sparseWeightBasedPCA Package

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`sparseWeightBasedPCA`: A package for Regularized weight based Simultaneous Component Analysis (SCA) and Principal Component Analysis (PCA)

Introduction

In this vignette we introduce an `R` package to perform regularized SCA and PCA with sparsity on the component weights, this package includes model selection procedures. The procedures developed are based on recent work by de Schipper and Van Deun. The main procedures of the package have been written in `C++` using Rcpp (Eddelbuettel and François 2011) and RcppArmadillo (Eddelbuettel and Sanderson 2014) to provide maximal efficiency of the underlying numerical computations. In this vignette we will introduce the reader to PCA and its multi-block extension SCA, followed by a substantiation of the models that the procedures in this package estimate. After that the `R` implementation of the package is discussed followed by detailed examples of data analysis and model selection.

Theoretical background

Principal Component Analysis

Principal component analysis (PCA) (Jolliffe 1986) is a widely used analysis technique for data reduction. It can give crucial insights in the underlying structure of the data when used as a latent variable model.

Let $\mathbf{X}$ be a data matrix that contains the scores for $i = 1...I$ objects on $j = 1...J$ variables — we follow the convention to present the J variable scores of observation i in row i, thus $\mathbf{X}$ has size $I \times J$ — PCA decomposes the data into Q components as follows,

$$\begin{aligned} &\mathbf{X} = \mathbf{X}\mathbf{W}\mathbf{P}^T + \mathbf{E} \\ &\text{subject to } \mathbf{P}^T\mathbf{P} = \mathbf{I}, \end{aligned} \tag{1}$$

where $\mathbf{W}$ is a $J \times Q$ component weight matrix, $\mathbf{P}$ is a $J \times Q$ loading matrix and $\mathbf{E}$ is a $I \times J$ residual matrix. The component weight matrix $\mathbf{W}$ will of main interest in this package, note that $\mathbf{T} = \mathbf{XW}$ represent the component scores.

The advantage of inspecting the component weights instead of the loadings is that you can directly derive meaning to $\mathbf{T}$, this because you see precisely in what way the items in $\mathbf{X}$ are weighted together by $\mathbf{W}$. The score on the qth component for object i is given by $t_{iq} = \sum_j w_{jq} x_{ij}$. Note that in Equation 1 the loadings are equal to the weights. This is not the case anymore when either the weights or loadings are penalized.

Simultaneous Component Analysis

The decomposition in (1) can be extended to the case of multi-block data by taking $\mathbf{X}_c = [\mathbf{X}_1 \dots \mathbf{X}_K]$; this is concatenating the K data blocks composed of different sets of variables of size J_k for the same units of observation. The decomposition of $\mathbf{X}_c$ has the same block structured decomposition as in (1) with $\mathbf{W}_c = [\mathbf{W}_1^T \dots \mathbf{W}_K^T]^T$ and $\mathbf{P}_c = [\mathbf{P}_1^T \dots \mathbf{P}_K^T]^T$. This multi-block formulation of PCA is known as the simultaneous component model:

$$\begin{aligned} &[\mathbf{X}_1 \dots \mathbf{X}_K] = [\mathbf{X}_1 \dots \mathbf{X}_K][\mathbf{W}_1^T \dots \mathbf{W}_K^T]^T[\mathbf{P}_1^T \dots \mathbf{P}_K^T] + \mathbf{E} \\ &\text{subject to } [\mathbf{P}_1^T \dots \mathbf{P}_K^T][\mathbf{P}_1^T \dots \mathbf{P}_K^T]^T = \mathbf{I}. \end{aligned} \tag{2}$$

When analyzing multi-block data with simultaneous component analysis (SCA), identifying meaningful relations between data blocks is of prime interest. In order to gain insight in how multiple data blocks relate to each other, we can search for block-wise structures in the component weights that tell us whether a component is uniquely determined by variables from one single data block (distinctive component), or whether it is a component that is determined by variables from multiple data blocks (common component). In other words, a distinctive component is a linear combination of variables of a particular data block only, whereas a common component is a linear combination of variables of multiple data blocks. An example of common and distinctive components with two data blocks is given below. The first two components are distinctive components, the third component is a common component,

$$\mathbf{T} = \begin{bmatrix}\mathbf{X}_1 & \mathbf{X}_2\end{bmatrix}\begin{bmatrix}\mathbf{W}_1 \\ \mathbf{W}_2\end{bmatrix} = \begin{bmatrix}\mathbf{X}_1 & \mathbf{X}_2\end{bmatrix}\begin{bmatrix} 0 & w_{1_1 2} & w_{1_1 3} \\ 0 & w_{2_1 2} & w_{2_1 3} \\ 0 & w_{3_1 2} & w_{3_1 3} \\ w_{1_2 1} & 0 & w_{1_2 3} \\ w_{2_2 1} & 0 & w_{2_2 3} \\ w_{3_2 1} & 0 & w_{2_2 3} \end{bmatrix}.$$

