estimation result. Thus, even there are several parameters in the FGSPCA, we do not need to worry about the parameter tuning issues here. In the above synthetic example with hidden groups, we just give the parameters arbitrary values, e.g. $\tau = 0.05, \lambda = 0.05, \lambda_1 = 0.1, \lambda_2 = 0.005$, while for the SPCA (Zou et al., 2006) we set up with the true number of hidden factors.

### 5.5 Limitation of FGSPCA

One limitation of FGSPCA is that it uses non-convex regularizers which are neither smooth nor differentiable. Recent research work (Birgin et al., 2021, Wen et al., 2018, Zhang et al., 2020b) has showed better denoising advantages of non-convex regularizers over convex ones. However, when solving the subproblem (4.1) with non-convex penalties, the proposed method could potentially lead to a local optimum, as the objective function in (4.1) is non-convex. As is pointed out in Wen et al. (2018), the performance of non-convex optimization problems is usually closely related to the initialization, which are inherent drawbacks of non-convex optimization problems. Hence, it is desirable to pick a suitable initial value of $\hat{\beta}^{(0)}$. Since each subprpblem (4.1) is a classical regression problem, possible candidate initial values are those estimated by any regression solver, such as the R package glmnet (Friedman et al., 2009) and the python sklearn. To keep simple, we use the result of SVD as the initialization in this paper.
6 Discussion

Extension to nnFGSPCA Since the FGSPCA problem contains $k$ independent FGS subproblems, and the FGS problem can be easily extended to the non-negative FGS problem (nnFGS) as the work in Qin et al. (2020), the FGSPCA can be easily extended to the settings with non-negative loadings, namely nnFGSPCA. By incorporating another regularization term, $p_3(\beta) = \sum_{l=1}^{p} (\min\{\beta_l, 0\})^2$, into the objective function, the nnFGSPCA can be easily obtained (See Appendix D for details).

7 Conclusion

In this paper, we propose the FGSPCA method to produce modified principal components which considers additional grouping structures where the loadings share similar coefficients (i.e., feature grouping), besides a special group with all coefficients being zero (i.e., feature selection). The proposed FGSPCA method can perform simultaneous feature clustering/grouping and feature selection by imposing a non-convex regularizer with naturally adjustable sparsity and grouping effect. Therefore, the grouping structure is learned from the model rather than from given prior information. Efficient algorithms are designed to solve our FGSPCA model and experiment results show that the proposed FGSPCA benefits from the grouping effect compared with methods without grouping effect.

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Appendices

An R implementation of FGSPCA\(^2\) can be found on github.

Notations For a vector \(w \in \mathbb{R}^p\), denote the squared \(L_2\) norm \(\|w\|_2^2 = \sum_{j=1}^{p} w_j^2\). Denote the \(L_1\) norm \(\|w\|_1 = \sum_{j=1}^{p} |w_j|\). For a matrix \(W\), denote the element-wise squared matrix norm \(\|W\|_F^2 = \|W\|_2^2 \triangleq \sum_{i,j} w_{ij}^2\), in which \(\|W\|_F\) is usually called the Frobenius norm. Note that \(\text{tr}(W^T W) = \|W\|_F^2\).

A Proof of Lemma 2

**Lemma 5** Consider the ridge regression criterion,

\[ J_\lambda(\beta) = \|y - X\beta\|_2^2 + \lambda\|\beta\|_2^2. \]

Denote the solution of ridge regression \(\hat{\beta} = \arg\min_\beta J_\lambda(\beta) = (X^T X + \lambda I)^{-1} X^T y\). Then

\[ J_\lambda(\hat{\beta}) = y^T (I - H_\lambda) y, \]

where

\[ H_\lambda = X(X^T X + \lambda I)^{-1} X^T. \]

**Proof of Lemma 2** We use the notation \(A_{p \times k} = [\alpha_1, \cdots, \alpha_k]\) and \(B_{p \times k} = [\beta_1, \cdots, \beta_k]\). Let

\[ J_\lambda(A, B) = \sum_{i=1}^{n} \|x_i - AB^T x_i\|_2^2 + \lambda\|\beta\|_2^2. \]

