Variable selection and covariance structure identification using sparse principal loading analysis

Jan O. Bauer
Faculty of Business and Economics, University of Basel
Faculty of Business Informatics,
Baden-Wuerttemberg Cooperative State University Mannheim
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Abstract

We provide sparse principal loading analysis which is a new concept that reduces dimensionality of cross sectional data and identifies the underlying covariance structure. Sparse principal loading analysis selects a subset of existing variables for dimensionality reduction while variables that have a small distorting effect on the covariance matrix are discarded. Therefore, we show how to detect these variables and provide methods to assess their magnitude of distortion. Sparse principal loading analysis is twofold and can also identify the underlying block diagonal covariance structure using sparse loadings. This is a new approach in this context and we provide required criteria to evaluate if the found block-structure fits the sample. The method uses sparse loadings rather than eigenvectors to decompose the covariance matrix which can result in a large loss of information if the loadings of choice are too sparse. However, we show that this is no concern in our new concept because sparseness is controlled by the aforementioned evaluation criteria. Further, we show the advantages of sparse principal loading analysis both in the context of variable selection and covariance structure detection, and illustrate the performance of the method with simulations and on real datasets. Supplementary material for this article is available online.

Keywords: Covariance Structure, Dimensionality Reduction, Sparse Principal Component Analysis, Sparsity, Variable Selection
1 Introduction

Principal loading analysis (PLA) is a method developed by Bauer and Drabant (2021) to reduce dimensionality using variable selection. The method chooses a subset of variables based on the impact of linked eigenvectors on the covariance matrix. PLA relies on hard-thresholding to link the eigenvectors to variables. Bauer and Drabant (2021) and Bauer (2021) provide recommendations for the threshold based on simulations in their work. However, since simulated results have their limitations, it is natural to search for an extension that does not rely on simulations. One approach by Bauer and Drabant (2023) is to analyze PLA from a regression point of view to obtain threshold values in line with coefficient significant tests of multivariate linear regression.

In this work, we provide the new concept of sparse principal loading analysis (SPLA) which gives two major contributions. First, SPLA does not rely on thresholding and therefore overcomes the concerns discussed above. The proposed concept is based on sparse loadings rather than eigenvectors to make the usage of a threshold redundant. Transforming a random vector using sparse loadings yields variables that are potentially correlated. Therefore, we propose the usage of a measure based on linear regression to correct calculation of the explained variance. Second, SPLA identifies the block covariance structure of the underlying random variables using sparse loadings. This is a new approach in this context. We contribute criteria to evaluate the detected structure which is necessary to find the one that fits the underlying block-structure.

Calculation of sparse loadings is not new and the respective literature is broad. Jolliffe et al. (2003) proposed a method that constrains the loadings using lasso regularization (see Tibshirani (1996)). Zou et al. (2006) formulated the calculation of the eigenvectors as a regression problem with quadratic penalization. The eigenvectors are then sparsed
using lasso regularization as well. Both regularizations together yield the elastic net (see Zou and Hastie (2005)). Qi et al. (2013) consider regularization by an elasticnet-type norm. On the other hand, Shen and Huang (2008) utilized the connection between the eigendecomposition of the covariance matrix and the singular value decomposition of the sample matrix to derive sparse loadings. Their approach is based on a regularized singular value decomposition which has also been used by Witten et al. (2009) for their method.

Our work is twofold since SPLA also identifies the underlying block-diagonal-structure of the covariance matrix. There are recent parametric (see, e.g., Srivastava and Reid (2012) and Yamada et al. (2017)) and non-parametric works (see, e.g., Pavlenko et al. (2012) and Devijver and Gallopin (2018)) especially in the high-dimensional context that have the same goal. The reason is that various techniques exist to estimate covariance matrices that follow a sparse structure (see, e.g., Ledoit and Wolf (2004), Karoui (2008), Bickel and Levina (2008), and many more). Further, detection of the block-diagonal structure prior to network inferences for Gaussian graphical models can improve performance (Tan et al., 2015).

This article is organized as follows: Section 2 provides notation needed for the remainder of this work. In Section 3, we motivate the new concept of SPLA. We discuss how SPLA is used to detect an underlying block-diagonal covariance structure in Section 4. In Section 5, we provide calculations of the explained total variance of SPLA which is required for application. Sparseness of the loadings to identify an underlying block-structure is essential for SPLA. We provide criteria to evaluate the found block covariance structure in Section 6. Further, we contribute the algorithm to conduct SPLA in practice. Although a sparser model is easier to interpret, it is problematic to work with a model that is sparser than the underlying covariance matrix since this results in too little explanatory power. Therefore,
we also discuss this variance-interpretability-trade-off and show respective solutions. A simulation study to evaluate the performance for block-diagonal covariance detection is given in Section 7. In Section 8 we provide real data examples for variable selection and block covariance structure detection, and we give an example for block covariance structure detection for synthetic data. SPLA will also be compared to PLA. We take a resume and suggest extensions in Section 9. Proofs and more detailed results are deferred to the supplementary material.

2 Setup

We first state some notation in this section. Afterwards, we give three assumptions used throughout this work and elaborate their respective objective.

We use the $\ell_2$ norm $\|v\|_2$ and the $\ell_\infty$ norm $\|v\|_\infty$ for column vectors. For any matrix $A$, $\|A\|$ denotes the matrix norm and we will use the spectral norm $\|A\|_2$ and the infinity norm $\|A\|_\infty$ as induced norms, and the Frobenius norm $\|A\|_F$. Further, $\text{tr}(A)$ denotes the trace and $A^+$ denotes the Moore–Penrose inverse of a matrix $A$. $O_p(\cdot)$ denotes stochastic boundedness.

We consider a random vector $X = (X_1, \ldots, X_M) \equiv (X_K, X_D) \in \mathbb{R}^M$ with $X_K^T \in \mathbb{R}^K$ and $X_D^T \in \mathbb{R}^D$ such that $K + D = M$. The covariance matrix of $X$ is given by $\hat{\Sigma} = (\hat{\sigma}_{i,j})$ for $i, j \in \{1, \ldots, M\}$, and the covariance matrices of $X_K$ and $X_D$ are $\Sigma_1$ and $\Sigma_2$ respectively. Further, we consider a perturbation matrix $E$ such that

$$
\hat{\Sigma} \equiv \begin{pmatrix} \hat{\Sigma}_1 & \hat{\Sigma}_{12} \\ \hat{\Sigma}_{12}^T & \hat{\Sigma}_2 \end{pmatrix} \equiv \Sigma + E \equiv \begin{pmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{pmatrix} + \begin{pmatrix} 0 & E_{12} \\ E_{12}^T & 0 \end{pmatrix},
$$

(1)
can be written as a sum of matrices. $E$ is a technical construction to extract the covariances between $X_K$ and $X_D$. The covariance matrix follows the eigendecomposition $\hat{\Sigma} = V \Lambda V^T$. 

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\( \Lambda \) is hereby a diagonal matrix containing the eigenvalues \( \lambda_1 > \cdots > \lambda_M \) of \( \tilde{\Sigma} \) in descending order, and \( V = (v_1, \ldots, v_M) \) is an orthonormal matrix containing the respective eigenvectors where \( v_i^\top = (v_i^{(1)}, \ldots, v_i^{(M)}) \) for all \( i \in \{1, \ldots, M\} \). Further, \( U = (u_1, \ldots, u_M) \) is a matrix containing the sparse loadings.

The independent and identically distributed (IID) sample \( x = (x_1, \ldots, x_M) \equiv (x_K, x_D) \in \mathbb{R}^{N \times M} \) contains \( N \) observations of the random vector \( X \). In general, the sample counterparts are indicated by the hat operator. For example, \( \hat{\Sigma} \equiv \hat{\Sigma} + \hat{E} \) is the sample covariance matrix of \( x \).