Content of the `sparseWeightBasedPCA`

The `sparseWeightBasedPCA` package provides functions that perform regularized PCA and SCA with regularization on the component weights. Furthermore the package will provide model selection procedures for the selection of the hyper parameters of the models. The core procedures of this package consist of the following functions:

1. `scads` Regularized SCA with common and distinctive component weights using constraints
2. `mmsca` Regularized SCA with common and distinctive component weights using the group LASSO
3. `ccpca` PCA with sparse component weights using cardinality constraints

Packages that provide similar functionality to the `sparseWeightBasedPCA` are: the elasticnet package (Zou and Hastie 2018) which provides sparse PCA for the component weights with ridge and LASSO regularization, the regularized SCA package (Gu and Van Deun 2018) which provides procedures for SCA/PCA with regularization on the loadings instead of the weights, sparse PCA using variable projection (Erichson et al. 2018) which also provides sparse PCA with regularization on the component weights with ridge and LASSO regularization including robust sparse PCA, the regularized PCA (Wang and Huang 2017) for sparse pca with spatial data, the mixOmics package (Rohart et al. 2017) that provides a sparse PCA function based on work from Shen and Huang (2008), penalized matrix decomposition package (Witten, Tibshirani, and Hastie

2009) that provides a penalized matrix decomposition with an application for sparse PCA. Note that this list is not exhaustive.

This packages is different from the aforementioned packages in that it provides functionality for SCA in order to analyze multi-block data for high-dimensional data with regularization on the component weights. It also provides procedures for model selection that can be applied to any sparse SCA/PCA procedure with regularization on the component weights, including procedures from other packages packages, albeit slightly modified.

Models of the `sparseWeightBasedPCA` package

Regularized SCA with sparse component weights using constraints

Here we present an approach of performing regularized SCA, with ridge and LASSO regularization and block wise constraints on $\mathbf{W}_c$ by solving,

$$\begin{aligned} L(\mathbf{W}_c, \mathbf{P}_c) = & \|\mathbf{X}_c - \mathbf{X}_c\mathbf{W}_c\mathbf{P}_c^T\|_2^2 + \lambda_L\|\mathbf{W}_c\|_1 + \lambda_R\|\mathbf{W}_c\|_2^2 \\ & \text{subject to } \mathbf{P}_c\mathbf{P}_c^T = \mathbf{I}, \text{ and } \lambda_L, \lambda_R \geq 0 \text{ and zero block constraints on } \mathbf{W}_c \end{aligned} \tag{3}$$

In order to get a minimum for (3) we alternate between the estimation of $\mathbf{W}_c$ and $\mathbf{P}_c$. Given $\mathbf{W}_c$ we can estimate $\mathbf{P}_c$ by using procruste rotation (Berge 1993; Zou, Hastie, and Tibshirani 2006), $\widehat{\mathbf{P}_c} = \mathbf{U}\mathbf{V}^T$, where $\mathbf{U}$ and $\mathbf{V}$ are the left and right singular vectors of $\mathbf{X}_c^T\mathbf{X}_c\widehat{\mathbf{W}}_c$. Given $\mathbf{P}_c$ we find estimates for $\mathbf{W}_c$ by using a coordinate descent algorithm that works by soft-thresholding the weights. For the specifics we refer the reader to (Schipper and Van Deun 2018). This iterative procedure stops when an optimum has been found (i.e. the loss function value is not decreasing anymore beyond pre-specified tolerance level). The optimization problem in (4) is non-convex and meaning there are local minima. In order to deal with local minima, multiple random starts can be used with different initializations of $\mathbf{W}_c$, the start leading to the lowest evaluation of (4) is retained. Typically starting the algorithm with the solution of PCA (e.g. the first Q right singular vectors of $\mathbf{X}_c$) will lead to smallest optimum.