Define \(I_{p \times p} = [A A_\perp]\). And \(A \in \mathbb{R}^{p \times k}\), \(A_\perp \in \mathbb{R}^{p \times (p-k)}\), \(B \in \mathbb{R}^{k \times k}\). With the orthogonal constraint, \(A^T A = I_{k \times k}\), \(B^T B = I_{k \times k}\), and constraint \(A^T A_\perp = 0_{k \times (p-k)}\), we have

\[
\sum_{i=1}^{n} \|x_i - AB^T x_i\|_2^2 = \|X - XBA^T\|_2^2
\]

\[
= \|X[A A_\perp] - XBA^T [A A_\perp]\|_2^2
\]

\[
= \|X A \ X A_\perp - [XBA^T A - XBA^T A_\perp]\|_2^2
\]

\[
= \|((XA - XB) \ XA_\perp)\|_2^2 \quad (A^T A = I_{k \times k}, A^T A_\perp = 0) \tag{A.1}
\]

\[
= \|XA - XB\|_2^2 + \|XA_\perp\|_2^2
\]

\[
= \sum_{j=1}^{k} \|X\alpha_j - X\beta_j\|_2^2 + \|XA_\perp\|_2^2.
\]

Therefore, when \(A\) is fixed, solving \(\arg \min_B J_\lambda(A, B)\) is equivalent to solving the series of ridge regressions

\[ \arg \min_{(\beta_j)_{j=1}^{k}} \sum_{j=1}^{k} \{\|X\alpha_j - X\beta_j\|_2^2 + \lambda\|\beta_j\|_2^2\}. \]

Denote the solutions

\[ \hat{\beta}_j = (X^T X + \lambda I)^{-1} X^T \alpha_j. \]

Using Lemma 5, (A.1) and (A.2), we have the partially optimized criterion

\[
J_\lambda(A, \hat{B}) = \|XA_\perp\|_2^2 + \sum_{j=1}^{k} \left\{\|X\alpha_j - X\hat{\beta}_j\|_2^2 + \lambda\|\hat{\beta}_j\|_2^2\right\} \tag{A.3}
\]

\[
= \|XA_\perp\|_2^2 + \text{tr}\{(X A)^T (I - H_\lambda) (X A)}\}.
\]

\(^2\text{https://github.com/ipapercodes/FGSPCA}\)
We consider the structured regularization functions of variables (factors) in regression models, as which should be minimized with respect to $A$

The first constraint induces sparsity in the coefficients; the second results in sparsity in their successive variable selection and model selection are two essential issues which have been extensively studied in the framework of regression, especially in the high-dimensional settings.

**Structured sparsity**

We consider the structured regularization functions of variables (factors) in regression models, as variable selection and model selection are two essential issues which have been extensively studied in the framework of regression, especially in the high-dimensional settings.

**Elastic net (Zou and Hastie, 2005)** The naive elastic net criterion (Zou and Hastie, 2005) is defined as

$$
\|Y - X\beta\|^2 \leq s_1 \sum_{j=1}^{p} |\beta_j| + \lambda \sum_{j=1}^{p} \|\beta_j\|_1.
$$

If there is a group of variables among which the pairwise correlations are very high, the lasso tends to select only one variable from the group and does not care which one is selected. Unlike the lasso, the elastic net encourages a grouping effect, where strongly correlated predictors tend to be in or out of the model together.

**Fused lasso (Tibshirani et al., 2005)** The fused lasso (Tibshirani et al., 2005) is defined as follows,

$$
\hat{\beta} = \arg\min_{\beta} \|Y - X\beta\|^2, \quad \text{subject to } \sum_{j=1}^{p} |\beta_j| \leq s_1, \sum_{j=2}^{p} |\beta_j - \beta_{j-1}| \leq s_2.
$$

The first constraint induces sparsity in the coefficients; the second results in sparsity in their successive differences, i.e. local constancy of the coefficient profiles $\beta_j$ as a function of $j$. The fused lasso gives a way to incorporate information about spatial or temporal structure in the data. However, it requires the features to be ordered in some meaningful way before the construction of the problem.