Variables or blocks of variables are linked to sparse loadings in SPLA. If we want to reduce dimensionality, we look for a set of variables \( D \) to discard while keeping the remaining variables \( K \). If we want to detect the underlying block covariance structure, our interest is to identify if two disjoint blocks of variables \( D \) and \( K \) do exist. Hence, we define \( D \subset \{1, \ldots, M\} \) with \( \text{card}(D) = D \) such that \( 1 \leq D < M \). \( D \) will contain the indices of a variable-block \( \{X_d\} \equiv \{X_d\}_{d \in D} \), and we introduce the quasi-complement \( K \equiv \{1, \ldots, M\} \setminus D \) with \( \text{card}(K) = K \) to label the remaining block of variables \( \{X_k\} \equiv \{X_k\}_{k \in K} \). In an analogous manner, \( \Delta \) with \( \text{card}(\Delta) = D \) will be used to index eigenvectors with respective eigenvalues linked to the \( \{X_d\} \).

For convenience purposes, we consider only the two blocks \( \{X_d\} \) and \( \{X_k\} \) throughout this work except for the examples in Section 8. Further, since \( X \equiv (X_K, X_D) \), the index sets are given by \( D = \{K + 1, \ldots, M\} \) and \( K = \{1, \ldots, K\} \) respectively. However, our results remain true for the trivial extension to any number of blocks and for the general case if \( D \subset \{1, \ldots, M\} \). All matrices following an analogous block-structure as \( \tilde{\Sigma} \) given in (1) are then to be replaced by their general form such as \( \tilde{\Sigma}_1 = \tilde{\Sigma}_{[K,K]}, \ \tilde{\Sigma}_2 = \tilde{\Sigma}_{[D,D]}, \ \tilde{\Sigma}_{12} = \tilde{\Sigma}_{[K,D]}, \ \text{and} \ \tilde{\Sigma}^\top_{12} = \tilde{\Sigma}_{[D,K]} \). For our purposes, this matrix-notation is only needed for
the proofs to which we refer for a more elaborate explanation.

Given the notation above, the following assumptions are made:

**Assumption 1.** \( \mathbb{E}(X) = 0 \).

We assume the random variables to have mean zero for convenience purposes to simplify the covariance matrix to \( \mathbb{E}(X^\top X) = \tilde{\Sigma} \).

**Assumption 2.** \( \tilde{\Sigma} \) is positive definite.

We want to extract the information contained in the \( \{X_d\} \) that can be explained by the \( \{X_k\} \). This is done by regression projection where \( \tilde{\Sigma} \) is required to be invertible. This corresponds to the full rank assumption of \( x \) in the sample case. Since \( \tilde{\Sigma} = \Sigma \) if \( \mathbb{E} = 0 \) by construction, we implicitly assume that \( \Sigma \) is positive definite as well.

**Assumption 3.** \( U \) is a block-diagonal matrix with \( U^\top U = I \).

Orthogonality of the sparse loadings is needed to obtain results regarding the explained total variance in this work. For convenience purposes, we therefore assume orthogonality throughout the whole work which holds without loss of generality: if \( U \) was not orthogonal, we would orthogonalize the loadings by using the singular value decomposition of \( U \) with singular values replaced by ones as it is done in a Procrustes problem (see, e.g., Mardia et al. (1979)). This can be done due to the block-diagonal shape of \( U \) which will be introduced in (3), and because the exact values of the non-zero components of \( U \) are not of concern. Both will be discussed elaborately in Section 3.

### 3 Methodology and Motivation

Firstly, we recap PLA in this section. The method relies on choosing a threshold value which, however, can be difficult in practice. Hence, we motivate the usage of SPLA based
on sparse loadings which does not require hard-thresholding anymore.

PLA is a concept for dimensionality reduction where a subset of existing variables is selected while the other variables are discarded. We refer to Bauer and Drabant (2021) for an elaborate explanation. However, the intuition is that blocks of variables are discarded which distort the covariance matrix only slightly. We scan for a block $X_D$ by checking if all $K$ elements $k \in K$ of $D$ eigenvectors $\{v^{(k)}_\delta\}_{\delta \in \Delta}$ of the covariance matrix $\tilde{\Sigma}$ are smaller in absolute terms than a certain cut-off value $\tau$. That is to say, we check if $|v^{(k)}_\delta| \leq \tau$ for all $(k, \delta) \in K \times \Delta \equiv \{(k, \delta) : k \in K, \delta \in \Delta\}$. For $X = (X_K, X_D)$, we therefore scan if the eigenvectors $V$ are of shape

$\begin{pmatrix} *_K \\ \varepsilon_D \end{pmatrix} \quad \text{for} \quad \delta^c \in \Delta^c \equiv \{1, \ldots, M\} \setminus \Delta \quad \text{with} \quad |\Delta^c| = K$

and hence represent the blocks $x_K$ and $x_D$ respectively. $*_K \in \mathbb{R}^K$, $*_D \in \mathbb{R}^D$ are hereby vectors containing components larger than $\tau$ in absolute terms, and $\varepsilon_K \in \mathbb{R}^K$, $\varepsilon_D \in \mathbb{R}^D$ are vectors containing components that are all smaller than $\tau$ in absolute terms respectively. The intuition comes from the special case when $\tau = 0$, i.e. when $E = 0$, since then the $\{v^{(\delta^c)}_\delta\}_{\delta \in \Delta^c}$ and $\{v_\delta\}_{\delta \in \Delta}$ represent the exclusive distortion of the covariance matrix by the $\{X_k\}$ and the $\{X_d\}$ respectively.

Lemma 1. The eigenvectors $V \equiv (v_1, \ldots, v_M)$ of the covariance matrix $\tilde{\Sigma} \equiv \Sigma + E$ from (2) are of shape $v^{(\delta^c)}_\delta = (*_K, 0_D)^\top$ and $v_\delta = (0_K, *_D)^\top$ if and only if $E = 0$.

In practice, we are more likely to face the situation that $E \neq 0$. However, if the perturbation $E$ is small, then the components of $\varepsilon_K$ and $\varepsilon_D$ are small as well because they are bounded by $E$. 
Corollary 1. For $\varepsilon_K \in \mathbb{R}^K$ and $\varepsilon_D \in \mathbb{R}^D$ from (2) it holds that $\|\varepsilon_K\|_\infty = O_p(\|E\|_l)$ and $\|\varepsilon_D\|_\infty = O_p(\|E\|_l)$ for $l \in \{2, \infty\}$.

Therefore, if the eigenvectors are of shape as in (2) with $\varepsilon_K$, $\varepsilon_D$ having all components smaller than $\tau$ in absolute terms, then most distortion of the variables $\{X_d\}$ is geometrically represented by the eigenvectors $\{v_\delta\}_{\delta \in \Delta}$. The explained variance of the $\{X_d\}$ can then be evaluated either by $\sum_{d \in D} \hat{\sigma}_{d,d}$ or approximated by $(\sum_m \lambda_m)^{-1}(\sum_{\delta \in \Delta} \lambda_\delta)$ where $\lambda_i$ is the eigenvalue corresponding to the eigenvector $v_i$. If the explained variance is sufficiently small for the underlying purpose of application, the variables $\{X_d\}$ are discarded. The same holds for the block $\{X_k\}$ in an analogous manner.