The main advantage of analyzing multi-block data by using this procedure is that it is fast and scalable to large data sets thanks to the coordinate descent implementation. The inclusion of the block-wise constraints on $\mathbf{W}_c$ make sure common and distinctive components are found, the ridge and LASSO regularizers are optional and facilitate extra sparsity within the component weights. A disadvantage of the method is that the common and distinctive structure for $\mathbf{W}_c$ is not known beforehand thus need to be selected using model selection, this can be computationally demanding depending on the number of total common and distinctive structures that need to be assessed.

This procedure has been implemented in the `scads` function. This function will be discussed in detail in the next section and examples will be given outlining the analysis including model selection.

Regularized SCA with sparse component weights using the group LASSO

Here we present a very flexible approach of performing regularized SCA using, ridge, LASSO, group LASSO and elitist LASSO regularization by solving:

$$\begin{aligned} L(\mathbf{W}_c, \mathbf{P}_c) = & \|\mathbf{X}_c - \mathbf{X}_c\mathbf{W}_c\mathbf{P}_c^T\|_2^2 + \lambda_L\|\mathbf{W}_c\|_1 + \lambda_R\|\mathbf{W}_c\|_2^2 \\ & + \sum_{q,k}(\lambda_G\sqrt{J_k}\|\mathbf{w}_q^{(k)}\|_2 + \lambda_E\|\mathbf{w}_q^{(k)}\|_{1,2}) \\ & \text{subject to } \mathbf{P}_c\mathbf{P}_c^T = \mathbf{I} \text{ and } \lambda_L, \lambda_R, \lambda_G, \lambda_E \geq 0 \end{aligned} \tag{4}$$

where $\mathbf{W}_c = [(\mathbf{W}^{(1)})^T \ldots (\mathbf{W}^{(K)})^T]^T$, and $\mathbf{w}_q^{(k)}$ denotes the qth column from the submatrix $\mathbf{W}^{(k)}$. In order to get a minimum for (4) we alternate between the estimation of $\mathbf{W}_c$ and $\mathbf{P}_c$. Given $\mathbf{W}_c$ we can estimate $\mathbf{P}_c$ by using using procruste rotation (Berge 1993; Zou, Hastie, and Tibshirani 2006), $\widehat{\mathbf{P}_c} = \mathbf{U}\mathbf{V}^T$, where $\mathbf{U}$ and $\mathbf{V}$ are the left and right singular vectors of $\mathbf{X}_c^T\mathbf{X}_c\widehat{\mathbf{W}}_c$. Given $\mathbf{P}_c$ we can find estimates for $\mathbf{W}_c$ by using the majorization minimization (MM) algorithm. For the specific we refer the reader to (de Schipper & Van Deun, TBA). This iterative procedure stops when an optimum has been found (i.e. the loss function value is not decreasing anymore beyond pre-specified tolerance level). The optimization problem in (4) is non-convex and meaning there are local minima. In order to deal with that multiple random starts can be used with different initializations of $\mathbf{W}_c$, the start leading to the lowest evaluation of (4) is retained. Typically starting the algorithm with the solution of PCA (e.g. the first Q right singular vectors of $\mathbf{X}_c$) will lead to smallest optimum.

The main advantage analyzing multi-block data by using this procedure is that it can automatically look for common and distinctive components by taking advantage of the properties of the group LASSO. Because the group LASSO is specified on the colored segments (see below), it will either include these segments or put them zero, uncovering common and distinctive components. This is especially useful if the number of blocks and the number of components are substantial and an exhaustive is computationally too demanding.

$$\mathbf{T} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{X}_2 \end{bmatrix} \begin{bmatrix} \mathbf{W}_1 \\ \mathbf{W}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{X}_2 \end{bmatrix} \begin{bmatrix} w_{1_1 1} & w_{1_1 2} & w_{1_1 3} \\ w_{2_1 1} & w_{2_1 2} & w_{2_1 3} \\ w_{3_1 1} & w_{3_1 2} & w_{3_1 3} \\ w_{1_2 1} & w_{1_2 2} & w_{1_2 3} \\ w_{2_2 1} & w_{2_2 2} & w_{2_2 3} \\ w_{3_2 1} & w_{3_2 2} & w_{2_2 3} \end{bmatrix}$$

The inclusion the LASSO and ridge regularization are optional and facilitate extra sparsity within the colored segments. The elitist LASSO has a very special use case, the elitist LASSO will include all colored segments and will put weights within each segment to zero. The elitist lasso can be used to force components to be common. It is not advised to use the group LASSO and the elitist LASSO together as they have opposing goals. A disadvantage of using this procedure is that is potentially slow, this because its implemented using a MM-algorithm which tend to be slow in convergence.