**Group lasso (Yuan and Lin, 2006)** Consider the general regression problem with $J$ groups/factors,

$$
Y = \sum_{j=1}^{J} X_j\beta_j + \epsilon.
$$

Here $Y \in \mathbb{R}^{n \times 1}$, $\epsilon \sim N_n(0, \sigma^2 I)$, $X_j$ is an $n \times p_j$ matrix corresponding to the $j$-th factor and $\beta_j$ is the coefficient vector of size $p_j$, $j = 1, \cdots, J$. For a vector $\eta \in \mathbb{R}^d$, $d \geq 1$, and a symmetric $d \times d$ positive definite matrix $K$, we denote $\|\eta\|_K = (\eta^TK\eta)^{1/2}$. Given positive definite matrices $K_1, \cdots, K_J$, the group lasso (Yuan and Lin, 2006) estimate is defined as the solution to the following minimization problem,

$$
\min_{\beta} = \frac{1}{2n} \|Y - \sum_{j=1}^{J} X_j\beta_j\|^2 + \lambda \sum_{j=1}^{J} \|\beta_j\|_K .
$$

In the group lasso problem, the non-squared Euclidean $L_2$-norm penalty encourages factor/group-level sparsity, where the entire group of predictors can be retained or discarded in the model. Thus the group lasso can conduct feature selection along the group level and select groups of variables. However, this kind of group-level sparsity depends on the predefined group partition.
Structured sparsity-inducing norms (Jenatton et al., 2011) Consider the empirical risk minimization problem for linear supervised learning, with regularization by structured sparsity-inducing norms (Jenatton et al., 2011),

\[
\min_w \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, x_i^T w) + \lambda \Omega(w),
\]

where \( \lambda \) is a regularization parameter, \( L(w) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, x_i^T w) \) the empirical risk of a weight vector \( w \in \mathbb{R}^p \), \( \ell(\cdot, \cdot) \) is a loss function which is usually assumed convex and continuously differentiable with respect to the second parameter. The \( \Omega(w) \) is a general family of sparsity-inducing norms that allow the penalization of subsets of variables grouped together; which is defined as follows,

\[
\Omega(w) = \sum_{G \in \mathcal{G}} \left[ \sum_{j \in G} (d_j^G)^2 |w_j|^2 \right]^{\frac{1}{2}} = \sum_{G \in \mathcal{G}} \| d^G \circ w \|_2.
\]

Here \( (d_j^G)_{G \in \mathcal{G}} \) is a \( |G| \)-tuple of \( p \)-dimensional vectors such that \( d_j^G > 0 \) if \( j \in G \) and \( d_j^G = 0 \) otherwise, and \( G \) denotes a subset of the power set of \( \{1, \cdots, p\} \) such that \( \sum_{G \in \mathcal{G}} = \{1, \cdots, p\} \), that is, a spanning set of subsets of \( \{1, \cdots, p\} \). It is possible for elements of \( \mathcal{G} \) to overlap. This general formulation has several important sub-cases such as \( L_2 \)-norm penalty, \( L_1 \)-norm penalty, group \( L_1 \)-norm penalty, and elastic net penalty. However, the structured sparsity-inducing regularization can only encode prior knowledge about the expected sparsity patterns.

### C Proof of Lemma 3 and the Procrustes problem

#### C.1 Proof of Lemma 3

**Proof of Lemma 3** The theoretical convergence guarantee for Algorithm 2 is stated in Lemma 3 is analogous to Theorem 3 in Qin et al. (2020). The proof just mimics the proof details of Theorem 1 in Shen et al. (2012) and Theorem 3 in Qin et al. (2020), thus we omit the proof.

#### C.2 The Procrustes problem

**Proof of Lemma 4** In the orthogonal Procrustes problem, we seek an orthonormal matrix such that

\[
A = \arg \min_A \| M - NA^T \|_2^2, \text{ s.t. } A^T A = I_{k \times k}.
\]

First, we expand the matrix norm in the above objective function

\[
\| M - N A^T \|_2^2 = \text{tr}(M^T M) + \text{tr}(A^T N A^T) - 2 \text{tr}(M^T N A^T).
\]

Since \( A^T A = I_{k \times k} \) and \( \text{tr}(AB) = \text{tr}(BA) \), then the second term becomes

\[
\text{tr}(A^T N A^T) = \text{tr}(N A^T A) = \text{tr}(N^T N).
\]

The problem is equivalent to finding an orthonormal matrix \( A \) which maximize \( \text{tr}(M^T N A^T) \). We proceed by substituting the SVD of \( M^T N = UDV^T \) and obtain

\[
\text{tr}(M^T N A^T) = \text{tr}(UDV^T A^T) = \text{tr}(UD(AV)^T) = \text{tr}((AV)^T UD).
\]