The concern in PLA is the proper choice of the threshold $\tau$ which is elementary for the detection of the blocks $\{X_d\}$ and $\{X_k\}$ respectively. There are no theoretical derivations for the choice of the threshold yet. Bauer and Drabant (2021) provided simulation results and Bauer and Drabant (2023) built a connection between $\tau$ and hypothesis testing in multivariate linear regression. However, if we use sparse loadings instead of eigenvectors, we do not rely on a threshold anymore. This is the intuition of the new concept of SPLA: Instead of checking if the eigenvectors follow a shape according to (2), we rather construct sparse loadings of shape

$$u_\delta^c = \begin{pmatrix} *_K \\ 0_D \end{pmatrix} \quad \text{for } \delta^c \in \Delta^c \equiv \{1, \ldots, M\} \setminus \Delta \text{ with } |\Delta^c| = K$$

$$u_\delta = \begin{pmatrix} 0_K \\ *_D \end{pmatrix} \quad \text{for } \delta \in \Delta \text{ with } |\Delta| = D$$

which represent the underlying covariance matrix. While eigenvectors follow a natural order due to the size of their respective eigenvalues, for our purposes such an order is not required for the sparse loadings. Instead, we will always consider $U$ to be a matrix of block
diagonal shape

\[ U \equiv \begin{pmatrix} *_{K \times K} & 0_{K \times D} \\ 0_{D \times K} & *_{D \times D} \end{pmatrix} \equiv \begin{pmatrix} U_1 & 0 \\ 0 & U_2 \end{pmatrix}, \]

which reduces \( \Delta^c = \{1, \ldots, K\} \) and \( \Delta = \{K + 1, \ldots, M\} \). If the sparse loadings do not follow this shape by construction, we will transform \( U \) to a matrix of block-diagonal shape \( P_1 U P_2 \) using permutation matrices \( P_1 \) and \( P_2 \) for row and column permutations respectively. We note that the exact component-values in \(*_{K \times K}\) and \(*_{D \times D}\) are not of concern, since we are only interested if an underlying structure representing the blocks \( \{X_k\} \) and \( \{X_d\} \) does exist. Therefore, we can always orthogonalize \( U \) as described in Assumption 3 despite of its changes of the component-values.

4 Block Covariance Structure Identification

In this section, we discuss how SPLA identifies if the random vector \( X \) follows a block covariance structure.

According to Lemma 1, it is reasonable to consider the eigenvectors for identification of the shape of the covariance matrix. Further, it holds that the covariance matrix follows a block-diagonal structure if all eigenvectors are either close to \((*_{K}, 0_{D})^\top\) or close to \((0_{K}, *_{D})^\top\).

**Lemma 2.** For \( \varepsilon_K \in \mathbb{R}^K \) and \( \varepsilon_D \in \mathbb{R}^D \) from (2) it holds that \( \|E\|_l = O_p(\|\varepsilon_K, \varepsilon_D\|^\top\|_\infty) \) for \( l \in \{2, F, \infty\} \).

Instead of checking if the eigenvectors are close to the aforementioned shape in the \( \mathcal{L}_1 \) norm, we rather suggest to check if sparse loadings exist that are not only of shape \( u_{\delta^c} = (*_{K}, 0_{D})^\top \) and \( u_\delta = (0_{K}, *_{D})^\top \) but also represent the underlying covariance matrix
adequately. Criteria to evaluate if the sparse loadings are representative for the covariance matrix and therefore for the random vector are provided in Section 6.

Note that using sparse loadings instead of eigenvectors loses the bounds on the perturbation. When using hard-thresholding on the eigenvectors in PLA, the magnitude of \( \mathbf{E} \) relates to the identification as a block-diagonal covariance matrix as follows:

**Corollary 2.** Let \( \tau \) be the threshold for PLA and \( \lambda_1 > \cdots > \lambda_M \) be the eigenvalues of \( \tilde{\Sigma} \) with \( \lambda_0 \equiv \infty \) and \( \lambda_{M+1} \equiv -\infty \). If the covariance matrix does not follow a block-structure in PLA-sense, then

\[
\| \mathbf{E} \|_l > \tau \cdot 2^{-3/2} \min_{j \in \{1, \ldots, M+1\}} (\lambda_{j-1} - \lambda_j),
\]

for \( l \in \{2, \infty\} \).

This bound on \( \mathbf{E} \) does not hold for the concept of SPLA when using sparse loadings however. The reason is that SPLA considers block covariance structure identification based on the covariance matrix and on the precision within a block, and not exclusively on the covariances between blocks. Hence, SPLA takes into account the relation between \( \mathbf{E} \) and \( \Sigma_1^{-1} \). This relation is important to evaluate if the found covariance structure is reasonable and will be considered more elaborately in Section 6.

## 5 Explained variance

Transforming the random vector using sparse loadings yields variables that are potentially correlated. This is a concern when calculating the explained variance for each loading or for each block of variables. Solutions to that issue will be addressed in this section.

Since \( \mathbb{E}[(\mathbf{Xv}_i)^\top \mathbf{Xv}_j] = 0 \) and \( \mathbb{E}[(\mathbf{Xv}_i)^\top \mathbf{Xv}_i] = \lambda_j \) for \( i, j \in \{1, \ldots, M\} \) and \( i \neq j \), it is well known that the eigenvalues contain the magnitude of dispersion of \( \mathbf{X} \) along the
eigenvectors. Hence, the overall distortion of the covariance matrix is given by $\sum_i \lambda_i$. In the sparse case, however, the projected variables $\{Xu_i\} \equiv \{Xu_i\}_{i \in \{1, \ldots, M\}}$ might be correlated such that $E[(Xu_i)^T Xu_j] \neq 0$ for $i, j \in \{1, \ldots, M\}$. Therefore, quasi-eigenvalues $E[(Xu_i)^T Xu_i] = u_i^T \tilde{\Sigma} u_i$ overvalue the explained total variance because the $\{Xu_i\}$ contain similar contributions.

To find a different measure for the explained variance, we recap that the partial covariance matrix $\tilde{\Sigma}_{2,1}$ contains the information left in $X_D$ after eliminating the effects of $X_K$ by regression projection.

**Remark 1.** Let $X \equiv (X_K, X_D)$ with $E[X^T X] = \tilde{\Sigma}$. It holds that

$$E[(X_D - X_K\beta)^T (X_D - X_K\beta)] = \Sigma_2 - E_{12}\Sigma_1^{-1}E_{12} \equiv \tilde{\Sigma}_{2,1}, \quad (4)$$

where $\beta$ contains the respective regression coefficients.

Hence, an initial proposal is to use a measure for the explained variance that is based on the partial covariance matrix $\tilde{\Sigma}_{2,1}$ to overcome the concern of correlation among the $\{Xu_i\}$. McCabe (1984) discussed several measures and we will use one of them for our examples in Section 8. However, in order to find the variables we want to discard as well as the number of variables we want to discard, each partial covariance matrix for any possible combination of variables $\sum_{m=1}^{M-1} \binom{M}{m} = 2^M - 2$ has to be calculated which is not feasible in practice. Further, calculating the partial covariance matrix is computationally demanding. Therefore, we suggest to firstly use a different evaluation of the explained variance to find possible blocks of variables we consider to discard.

Zou et al. (2006) proposed to correct the explained variance using regression projection as well. For calculating the explained variance of $Xu_i$, they suggest to correct upwardly for $\{Xu_j\}_{j \in \{1, \ldots, i-1\}}$ and therefore to use

$$E[(Xu_i - XU_{i-1}\beta)^T (Xu_i - XU_{i-1}\beta)] \equiv r_{i,i}^2, \quad (5)$$
where $\mathbf{U}_{i-1} \equiv (\mathbf{u}_1, \ldots, \mathbf{u}_{i-1})$, and $\mathbf{\beta}$ contains the respective regression coefficients. The advantage is the following computationally more efficient measure for application in the sample case using a QR decomposition.