This procedure has been implemented in the `mmsca` function. This function will be discussed in detail in the next section and examples will be given outlining the analysis including model selection.

PCA with sparse component weights using cardinality constraints

Here we present an approach of solving PCA by applying cardinality constraints to the component weights by solving:

$$\begin{aligned} &L(\mathbf{W}, \mathbf{P}) = \|\mathbf{X} - \mathbf{X}\mathbf{W}\mathbf{P}^T\|_2^2 \\ &\text{subject to } \mathbf{W} \text{ including } K \text{ zeros.} \end{aligned} \tag{5}$$

In order to get a minimum for (5) we need to alternate between the estimation of $\mathbf{W}$ and $\mathbf{P}$. Given $\mathbf{W}$ we can estimate $\mathbf{P}$ by using procruste rotation (Berge 1993; Zou, Hastie, and Tibshirani 2006), $\mathbf{P} = \mathbf{U}\mathbf{V}^T$, where $\mathbf{U}$ and $\mathbf{V}$ are the left and right singular vectors of $\mathbf{X}^T\mathbf{X}\widehat{\mathbf{W}}$. Given $\mathbf{P}$ we can find estimates for $\mathbf{W}$ given the cardinality constraints using the cardinality constraint regression algorithm for detail see (de Schipper & Van Deun TBA). The optimization problem in (5) is non-convex meaning there are local minima. In order to deal with that multiple random starts can be used with different initializations of $\mathbf{W}$, the start leading to the lowest evaluation of (5) is retained. Typically starting the algorithm with the solution of PCA (e.g. the first Q right singular vectors of $\mathbf{X}$) will lead to smallest optimum.

The main advantage of solving (5) is that this model tries to directly tackle the problem of finding the underlying subset of weights, in contrast to the usage of a penalty that shrinks the weights and also induces sparsity such as the LASSO. This approach can lead to better discovery of the underlying weights compared to LASSO (de Schipper & Van Deun TBA). Another advantage is that you directly impose cardinality constraints on $\mathbf{W}$. This gives the user total control over the amount of sparsity. This can be desirable if there is already an idea about the level of sparsity in the final model. A disadvantage of using this procedure is that is potentially slow, this because the cardinality constraint algorithm regression is an MM-algorithm which tend to be slow in convergence. Another potential downside could be the absence of regularizers, they tend to shrink the variance of the estimators leading to more efficiency. In noisy situations other procedures might outperform this procedure.

This model has been implemented in the `ccpca` function. This function will be discussed in detail in the next section.

The implementation in `R` of the `sparseWeightBasedPCA` package

The `sparseWeightBasedPCA` package provides functions for the aforementioned models. Model selection procedures are also provided in order to tune the hyper parameters. The main functions: `scads, mmsca` and `ccpca` are implemented in `C++` using the packages Rcpp (Eddelbuettel and François 2011) and RcppArmadillo (Eddelbuettel and Sanderson 2014). The model selection procedures are implemented in `R`. The functions of the package will be discussed after which detailed examples will be given.

Implementation of the main functions of the `sparseWeightBasedPCA` package

The main functions: `scads`, `mmsca` and `ccpca` are all implemented in a similar manor. At the core they perform SCA/PCA with variations depending on the goals of the user. An typical minimal example of `scads` given below (`mmsca` and `ccpca` are implemented very similarly) first generate some data:

```
J <- 30
I <- 100
X <- matrix(rnorm(I*J), I, J)
```

With this data `scads` can be run with supplied values for the minimal required arguments. This minimal example performs PCA, with no constraints and, ridge and LASSO regularization.

```
ncomp <- 3 # The number of components to estimate
constraints <- matrix(1, J, ncomp) # No constraints
res <- scads(X,
             ncomp = ncomp,
             ridge = 10e-8,
             lasso = rep(1, ncomp),
             constraints = constraints,
             Wstart = matrix(1, J, ncomp),
             itr = 10e5)
```

`scads`, `mmsca` and `ccpca` return a list with the following elements:

- `W` A matrix containing the component weights
- `P` A matrix containing the loadings
- `loss` A numeric variable containing the minimum loss function value of all the `nStarts` starts
- `converged` A boolean containing `TRUE` if the algorithm converged, `FALSE` if the algorithm did not converge

Details examples of data analysis will follow in the next section or see the documentation `?scads` et cetera. The main functions `scads`, `mmsca` and `ccpca` have a slightly different set of arguments. See the following lists for the specifics.