As \( V \) is \( k \times k \) orthonormal, we have \( (AV)^T (AV) = V^T A^T AV = I_{k \times k} \). Note that \( D \) is diagonal with non-negative entries, \( \text{tr}((AV)^T UD) \) is maximized when the diagonal of \( (AV)^T U \) is positive and maximized. By Cauchy-Schwartz inequality, this is achieved when \( (AV) = U \), and in this case the diagonal elements are all ones, \( (AV)^T U = I_k \). Hence, an optimal solution is given by \( \hat{A} = UV^T \).
D Extension to nnFGSPCA

The nnFGSPCA criterion For the FGSPCA criterion, by adding another regularization function controlling the non-negativity of the loadings, we can obtain the nnFGSPCA criterion (D.1) easily,

$$\min_{A,B} \sum_{i=1}^{n} \|x_i - AB^T x_i\|_2^2 + \Psi(B),$$

subject to $A^T A = I_{k \times k}$,

where

$$\Psi(B) = \lambda \sum_{j=1}^{k} \|\beta_j\|_2^2 + \lambda_1 \sum_{j=1}^{k} p_1(\beta_j) + \lambda_2 \sum_{j=1}^{k} p_2(\beta_j) + \lambda_3 \sum_{j=1}^{k} p_3(\beta_j).$$

(D.2)

Here $p_1(\beta)$ and $p_2(\beta)$ are the same regularization functions as that in the FGSPCA criterion, and $p_3(\beta)$ is a new regularization function controlling the non-negativity of the loadings, which takes the following penalty form,

$$p_3(\beta_j) = \sum_{l=1}^{p} \left[ \min \left( \beta_{ij}, 0 \right) \right]^2.$$

(D.3)

In order to be self-contained, we also list here the regularization functions of $p_1(\beta)$ and $p_2(\beta)$

$$p_1(\beta_j) = \sum_{l=1}^{p} \min \left\{ \frac{|\beta_{ij}|}{\tau}, 1 \right\}, \quad p_2(\beta_j) = \sum_{l<l', (l,l') \in E} \min \left\{ \frac{|\beta_{ij} - \beta_{lj'}|}{\tau}, 1 \right\}.$$

The algorithm to solve the nnFGSPCA problem should be the same as Algorithm 1 and Algorithm 2. The procedure of updating $A$ is the same, only the updating of $\beta^{(m,k)}_l$ is slightly different.

To calculate $B$ If $A$ is given, for each $j$, denote $Y_j = X\alpha_j$. To estimate $\hat{B} = [\hat{\beta}_1, \cdots, \hat{\beta}_k]$, the nnFGSPCA criterion is equivalent to $k$ independent non-negative feature-grouping-and-sparsity constrained regression subproblems (nnFGS) defined in the following

$$\min_{\beta} \left\{ S(\beta) = \|Y_j - X\beta\|_2^2 + \lambda \|\beta\|_2^2 + \lambda_1 p_1(\beta) + \lambda_2 p_2(\beta) + \lambda_3 p_3(\beta) \right\}.$$  

(D.4)

Each $\hat{\beta}_j = \arg\min_{\beta} S(\beta)$ is a solution of the nnFGS problem, which can be obtained through a slightly different updating process of $\beta^{(m,k)}_l$.

Note that $p_3(\beta)$ should be decomposed by the difference-of-convex programming just as $p_1(\beta)$ and $p_2(\beta)$ do. In particular, $S(\beta)$ can be decomposed as follows,

$$S(\beta) = S_1(\beta) - S_2(\beta),$$

where the two convex functions $S_1(\beta)$ and $S_2(\beta)$ are given respectively by

$$S_1(\beta) = \sum_{i=1}^{n} \left( y_i - x_i^T \beta \right)^2 + \lambda \sum_{l=1}^{p} \beta_l^2 + \lambda_1 \sum_{l=1}^{p} \frac{|\beta_l|}{\tau} + \lambda_2 \sum_{l<l', (l,l') \in E} \frac{|\beta_l - \beta_{l'}|}{\tau} + \lambda_3 \sum_{l=1}^{p} \beta_l^2,$$

$$S_2(\beta) = \lambda_1 \sum_{l=1}^{p} \left( \frac{|\beta_l|}{\tau} - 1 \right) + \lambda_2 \sum_{l<l', (l,l') \in E} \left( \frac{|\beta_l - \beta_{l'}|}{\tau} - 1 \right) + \lambda_3 \sum_{l=1}^{p} \left( |\beta_l| \right)^2.$$