**Remark 2.** Let $\mathbf{x}\hat{\mathbf{U}} = \hat{\mathbf{Q}}\hat{\mathbf{R}}$ with $\hat{\mathbf{R}} = (\hat{r}_{i,j})$ be the QR decomposition of the sample $\mathbf{x}\hat{\mathbf{U}}$. It holds that

$$
\|\mathbf{x}\hat{\mathbf{u}}_i - \mathbf{x}\hat{\mathbf{U}}_{i-1}\hat{\mathbf{\beta}}\|^2 = \hat{r}_{i,i}^2,
$$

where $\hat{\mathbf{U}}_{i-1} \equiv (\hat{\mathbf{u}}_1, \ldots, \hat{\mathbf{u}}_{i-1})$, and $\hat{\mathbf{\beta}}$ contains the respective regression coefficients. Further, $(N - 1)^{-1}\hat{r}_{i,i}^2 \xrightarrow{p} r_{i,i}^2$ is the sample counterpart of $r_{i,i}^2$ for $i \in \{1, \ldots, M\}$.

Hence, in the sample case the explained variance of $\mathbf{X}\mathbf{u}_i$ corrected by $\{\mathbf{X}\mathbf{u}_j\}_{j \in \{1, \ldots, i-1\}}$ can be estimated by $(N - 1)^{-1}\hat{r}_{i,i}^2$, and the explained total variance can be estimated by $(N - 1)^{-1}\sum_i \hat{r}_{i,i}^2$ respectively. However, while (6) gives a computationally efficient measure, there are also two downsides: Firstly, the evaluation of blocks of variables is not taken into account since the measure considers each sparse loading as an $1 \times 1$ block. Secondly, the measure is biased because we do not correct for all sparse loadings. Since we correct for more loadings when $i$ increases, it holds that this bias decreases the larger $i$. However, (6) still provides a good first intuition regarding the explained variance which benefits from the efficient calculation. Therefore, we propose that SPLA is based on (6) for a first analysis to reduce the number of block-combinations that have to be evaluated as well as on the partial covariance matrix (4) for the final evaluation.

### 6 Identifying the Underlying Block-Structure

When calculating sparse loadings, we might create sparse loadings even if the underlying eigenvector structure is not sparse-ish, or we might create loadings that are sparser than
the underlying eigenvector structure. In Section 6.1, we therefore discuss how to evaluate if
the obtained sparse loadings are reasonable or not. Further, we recap methods to calculate
sparse loadings. Afterwards, we have all pieces together to provide the algorithm for SPLA
in Section 6.2. Additionally, we show in Section 6.3 that the explained total variance of
the sparse model is controlled by the introduced evaluations in Section 6.1.

6.1 Sparseness Evaluation Criteria

The sparser the loadings, the easier it is to interpret the underlying structure of the sample.
Of course, it is only reasonable to enforce sparse loadings in application if the underlying
population eigenvectors are sparse-ish. However, since we have only access to the sample
eigenvectors in practice, we need a criterion to decide if the found sparseness is reasonable
or not.

Let therefore \( u_{\delta^*} \) be the sparse loading associated with the block \( \{X_d\} \) with the smallest
index. As a sparseness criterion, we propose to evaluate the ratio between the corrected
explained variance \( r_{\delta^*,\delta^*} \) of \( u_{\delta^*} \) and its uncorrected variance \( \mathbb{E}[(X u_{\delta^*})^2] = u_{\delta^*}^\top \tilde{\Sigma} u_{\delta^*} \). We
use \( u_{\delta^*} \) because if we used another \( u_d \) with \( d < \delta^* \), then this sparse loading would be
corrected by \( u_{\delta^*} \) i.e. it would be corrected by variables included in the same block. It
holds the following result for the corrected explained variance given by the largest sparse
loading \( u_{\delta^*} \):

**Theorem 1.** Let \( \delta^* \in \Delta \) and let \( \{u_\delta\}_{\delta \in \Delta} \) be the sparse loadings associated with the block
\( \{X_d\} \). It holds for \( r_{\delta^*,\delta^*} \equiv \mathbb{E}[(X u_{\delta^*} - X U_{\delta^*-1} \beta)^\top (X u_{\delta^*} - X U_{\delta^*-1} \beta)] \) that

\[
r_{\delta^*,\delta^*} = u_{\delta^*}^\top \tilde{\Sigma} u_{\delta^*} - O_p(\|E u_{\delta^*}\|_2^2 \|\Sigma^{-1/2}\|_2),
\]

where \( \delta^* \equiv \min \Delta \) is the smallest index of the sparse loadings associated with the \( \{X_d\} \),
\( U_{\delta^*-1} \equiv (u_1, \ldots, u_{\delta^*-1}) \), and \( \beta \) contains the respective regression coefficients.
The bound depends on the covariances between the \( \{X_d\} \) and the \( \{X_k\} \), and on the precision matrix of the \( \{X_k\} \). The latter one follows the indication by Bauer and Drabant (2021) that blocks become more distinguishable the stronger the relation is within the blocks. In case the underlying covariance matrix follows a perfect block-diagonal structure, i.e. if \( E = 0 \), we can conclude that \( r_{\delta^*,\delta^*}^2 = u_{\delta^*}^\top \Sigma u_{\delta^*} \) reduces to the largest sparse quasi-eigenvalue. Therefore, the closer the ratio of the following criterion is to one, the more likely we detected the correct underlying sparse structure.

**Remark 3.** Let \( 1 \notin \Delta \) and let \( \delta^* \equiv \min \Delta \) be the smallest index of the sparse loadings associated with the \( \{X_d\} \). The block evaluation criterion (EC) for \( \{X_d\} \) is given by

\[
EC \equiv \frac{r_{\delta^*,\delta^*}^2}{u_{\delta^*}^\top \Sigma u_{\delta^*}} \in (0, 1]
\]

and it holds that

\[
EC = \frac{u_{\delta^*}^\top \Sigma u_{\delta^*} - O_p(\|Eu_{\delta^*}\|_2^2 \|\Sigma_1^{-1}\|_2)}{u_{\delta^*}^\top \Sigma u_{\delta^*}}
\]

due to Theorem 1.

Clearly, (7) equals one for the extreme case when \( \Sigma_{12} \equiv E_{12} = 0 \). Further, the criterion is positive by construction because it is a scaled variance term with \( \Sigma \) being positive definite (Assumption 2).

For completion, we shall mention that we obtain similar bounds to Theorem 1 also for the case when the block-diagonal shape of the loadings given in (3) is not satisfied. However, in this case it is not feasible to correct for all \( K \) loadings associated with the block \( \{X_k\} \) since we would correct for variables contained in the same block otherwise.

**Lemma 3.** Let \( 1 \notin \Delta \) and let \( \{u_{\delta}\}_{\delta \in \Delta} \) be the sparse loadings associated with the block \( \{X_d\} \). If the block-diagonal condition of \( U \) in Assumption 3 is violated, it holds for \( r_{\delta^*,\delta^*}^2 \equiv \)
\[
E[(Xu_{\delta^*} - XU_{\delta^*-1}\beta)^\top (Xu_{\delta^*} - XU_{\delta^*-1}\beta)] \text{ that }
\]
\[
\frac{r_{\delta^*,\delta^*}^2}{u_{\delta^*}\tilde{\Sigma}u_{\delta^*}} = \mathcal{O}_p(\|\mathbf{E}u_{\delta^*}\|^2_2\|\Sigma_1^{-1}\|_2),
\]
where \(\delta^* \equiv \min \Delta\) is the smallest index of the sparse loadings associated with the \(\{X_d\}\), \(U_{\delta^*-1} \equiv (u_{\kappa_1}, u_{\kappa_2}, \ldots)\) with \(\kappa_1, \kappa_2, \ldots < \delta^*\) and \(\text{card}(\{\kappa_1, \kappa_2, \ldots\}) < K\), and \(\beta\) contains the respective regression coefficients.