Overview of the `scads` arguments

- `X` A data matrix of class `matrix`
- `ncomp` The number of components to estimate (an integer)
- `ridge` A numeric value containing the ridge parameter for ridge regularization on the component weight matrix W
- `lasso` A vector containing a ridge parameter for each column of W separately, to set the same lasso penalty for the component weights W, specify: lasso = `rep(value, ncomp)`
- `constraints` A matrix of the same dimensions as the component weights matrix W (`ncol(X)}` x `ncomp`). A zero entry corresponds in constraints corresponds to an element in the same location in W that needs to be constraint to zero. A non-zero entry corresponds to an element in the same location in W that needs to be estimated.

- `itr` The maximum number of iterations (an integer)
- `Wstart` A matrix of `ncomp` columns and `nrow(X)` rows with starting values for the component weight matrix W, if `Wstart` only contains zeros, a warm start is used: the first `ncomp` right singular vectors of X
- `tol` The convergence is determined by comparing the loss function value after each iteration, if the difference is smaller than tol, the analysis is converged. The default value is `10e-8`.
- `nStarts` The number of random starts the analysis should perform. The first start will be performed with the values given by `Wstart`. The consecutive starts will be `Wstart` plus a matrix with random uniform values times the current start number (the first start has index zero).
- `printLoss` A boolean: `TRUE` will print the loss function value each 10th iteration.

Overview of the `mmsca` arguments

- `X` A data matrix of class `matrix`
- `ncomp` The number of components to estimate (an integer)
- `ridge` A vector containing a ridge parameter for each column of W separately, to set the same ridge penalty for the component weights W, specify: ridge = `rep(value, ncomp)`, value is a non-negative double
- `lasso` A vector containing a ridge parameter for each column of W separately, to set the same lasso penalty for the component weights W, specify: lasso = `rep(value, ncomp)`, value is a non-negative double
- `grouplasso` A vector containing a grouplasso parameter for each column of W separately, to set the same grouplasso penalty for the component weights W, specify: grouplasso = `rep(value, ncomp)`, value is a non-negative double
- `elitistlasso` A vector containing a elitistlasso parameter for each column of W separately, to set the same elitistlasso penalty for the component weights W, specify: elitistlasso = `rep(value, ncomp)`, value is a non-negative double
- `groups` A vector specifying which columns of `X` belong to what block. Example: `c(10, 100, 1000)`. The first 10 variables belong to the first block, the 100 variables after that belong to the second block etc.
- `constraints` A matrix of the same dimensions as the component weights matrix W (`ncol(X)` x `ncomp`). A zero entry corresponds in constraints corresponds to an element in the same location in W that needs to be constraint to zero. A non-zero entry corresponds to an element in the same location in W that needs to be estimated.
- `itr` The maximum number of iterations (a positive integer)
- `Wstart` A matrix of `ncomp` columns and `nrow(X)` rows with starting values for the component weight matrix W, if `Wstart` only contains zeros, a warm start is used: the first `ncomp` right singular vectors of `X`
- `tol` The convergence is determined by comparing the loss function value after each iteration, if the difference is smaller than `tol`, the analysis is converged. Default value is `10e-8`
- `nStarts` The number of random starts the analysis should perform. The first start will be performed with the values given by `Wstart`. The consecutive starts will be `Wstart` plus a matrix with random uniform values times the current start number (the first start has index zero).
- `printLoss` A boolean: `TRUE` will print the loss function value each 10th iteration.
- `coorDes` A boolean with the default `FALSE`. If coorDes is `FALSE` the estimation of the majorizing function to estimate the component weights W conditional on the loadings P will be found using matrix inverses which can be slow. If set to true the majorizing function will be optimized (or partially optimized) using coordinate descent, in many cases coordinate descent will be faster
- `coorDesItr` An integer specifying the maximum number of iterations for the coordinate descent algorithm, the default is set to 1. You do not have to run this algorithm until convergence before alternating back to the estimation of the loadings. The tolerance for this algorithm is hard coded and set to `10^-8`.

Overview of the `ccpca` arguments

- `X` A data matrix of class `matrix`
- `ncomp` The number of components to estimate (an integer)
- `nzeros` A vector of length `ncomp` containing the number of desired zeros in the columns of the component weight matrix `W`
- `itr` The maximum number of iterations (an integer)
- `Wstart` A matrix of `ncomp` columns and `nrow(X)` rows with starting values for the component weight matrix `W`, if `Wstart` only contains zeros, a warm start is used: the first `ncomp` right singular vectors of `X`
- `nStarts` The number of random starts the analysis should perform. The first start will be performed with the values given by `Wstart`. The consecutive starts will be `Wstart` plus a matrix with random uniform values times the current start number (the first start has index zero). The default value is 1.
- `tol` The convergence is determined by comparing the loss function value after each iteration, if the difference is smaller than `tol` the analysis is converged. The default value is `10e-8`
- `printLoss` A boolean: `TRUE` will print the loss function value each 10th iteration.