For the $m$-th iteration, we replace $S_2(\beta)$ with its affine minorization at the $(m-1)$-th iteration.

$$S_2^{(m)}(\beta) \approx S_2(\beta^{(m-1)}) + \left( \beta - \beta^{(m-1)} \right), \quad \partial S_2(\beta) = \beta^{(m-1)}.$$}

$$\propto S_2(\beta^{(m-1)}) + \frac{\lambda_1}{\tau} \sum_{l=1}^{p} \mathbf{1}_{\{|\beta_l^{(m-1)}| \geq \tau\}} \cdot |\beta_l| + \frac{\lambda_2}{\tau} \sum_{l<l', (l,l') \in E} \mathbf{1}_{\{|\beta_l^{(m-1)} - \beta_{l'}^{(m-1)}| \geq \tau\}} \cdot |\beta_l - \beta_{l'}| + \lambda_3 \sum_{l=1}^{p} \mathbf{1}_{\{|\beta_l^{(m-1)}| \geq 0\}} \cdot \beta_l^2.$$
For the $m$-th approximation, an upper convex approximating function to $S(\beta)$ can be obtained by

$$S(m)_1(\beta) = S_1(\beta) - S_2(m)_2(\beta),$$

which formulates the following subproblem.

$$\min_{\beta} \sum_{i=1}^{n} (y_i - x_i^T \beta)^2 + \lambda \sum_{l=1}^{p} \beta_l^2 + \frac{\lambda_1}{\tau} \sum_{l \in \mathcal{F}(m-1)} |\beta_l| + \frac{\lambda_2}{\tau} \sum_{l < l', (l, l') \in \mathcal{E}(m-1)} |\beta_l - \beta_{l'}| + \lambda_3 \sum_{l \in \mathcal{N}(m-1)} \beta_l^2,$$

where

$$\mathcal{F}(m-1) = \{ l : |\hat{\beta}_l^{(m-1)}| < \tau \},$$

$$\mathcal{E}(m-1) = \{ (l, l') \in \mathcal{E}, |\hat{\beta}_l^{(m-1)} - \hat{\beta}_{l'}^{(m-1)}| < \tau \},$$

$$\mathcal{N}(m-1) = \{ l : \hat{\beta}_l^{(m-1)} < 0 \}. \quad (D.5)$$

Denote $\beta_{l'} = \beta_l - \beta_{l'}$ and define $\xi = (\beta_1, \cdots, \beta_p, \beta_{12}, \cdots, \beta_{1p}, \cdots, \beta_{(p-1)p})$. The $m$-th subproblem can be reformulated as an equality-constrained convex optimization problem,

$$\min_{\xi} \sum_{i=1}^{n} (y_i - x_i^T \beta)^2 + \lambda \sum_{l=1}^{p} \beta_l^2 + \frac{\lambda_1}{\tau} \sum_{l \in \mathcal{F}(m-1)} |\beta_l| + \frac{\lambda_2}{\tau} \sum_{l < l', (l, l') \in \mathcal{E}(m-1)} |\beta_{l'}| + \lambda_3 \sum_{l \in \mathcal{N}(m-1)} \beta_l^2,$$

subject to $\beta_{l'} = \beta_l - \beta_{l'}$, $\forall l < l' : (l, l') \in \mathcal{E}(m-1)$.

The only difference for nnFGSPCA is the updating rule of $\hat{\beta}_l^{(m,k)}$, since $p_3(\beta)$ does not involve other variables but only $\beta_l$. In particular, when updating by

$$\hat{\beta}_l^{(m,k)} = \alpha^{-1} \gamma,$$

$\alpha$ is a little different compared to the solution of FGSPCA and $\gamma$ stays the same. The new $\alpha$ is formulated as follows,

$$\alpha = 2\lambda + 2\lambda_3 I_{\{\hat{\beta}_l^{(m-1)} < 0\}} + 2 \sum_{i=1}^{n} x_i^2 + \nu^k \sum_{l' : (l, l') \in \mathcal{E}(m-1)} \left| l' \right|. \quad (D.6)$$