We evaluate the sparseness only in an upward manner in the EC due to the nature of the measure \(r_{ij}^2\) from (5) as discussed in Section 5 in relation to Remark 2. Further, following Theorem 1 we evaluate a block with respect to its largest associated sparse loading. If we used a different loading \(u_{\delta}\) with \(\delta \neq \delta^* \equiv \min \Delta\), the bound on the quasi-eigenvalue would not only depend on \(E_{12}\) and \(\Sigma_1^{-1}\), but also on \(\Sigma_2\).

So far, we have not yet discussed that the EC considers not the plain covariances between the blocks but rather a weighted covariance \(E_{\delta^*}\) with weights \(u_{\delta^*}\). This is problematic because different loadings of same shape yield different evaluation outcomes. Additionally, variables with zero-components in the corresponding loading are not considered in the criterion. However, we can fix this issue by giving equal weights to all variables which motivates another evaluation criterion.

**Remark 4.** Let \(1 \notin \Delta\) and let \(\delta^* \equiv \min \Delta\) be the smallest index of the sparse loadings associated with the \(\{X_d\}\). Let further \(w_{\delta^*} \equiv (0_K, 1_D)^\top\). We replace the \(\delta^*\)th loading by \(u_{\delta^*} = w_{\delta^*}/\|w_{\delta^*}\|_2 = D^{-1/2}w_{\delta^*}\) and we replace \(\{u_i\}_{i \neq \delta^*}\) such that Assumption 3 is satisfied. The weight-corrected block evaluation criterion (CEC) for \(\{X_d\}\) is given by

\[
CEC \equiv \frac{r_{\delta^*,\delta^*}^2}{u_{\delta^*}\tilde{\Sigma}u_{\delta^*}} \in (0, 1]
\]

and it holds that

\[
CEC = \frac{u_{\delta^*}\tilde{\Sigma}u_{\delta^*}}{u_{\delta^*}\tilde{\Sigma}u_{\delta^*}} - \mathcal{O}_p(D^{-1/2}\|E_{12}1_D\|^2_2\|\Sigma_1^{-1}\|_2).
\]
Clearly, the vector $\mathbf{w}_{\delta^*}$ weighs all covariances between $\{X_d\}$ and $\{X_k\}$ equally making CEC a corrected criterion. When replacing a loading $\mathbf{u}_{\delta^*}$, we have to change all remaining loadings $\{\mathbf{u}_i\}_{i \neq \delta^*}$ to maintain orthogonality of $\mathbf{U}$. However, such a change is quickly implemented and a respective procedure is given in Supplementary Material [1].

Note that $\delta^* = 1$, i.e. using the first loading $\mathbf{u}_1$, is not feasible for the evaluation criteria EC and CEC. We have to keep this in mind for the general case with more than two blocks. Despite $\delta^* = 1$ is mathematically possible in [6], no additional information is provided since loadings are corrected only in an upward direction. Therefore, the first loading is not corrected for the effect of other loadings and therefore the EC and CEC always equal one in this case.

**Corollary 3.** Let $\{\mathbf{u}_d\}_{\delta \in \Delta}$ be the sparse loadings associated with the block $\{X_d\}$. If $\delta^* \equiv \min \Delta = 1$, then both block-structure evaluation criteria EC [7] and CEC [8] reduce to one.

If this situation arises, however, one evaluates the block $\{X_k\}$ instead of $\{X_d\}$ by using its largest loading $\mathbf{u}_{\kappa^*}$ with $\kappa^* = \min\{1, \ldots, M\} \setminus \Delta$. Clearly, verifying the block $\{X_k\}$ implies verification of $\{X_d\}$ as a block. The condition that $1 \notin \Delta$ in Theorem [1] is fulfilled by construction in this work since we assumed for convenience that $\mathcal{D} = \Delta = \{K + 1, \ldots, M\}$ and therefore that $\delta^* \equiv \min \Delta = K + 1$. However, in a more general setting $1 \in \Delta$ is possible as can be seen in the examples in Section [8].

We note that other evaluation criteria based on the partial covariance matrix can also be used.
Lemma 4. Let $\tilde{\Sigma}_{2,1} \equiv \Sigma_2 - E_{12}^T \Sigma_1^{-1} E_{12}$ be the partial covariance matrix. It holds that

$$\frac{\|\tilde{\Sigma}_{2,1}\|}{\|\Sigma_2\|} = \frac{\|\Sigma_2\| - O_p(\|E_{12}\|^2 \|\Sigma_1^{-1}\|)}{\|\Sigma_2\|} \in (0, 1).$$

As mentioned in Section 5, however, calculation of the partial covariance matrix is computationally costly.

### 6.2 Sparse Principal Loading Analysis

In Section 5, we proposed that a measure for the explained variance in SPLA should be based on the QR decomposition (6) for a first analysis as well as on the partial covariance matrix (4) for the final evaluation. To decide if the found block-structure is reasonable, we additionally check the evaluation criteria.

The missing piece is the calculation of the sparse loadings. Guerra-Urzola et al. (2021) compared the performance of several methods and assessed that the one by Shen and Huang (2008) performs best. Since it is a special case of the approach by Witten et al. (2009), we use their method for the majority of this work. For some of our examples, however, we applied the procedure of Zou et al. (2006). The latter one allows sparsening of each loading individually by penalization which allows to create any composition of sparse loadings and has been used for the examples in Section 8.1 and Section 8.2 respectively. Both methods are recapped in Supplementary Material 1, however, we refer to the original works for elaborate explanations.

We can now contribute an algorithm for SPLA. Discard $\{X_d\}$ according to SPLA proceeds as follows:

In case we are only interested in finding the underlying block covariance structure, the first three steps 1 to 3 of Algorithm 1 are sufficient.

Despite the usage of methods to calculate sparse loadings, we experienced that com-
Algorithm 1 Sparse principal loading analysis

1: Calculate the sparse loadings \( \{u_i\} \).

2: Assess if the detected sparseness is meaningful by checking the sparseness evaluation criterion (7) or (8). Repeat step 1-2 as long as the sparseness is reasonable.

3: Evaluate the detected blocks of variables using their explained variances from (6) and select potential blocks for discarding accordingly.

4: Check the choice in step 3 using the partial covariance matrices from (4). Discard the blocks if selection is verified.

Components become very close but not equal to zero in practice. Therefore, we recommend to use a small cut-off value for the sparse loadings in step 1. Further, in step 2 we decide that the detected sparseness is not reasonable when the evaluation criteria falls below a fixed parameters \( c_{EC} \) or \( c_{CEC} \) respectively.

6.3 Variance-Interpretability-Trade-Off

In this section, we discuss the trade-off between the explained total variance and interpretability, and elaborate the importance of a large explained total variance. We will show that the variance-interpretability-trade-off is addressed appropriately when the evaluation of the underlying sparseness discussed in Section 6.1 is considered.

For applications, we have to be aware of the trade-off between the explained total variance and interpretability of SPLA. We discussed in Section 6.1 that the more sparse the loadings, the easier it is to interpret the underlying sample. However, this comes at the price of a small explained total variance which, on the other hand, might make interpretation not reasonable anymore because the sparse loadings simply provide too little information.