Implementation of the model selection functions of the `sparseWeightBasedPCA` package

The to execute the `scads`, `mmsca` and `ccpca` arguments for the hyper parameters need to selected. For example the number of components or values for the `lasso` arguments. The `sparseWeightBasedPCA` package provides three procedures for selecting the hyper-parameters of the model: Cross-validation using the EigenVector method, the Index of Sparseness (IS) and the Bayesian Information Criterion (BIC), for details see (de Schipper & Van Deun TBA). The procedures are implemented in the functions: `CVforPCAwithSparseWeights`, `ISforPCAwithSparseWeights` and `BICforPCAwithSparseWeights`. They are parametrized as follows: first come the arguments specific to the model selection function, followed by a pointer to the function (In `R` that is the function name with no brackets) that does the analysis, followed by arguments to that function. An example is given here:

```
J <- 30
I <- 100
X <- matrix(rnorm(I*J), I, J)
```

With this data, `CVforPCAwithSparseWeights` using `scads` works as follows,

```
ncomp <- 3
res <- CVforPCAwithSparseWeights(X = X,
                                 nrFolds = 10,
                                 FUN = scads, # Pointer to scads(), function name withou
                                 ncomp = ncomp, # Followed by the arguments
                                 ridge = 0,
                                 lasso = rep(0.1, ncomp),
                                 constraints = matrix(1, J, ncomp),
                                 Wstart = matrix(0, J, ncomp),
                                 itr = 10e5,
                                 printLoss = FALSE)
```

This function returns a list with the following elements:

- `MSPE` The mean squared prediction error given the tuning parameters
- `MSPEstdError` The standard error of the `MSPE`
- `nNonZeroCoef` The number of non-zero coefficients in the model

Model selection of the hyper-parameters can be based on the model that results in the lowest mean squared prediction error, or a model can be picked with the least number of non-zero coefficients still within one standard error of the model with the lowest mean squared prediction error. The other functions work similar, see `?BICforPCAwithSparseWeights` and `?ISforPCAwithSparseWeights` for more detailed information.

Additional tuning functions for mmsca

This package provides more elaborate model selection functions for `mmsca`. Because of its flexibility it can be overwhelming to use the basic tuning functions described in the previous section. Therefore two additional functions are provided: `mmscaModelSelection` and `mmscaHyperCubeSelection`. `mmscaModelSelection` uses a fixed grid of all combinations of the hyper-parameters to pick the best combination from, whereas `mmscaHyperCubeSelection` uses an adaptive grid that zooms in on a good combination of hyper-parameters until it converges on a certain combination. Note that `mmscaHyperCubeSelection` is experimental, it could potentially speed up the process of tuning enormously but it has not been scrutinized using a simulation study. A basic example of both is given here:

To perform model selection with `mmsca` using an exhaustive grid of all combinations of the tuning parameters the following can be done:

```r
J <- 30
I <- 100
X <- matrix(rnorm(I*J), I, J)

out <- mmscaModelSelection(X,
            ridgeSeq = seq(0, 1, by = 0.1), # Sequences of the hyper parameter
            lassoSeq = 0:100,
            grouplassoSeq = 0, # No group lasso and no elitist lasso
            elitistlassoSeq = 0,
            ncompSeq = 1:3,
            tuningMethod = "CV", # Indicate the tuning method
            nrFolds = 10,
            groups = ncol(X), # Arguments for mmsca()
            itr = 100000,
            nStart = 1,
            coorDes = FALSE,
            coorDesItr = 100,
            printProgress = TRUE)
```

This function returns a list with two elements:

- `results` A list with `ncomp` elements each containing the following elements
  - `"BIC, IS or MSPE"` The index chosen in tuningMethod for all combinations of ridge, lasso, grouplasso and elististlasso
  - `"bestBIC, bestIS, bestMSPE or bestMSPE1stdErrorRule"` The best index according to the chosen tuning method
  - `"nNonZeroCoef"` The number of non zero weights in the best model
  - `"ridge"` The value of the ridge penalty corresponding to the best model
  - `"lasso"` The value of the lasso penalty corresponding to the best model
  - `"grouplasso"` The value of the group lasso penalty corresponding to the best model
  - `"elististlasso"` The value of the elitist lasso penalty corresponding to the best model
  - `"ncomp"` The number of component that was used for these items
  - `"ridge1stdErrorRule"` In case tuningMethod == "CV", the value of the ridge penalty according to the 1 standard error rule: the most sparse model within one standard error of the model with the lowest MSPE
  - `"lasso1stdErrorRule"` In case tuningMethod == "CV", the value of the lasso penalty according to the 1 standard error rule: the most sparse model within one standard error of the model with the lowest MSPE
  - `"grouplasso1stdErrorRule"` In case tuningMethod == "CV", the value of the group lasso penalty according to the 1 standard error rule: the most sparse model within one standard error of the model with the lowest MSPE
  - `"elitistlasso1stdErrorRule"` In case tuningMethod == "CV", the value of the elitist lasso

penalty according to the 1 standard error rule: the most sparse model within one standard error of the model with the lowest MSPE
    - `"ridge1stdErrorRule"` In case tuningMethod == "CV", the value of the ridge according to the 1 standard error rule: the most sparse model within one standard error of the model with the lowest MSPE
- `bestNcomp` The number of component with the best value for the chosen tuning index

For more details `?mmscaModelSelection`. This procedure can be slow because the number of combinations can be great it takes a lot of time to evaluate them all in order to pick the best one. To that end we also provide an alternative way of tuning using `mmscaHyperCubeSelection`. This function tunes a grid of the tuning parameters determined by the min and max of their corresponding sequences and a step size the provided by `stepsize` argument. It picks out the best combination of that grid, and zooms in on that combination, by making a new, smaller grid around the previous best combination. This process continues until the average range of the sequences is less than a specified criterion. The new sequences are determined by taking the minimum value to be: best value - range, and maximum value by: best value + range, and a pre-specified step size in `stepsize`. In order for this procedure to work well, the grid needs to include an optimal combination of tuning parameters, and it needs a reasonable step size (at least 3, 5 is better, 2 is too small). This approach assumes that a local optimum of tuning parameters is good enough to get interpretable results. Note that this function is experimental and has not been scrutinized using a simulation study.

This procedure can be performed as follows,

```
out <- mmscaHyperCubeSelection(X,
              ncomp = 3, # This function works with a fixed number of components
              ridgeSeq = 0:3,
              lassoSeq = 0:10,
              grouplassoSeq = 0,
              elitistlassoSeq = 0,
              stepsize = 5, # Step size of the sequences
              logscale = FALSE, # Sequences can be on the log-scale
              stopWhenRange = 0.01, # stop when average range is < 0.01
              method = "CV1stdError", # Tuning method
              groups = ncol(X), # Arguments for mmsca()
              nStart = 1,
              itr = 100000,
              printProgress = TRUE,
              coorDes = FALSE,
              coorDesItr = 1,
              tol = 10e-5,
              nrFolds = 10)
```

This function returns a list with the following elements:

- `ridge` A vector with `ncomp` elements all equal to the chosen ridge value
- `lasso` A vector with `ncomp` elements all equal to the chosen lasso value
- `grouplasso` A vector with `ncomp` elements all equal to the chosen group lasso value
- `elitistlasso` A vector with `ncomp` elements all equal to the chosen elitist lasso value

For more details see `?mmscaHyperCubeSelection`.

Detailed examples of SCA and PCA with the `sparseWeightBasedPCA` package

In this section we will give some detailed examples where we analyze multi- and single block data with SCA and PCA including the model selection process. We given an examples of `scads`, `mmsca` and `ccpca` and the model selection functions. We will demonstrate these procedures using simulated data, for that purpose the package includes data generating functions that simulate data according to the following structure:

$$\mathbf{X} = \mathbf{XWP}^T, \tag{6}$$

where $\mathbf{W}$ is $J \times J$, $\mathbf{W}^T\mathbf{W} = \mathbf{I}$ and $\mathbf{W} = \mathbf{P}$. $\mathbf{W}$ is manipulated such that it contains a specified level of sparsity in the first Q columns. The covariance matrix of $\mathbf{X}$ can be constructed by taking $\mathbf{\Sigma} = \mathbf{W}\mathbf{\Lambda}\mathbf{W}^T$, the eigenvalues in $\mathbf{\Lambda}$ can be manipulated to control the variance of the signal components versus the variance of the noise components. Using the covariance matrix data can be sampled from the multivariate normal distribution using `mvrnorm` from the `MASS` package (Venables and Ripley 2002). Functions for data generation are provided by:

- `sparsify` to put sparsity in $\mathbf{W}$
- `makeVariance` to manipulate the eigenvalues in $\mathbf{\Lambda}$
- `makeDat` to simulate the data.