In application, the explained total variance of the sample sparse loadings according
to (6) relative to the total variance of $\mathbf{x}$ is given by $(N - 1)^{-1} \sum_i \hat{r}_{i,i}^2 / \text{tr}(\hat{\Sigma})$. Due to the perturbation $\hat{\mathbf{E}} \equiv \hat{\Sigma} - \hat{\Sigma}$, we obtain the following result:

**Theorem 2.** Let $\varepsilon(\mathbf{x})$ be a perturbation of the sample such that $\hat{\mathbf{x}} \equiv \mathbf{x} - \varepsilon(\mathbf{x})$ has covariance matrix $\hat{\Sigma}$. It holds that

$$\|\varepsilon(\mathbf{x})\| = \mathcal{O}_p(\|\hat{\mathbf{E}}\|).$$

If further $(N - 1)^{-1} \|\hat{\Sigma}^{-1}\|_2^{1/2} \|\varepsilon(\mathbf{x})\|_2 < 1$, it holds that

$$(N - 1)^{-1} \sum_i \hat{r}_{i,i}^2 = \text{tr}(\hat{\Sigma}) - (N - 1)^{-1} \mathcal{O}_p(\|\hat{\mathbf{E}}\|_F^2).$$

Theorem 2 contains two implications. Firstly, since $\|\varepsilon(\mathbf{x})\| = \mathcal{O}_p(\|\hat{\mathbf{E}}\|)$, the condition that $(N - 1)^{-1} \|\hat{\Sigma}^{-1}\|_2^{1/2} \|\varepsilon(\mathbf{x})\|_2 < 1$ evaluates the relation within blocks in comparison to the relation between blocks as discussed in Section 6.1. Secondly, the explained total variance drops in case we erroneously assign a block. In turn, the explained total variance is large in case we correctly detect a block. However, recall that we already control for correct specification of blocks in SPLA due to the EC and the CEC from (7) and (8) respectively. We can conclude that the variance-interpretability-trade-off is of no concern when we follow Algorithm 1 and therefore evaluate the sparseness according to the evaluation criteria.

### 7 Simulation Study

In this section, we deepen the understanding of SPLA based on simulations. In Section 7.1, we analyse the behaviour of the CEC from Section 6 for block-diagonal covariance detection when the correlation among blocks varies. Afterwards, we evaluate the percentage of identified block-diagonal covariance matrices (identification rate) of SPLA in Section 7.2. We further discuss considerations regarding our simulation design in Section 7.3. Code to replicate all simulation results is provided in Supplementary Material 2.
7.1 Corrected Evaluation Criterion Analysis

In this section, we simulate a sample following a block-diagonal correlation matrix of six blocks to demonstrate the evaluation using the CEC.

Let therefore $Y$ and $Z_i$ for $i \in \{1, \ldots, 5\}$ be IID $N(0, 10)$ distributed, and let $W$ be $N(0, 1)$ distributed. We consider a random vector $X^{[\rho]} = (X_1, \ldots, X_{14})$ with $X_j = \sqrt{1-\rho} Z_i + \sqrt{\rho} Y + W$ for $(j, i) \in \{(1,1), (2,1), (3,2), (4,2), \ldots, (13,6), (14,6)\}$ such that $X^{[\rho]}$ has a covariance matrix with six $2 \times 2$ blocks on the diagonal. Hereby, $\rho$ reflects the approximate correlation between the blocks. We simulate a sample $x^{[\rho]}$ by firstly drawing $N = 100$ observations from $X^{[\rho]}$ and secondly standardizing the sample. Therefore, the sample covariance matrix equals the sample correlation matrix which is illustrated in Figure 1 for $\rho \in \{0.1, 0.2, 0.4, 0.5\}$. Afterwards, we redraw $s \in \{1, \ldots, 100\}$ samples $x^{[\rho,s]}$ with $N = 100$ observations and calculate the respective CEC according to (8) for block two, four, and six. The results are illustrated as boxplots in Figure 2.

The CEC decreases with an increase of the correlation among the blocks and, therefore, with an increase of $\rho$. Further, the CEC decreases when evaluating more blocks. This is due to the construction of the corrected measure for the explained variance in (6) because we control in an upward direction.

According to the CEC for the sixth block in Figure 2, $c_{CEC} = 0.6$ seems appropriate.
Figure 2: CEC for block two, four, and six for each of the $s \in \{1, \ldots, 100\}$ samples $\mathbf{x}^{[\rho,s]}$ drawn from $\mathbf{X}^{[\rho]}$ for $\rho \in \{0.1, 0.2, 0.3, 0.4, 0.5\}$ respectively.

because it confirms the block for $\rho < 0.3$ and rejects the block for $\rho > 0.5$. This is meaningful, since strong correlation among variables tells us that they are not separated into different blocks. We therefore use $c_{CEC} = 0.6$ for the remainder of this work. For completion, we shall emphasize that choosing the appropriate sparseness depends on application. Choosing a too small $c_{CEC}$, however, is no concern because erroneously detected blocks are corrected in step 4 of Algorithm 1 using the partial covariance matrix.

### 7.2 Performance

In this section, we compare the performance of block-diagonal covariance structure detection. Recently, [Devijver and Gallopin (2018)](Devijver2018) derived nonasymptotic approaches that select the number of blocks either using a slope heuristic robust regression (SHRR) or using a slope heuristic dimension jump (SHDJ). We refer to their work for an elaborate explanation. These approaches outperform existing methods when the number of blocks is unknown a priori and we therefore compare SPLA to them.

Similar to Section 7.1, we simulate $s \in \{1, \ldots, 100\}$ samples $\mathbf{x}^{[\rho,s]}$ for $\rho \in \{0, 0.1, \ldots, 0.9\}$ with number of observations $N \in \{1000, 500, 100, 50, 20\}$. We compare the performance of the methods according to the identification rate and the results are illustrated in Figure 3.
Figure 3: Performance of the block-diagonal covariance structure detection by SHDJ, SHRR, and SPLA with $c_{CEC} = 0.6$ measured by the identification rate (the percentage of samples where all blocks were identified) on $s \in \{1, \ldots, 100\}$ samples $x^{[\rho,s]}$ for $\rho \in \{0, 0.1, \ldots, 0.7\}$ with number of observations $N \in \{1000, 500, 100, 50, 20\}$. Further, the CEC for each block is illustrated for the case when $N = 100$.

SPLA performs best for large sample sizes. The identification rate decreases for larger $\rho$ since the covariance matrix can no longer be considered to be a block-diagonal matrix due to the increasing correlation among variables. This is illustrated by the decreasing CEC. Still, we could increase identification rate by assuming a small CEC to be reasonable as well. This is illustrated in Figure 4 where the identification rate continues to be high for an increasing $\rho$. However, this demonstration of adapting $c_{CEC}$ is only given for completion since it might be useful for a different context. One should be aware that a small CEC might not reflect a reasonable block-structure as discussed in Section 6.

SHDJ and SHRR increase performance the smaller the sample size because they are nonasymptotic approaches. Further, they can also be applied for the case when $M > N$
Figure 4: Performance of the block-diagonal covariance structure detection by SPLA for \( c_{CEC} \in \{0.1, 0.2, 0.3, 0.4, 0.5, 0.6\} \) measured by the identification rate (the percentage of samples where all blocks were identified) on \( s \in \{1, \ldots, 100\} \) samples \( x^{[\rho|s]} \) for \( \rho \in \{0, 0.1, \ldots, 0.9\} \) with number of observations \( N \in \{500, 100, 20\} \). Identification rates for SHDJ are drawn to make the graphics comparable to Figure 3 which is not discussed for SPLA in this work.

7.3 Considerations about the Simulation Design

Simulations always face limitations due to their artificialness. However, there are further considerations due to the nature of SPLA. In the previous sections, we constructed a spiked covariance model \( (\text{Johnstone, 2001}) \) similar to \( \text{Zou et al., (2006)} \) and \( \text{Shen and Huang, (2008)} \) respectively to cause strong correlations within each block. The reason is that SPLA might rightfully split an intended block into several blocks if the within-block-correlation is small, making it difficult to analyse the obtained results. As an illustration, we simulated 1000 times the matrix \( A \in \mathbb{R}^{3 \times 3} \) by drawing each element \( a_{i,j} \) from a uniform \( U(0, 1) \) distribution. The covariance matrix \( \hat{\Sigma} = A^\top A \) was constructed accordingly and we consider the respective correlation matrix. By construction, the correlation matrix reflects three correlated variables. However, in Figure 5 we see that SPLA detected one, two, or three blocks respectively for different realisations. The CEC is small when SPLA detected one block (i.e. no split of the variables) and large for two or three blocks respectively which
Figure 5: Number of detected blocks by SPLA in relation to the CEC for simulated samples with correlation matrices obtained from the simulated covariance matrix $\hat{\Sigma} = A^T A$.

indicates that the found block-structure was reasonable.

Therefore, our simulations follow a spiked covariance model having a large within-block-correlation to ensure that an intended block cannot be interpreted as several blocks from a SPLA perspective.

8 Examples

We provide two examples for SPLA on real data and one example on synthetic data in this section. The first example in Section 8.1 mainly serves to illustrate detection of the underlying block covariance structure and results are compared to the ones obtained by PLA. In the second example in Section 8.2, the principal focus lies on variable selection by SPLA. Afterwards, we discuss a synthetic example from the sparse principal component analysis context in Section 8.3. Code to replicate all examples is provided in Supplementary Material 3.

8.1 OECD Sample

For the first example, we use data from Mankiw et al. (1992) that consist of $N = 22$ OECD countries with population larger than one million. The sample contains the real
GDP in 1960 ($Y_{60}$) and in 1985 ($Y_{85}$) per person of working age respectively. Further, it consists of the average annual ratios of real investment to GDP ($I/Y$), the percentage of working-age population that is in secondary school ($SCH$), the annual population growth from 1960 to 1985 ($POP$), and the average of annual ratios of gross domestic expenditure on research and development to nominal GDP ($RD$). Data are available in the CRAN contributed package **AER** by [Kleiber and Zeileis (2008)](http://cran.r-project.org/web/packages/AER). We standardized the sample i.e. we consider the correlation matrix rather than the covariance matrix because the variables have different scales.

The detected blocks by both PLA and SPLA are summarized in Table 1. A large number of blocks $K$ eases interpretation while a large CEC indicates that the block-structure represents the underlying sample. Therefore, splitting the OECD sample into the four blocks $\{I/Y\}$, $\{SCH\}$, $\{POP\}$, and $\{RD, Y_{85}, Y_{60}\}$ with CEC = 0.84 is an appropriate choice since this provides a reasonable as well as more detailed representation of the underlying sample. The corresponding sparse loadings which we obtain when performing SPLA according to Algorithm 1 are given in Table 2. In general, we continuously increase the sparseness of the loadings to find the underlying structure until the CEC indicates that sparseness is too large. This procedure is indicated in Table 1 where we stop with four blocks since five blocks result in a small CEC.

Note that PLA does not detect as many combinations as SPLA due to its nature of hard-thresholding. Further, PLA does not provide information to decide which number of blocks to choose. This is a concern because the detected blocks with $\tau = 0.5$ could be chosen which are a poor representation of the underlying sample according to the CEC.

Variable selection appears not to be feasible in this case, because no block has a small cumulative share of explained total variance and, therefore, there is no block that distorts
Table 1: Number of blocks $K$ of the OECD sample detected by PLA and SPLA. For PLA, we either provide the threshold $\tau$ or we denote $--$ if the structure cannot be identified by any threshold. For SPLA, we give the smallest CEC of all detected blocks to evaluate if the respective structure is reasonable.

| $K$ | Blocks | PLA | SPLA |
|-----|--------|-----|------|
| 2   | $\{I/Y, \text{POP}\}, \{\text{SCH, RD, Y85, Y60}\}$ | $--$ | 0.96 |
| 2   | $\{I/Y, \text{POP, SCH}\}, \{\text{RD, Y85, Y60}\}$ | 0.40 | 0.84 |
| 3   | $\{I/Y\}, \{\text{POP}\}, \{\text{SCH, RD, Y85, Y60}\}$ | $--$ | 0.96 |
| 3   | $\{\text{RD}\}, \{\text{Y85, Y60}\}, \{I/Y, \text{SCH, POP}\}$ | 0.50 | 0.53 |
| 4   | $\{I/Y\}, \{\text{POP}\}, \{\text{SCH}\}, \{\text{RD, Y85, Y60}\}$ | $--$ | 0.84 |
| 5   | $\{I/Y\}, \{\text{POP}\}, \{\text{SCH}\}, \{\text{RD}\}, \{\text{Y85, Y60}\}$ | $--$ | 0.45 |

the covariance matrix only a little. As discussed in Section 5 however, we have to be aware that the explained variance given by $R$ is biased. Following Algorithm 1, we therefore check the results using the partial covariance matrices. Instead of calculating the partial covariance matrix for all possible combinations $\sum_{m=1}^{6-1} \binom{6}{m} = 62$, we are now left with calculations for the three respective blocks. The partial covariance does not indicate that any block should be discarded either and the respective results can be found in Table 5 for completion.

### 8.2 EXAM Sample

The second example deals with the EXAM sample from Mardia et al. (1979), where we have access to grades of $N = 88$ students in a five part exam containing the subjects Mechanics ($mec$), Vectors ($vec$), Algebra ($alg$), Analysis ($ana$), and Statistics ($stat$). Each subject
Table 2: Sample sparse loadings $\hat{u}_i$ with $i \in \{1, \ldots, 6\}$ of the covariance matrix of the standardized OECD sample. All loading components equal to zero are left blank. $SV \equiv \hat{r}_{ii}^2 / \text{tr}(\hat{\Sigma})$ denotes the share of explained total variance (in percent), CV denotes the cumulative share of explained total variance for each block (in percent).

|     | $\hat{u}_1$ | $\hat{u}_2$ | $\hat{u}_3$ | $\hat{u}_4$ | $\hat{u}_5$ | $\hat{u}_6$ |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| I/Y | 1.00        |             |             |             |             |             |
| SCH |             | 1.00        |             |             |             |             |
| RD  |             |             | 1.00        |             |             |             |
| POP |             |             |             | 0.50        | -0.87       | 0.00        |
| Y85 |             |             |             | 0.64        | 0.36        | 0.68        |
| Y60 |             |             |             | 0.59        | 0.34        | -0.73       |
| CEC |             |             |             |             | 0.96        | 0.93        | 0.84        |
| SV  | 16.67       | 16.04       | 15.57       | 40.26       |             |             |
| CV  | 16.67       | 32.71       | 48.28       | 88.54       |             |             |

has been scored separately. The sample was taken from the CRAN contributed package bootstrap by Tibshirani (2019). Following the procedure in Algorithm 1, we obtain the results given in Table 3.

Due to the evaluation criteria of 0.74 and 0.72, we can conclude that the block-structure consisting of the three blocks $\{\text{vec}\}$, $\{\text{mec}\}$, and $\{\text{alg, ana, sta}\}$ reflects the EXAM sample well. Further, the shared explained total variance of $\{\text{vec}\}$ equals 13.21%. Since a single variable out of five should on average explain 20% and since the 13.27% are biased upwardly as discussed in Section 5, we consider to discard this variable. We verify or falsify this
Table 3: Sparse loadings $u_i$ with $i \in \{1, \ldots, 5\}$ of the covariance matrix of the EXAM sample. All loading components equal to zero are left blank. $SV \equiv r_{i,i}^2 / \text{tr}(\tilde{\Sigma})$ denotes the share of explained total variance (in percent), CV denotes the cumulative share of explained total variance for each block (in percent).

|   | $u_1$ | $u_2$ | $u_3$ | $u_4$ | $u_5$ |
|---|---|---|---|---|---|
| vec | 1.00 |   |   |   |   |
| mec | 1.00 |   |   |   |   |
| alg |   | -0.09 | -0.99 | 0.00 |   |
| ana |   | -0.65 | 0.06 | -0.756 |   |
| sta |   |   | -0.75 | 0.06 | 0.66 |
| CEC |   |   |   |   | 0.74 |
| SV  | 13.21 | 19.28 | 38.98 |   |   |
| CV  | 13.21 | 32.49 | 71.47 |   |   |

selection by checking the partial covariance matrix. Accordingly, the block $\{\text{vec}\}$ explains only 7.45% (Table 5) and discarding is verified.

8.3 Synthetic Example

We use an example based on Zou et al. (2006) and Shen and Huang (2008) to illustrate the block covariance structure detection of a synthetic sample. First, we consider a random vector $X = (X_1, \ldots, X_8)$ with $X_j = Z_1 + \theta_j$ for $j \in \{1, \ldots, 4\}$ and $X_j = Z_2 + \theta_j$ for $j \in \{5, \ldots, 8\}$. $Z_1$, $Z_2$, and the $\theta_j$ are independent and we let $Z_1 \sim N(0, 290)$, $Z_2 \sim N(0, 300)$ and $\theta_j \sim N(0, 1)$ for $j \in \{1, \ldots, 10\}$. A synthetic sample $x$ consisting of $N = 5000$
observations is generated accordingly. By construction, the sample consists of the two blocks \( \{ X_1, \ldots, X_4 \} \) and \( \{ X_5, \ldots, X_8 \} \). SPLA detects this underlying block-structure which is reflected by a CEC of 0.9998 (Table 4).

We extend the synthetic example and add the two random variables \( X_j = -0.3 \cdot Z_1 + 0.925 \cdot Z_2 + \theta_j \) for \( j \in \{9, 10\} \) to the random vector \( X = (X_1, \ldots, X_{10}) \). Both Zou et al. (2006) and Shen and Huang (2008) discuss the appropriate sparseness of the loadings. Hereby, Zou et al. (2006) use the knowledge about the synthetic sample while the approach of Shen and Huang (2008) is based on the explained variance of the most important loadings in a variance-sense. Expressing their results in SPLA-sense, they discuss if the loadings are of shape

\[
\begin{pmatrix}
*_{4 \times 4} & 0 & 0 \\
0 & *_{4 \times 4} & 0 \\
0 & 0 & *_{2 \times 2}
\end{pmatrix}
\quad \text{or} \quad
\begin{pmatrix}
*_{4 \times 4} & 0 \\
0 & *_{6 \times 6}
\end{pmatrix}
\]

respectively and therefore if the three blocks \( \{ X_1, \ldots, X_4 \} \), \( \{ X_5, \ldots, X_8 \} \) and \( \{ X_9, X_{10} \} \), or if the two blocks \( \{ X_1, \ldots, X_4 \} \) and \( \{ X_5, \ldots, X_{10} \} \) represent the random vector. From a SPLA-perspective, we clearly confirm the two-block-structure with a CEC of 0.9910 and results can be found in Table 4. The block \( \{ X_9, X_{10} \} \) in the three-block-scenario has a CEC of 0.0009 and we can therefore conclude that it is not adequate to split \( \{ X_1, \ldots, X_{10} \} \) into \( \{ X_5, \ldots, X_8 \} \) and \( \{ X_9, X_{10} \} \).

9 Concluding Remarks

We introduced SPLA as a new concept for variable selection and block covariance structure identification based on sparse loadings. We proposed how the sparse loadings can be used to identify the underlying block-structure, and gave criteria to evaluate if the detected
Table 4: Block indices $j$ for the $\{X_j\}$ of the synthetic examples given by $X = (X_1, \ldots, X_8)$ and $X = (X_1, \ldots, X_{10})$ respectively. CEC is the respective criterion for the blocks according to Remark 4.

| $X$ | $X = (X_1, \ldots, X_8)$ | $X = (X_1, \ldots, X_{10})$ |
|-----|----------------|----------------|
| $j$ | $\{1, \ldots, 4\}$ | $\{1, \ldots, 4\}$ | $\{1, \ldots, 4\}$ |
| CEC | 0.9998 | 0.9910 | 0.9998 | 0.0009 |

structure fits the covariance matrix. Regarding dimensionality reduction, calculation of the explained total variance is a concern and we provided an eligible measure to control the loss of explanatory power. Algorithm 1 can be used to apply SPLA for variable selection and block covariance structure identification in practice. The algorithm is available in the CRAN contributed package prinvars by Bauer and Holzapfel (2023).

Some improvements have to be addressed in future research. From an applied perspective, the choice of the method to calculate the sparse loadings needs to be discussed. This should address the computational speed by comparing existing methods that calculate sparse loadings. However, the methods need also be evaluated with respect to the created block-structure. From a theoretical perspective, considering how SPLA is related to the optimal variable selection based on the partial covariance matrix is of interest. While SPLA yields blocks that possibly explain only little of the overall variance, it is not clear yet how optimal these blocks are in a variable selection-sense.

There are methods to calculate sparse loadings that are stable in the high-dimensional setting. This motivates block covariance structure identification in the generalized spiked covariance model (Bai and Yao 2012) or the spiked population model (Johnstone 2001).
as a special case where the $M \times M$ population covariance matrix is assumed to be of form
\[
\begin{pmatrix}
\text{Cov}(X) & 0 \\
0 & V_{M'}
\end{pmatrix}
\]
where $M' = M - P$ and $M = M(N)$ such that $M/N \to \theta > 0 \ (N \to \infty)$. A natural extension of SPLA would be the identification of this block covariance structure in this high dimensional scenario.

Further, SPLA in time series analysis and functional data analysis is of interest. Let therefore $\{X_t\}_{t \in \mathcal{T}}$ be a stochastic process where $\mathcal{T}$ is discrete. In time series analysis, the autocovariance function $\gamma_X(s,t) \equiv \text{Cov}(X_s,X_t)$ gives the covariance with itself at pairs of time points. Further, weak stationarity of time series requires that $\gamma_X(h) \equiv \text{Cov}(X_t,X_{t+h})$ for $t,h \in \mathbb{Z}$ does not depend on time and therefore assumes that the autocovariance matrix consists of one block in a SPLA-sense. Hence, if the autocovariance matrix consists of several blocks, SPLA detects structural breaks where the weak stationary assumption is violated. On the other hand, SPLA can be used for functional (time) data analysis to detect time intervals that are less important from a variance perspective. This can be done by extending the concept of SPLA to the eigenfunctions of the covariance function of the underlying stochastic process.

A Complementary Results

This section provides complementary results about the partial covariance matrix for both examples discussed in Section 8.1 and Section 8.2 respectively.

Table 5 contains the trace of the sample partial covariance matrix for each of the identified blocks from Section 8. Considering the trace is in line with one of the measures given by McCabe (1984). Further, scaling the matrices by the overall explained variance
tr(\(\hat{\Sigma}\)) gives us the contribution of each block corrected by all remaining blocks in percent.

Table 5: Share of the total variance explained by the sample partial covariance matrix \(\hat{\Sigma}_{2,1}\) of the variables \(\{X_d\}\) eliminating the effects of the remaining variables \(\{X_k\}\) such that 
\(\{X_d\} \cup \{X_k\} = \{X_j\}_{j \in \{1,...,M\}}\) both for the OECD and for the EXAM sample respectively.

| \(D\)            | \(\frac{\text{tr}(\hat{\Sigma}_{2,1})}{\text{tr}(\hat{\Sigma})} \times 100\) | \(D\)            | \(\frac{\text{tr}(\hat{\Sigma}_{2,1})}{\text{tr}(\hat{\Sigma})} \times 100\) |
|------------------|---------------------------------|------------------|---------------------------------|
| \{I/Y\}          | 10.23                           | \{vec\}          | 7.45                            |
| \{SCH\}          | 12.41                           | \{mec\}          | 17.97                           |
| \{POP\}          | 12.94                           | \{alg, ana, sta\}| 46.49                           |
| \{RD, Y85, Y60\} | 41.73                           |                  |                                 |

SUPPLEMENTARY MATERIAL

1. Methods to calculate sparse loadings and weight matrix construction for Remark 4.
2. Simulation results
3. Examples
4. Proofs

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