Check the package documentation for more details. In general data are not simulated and need to be pre-processed before hand. The `RegularizedSCA` package (Gu and Van Deun 2018) provides functionality for this with `pre_process`, see their documentation for more details.

Example of SCA with `scads`

Here we will demonstrate data analysis using `scads`. In this example we will have 2 data blocks each with 15 variables and 3 components. First we create a common and distinctive structure for the component weights to generate data from, we will use a structure with 2 distinctive components and 1 common component.

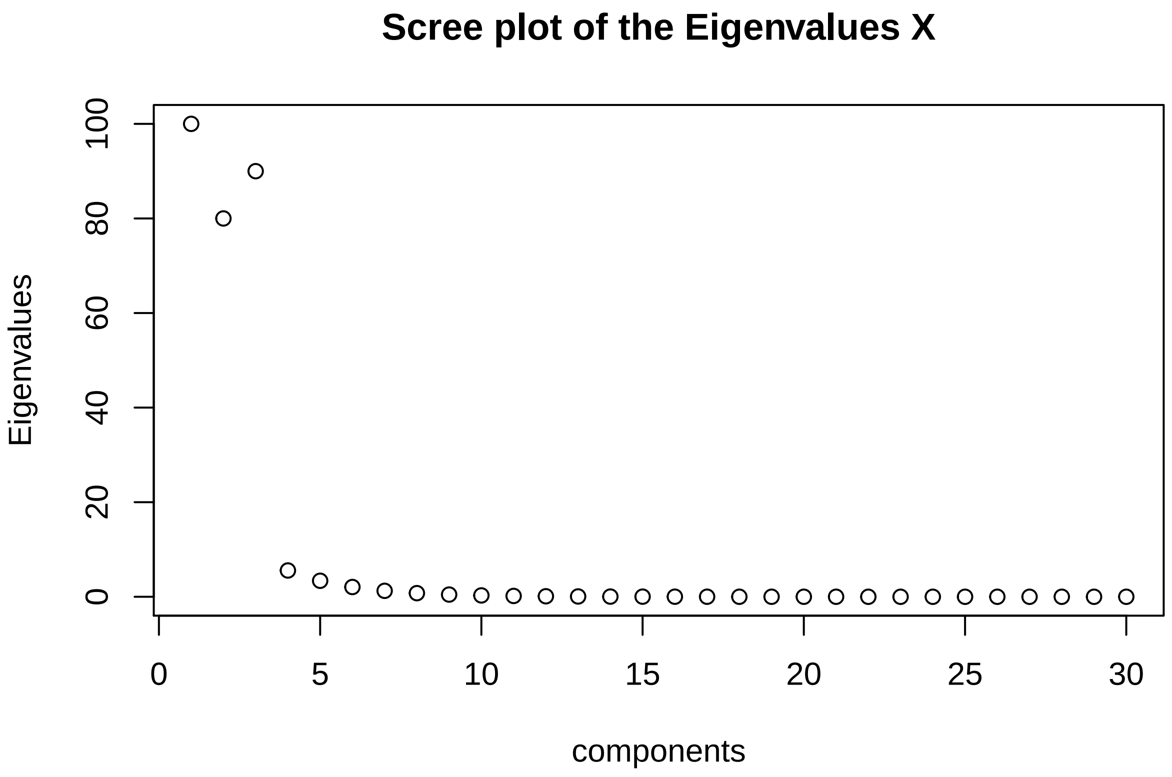
```r
set.seed(1)
ncomp <- 3
J <- 30
comdis <- matrix(1, J, ncomp) # Component weight structure
comdis[1:15, 1] <- 0 # The first component is distinctive for the first block
comdis[16:30, 2] <- 0 # The second component is distinctive for the second block
comdis <- sparsify(comdis, 0.2) #set 20 percent of the 1's to zero

# inspect the component weight structure, weights indicated with a 1,
# will in the data generating model
comdis
```

```
##       [,1] [,2] [,3]
##  [1,]    0    0    0
##  [2,]    0    0    1
##  [3,]    0    1    1
##  [4,]    0    1    1
##  [5,]    0    1    1
##  [6,]    0    1    1
##  [7,]    0    1    1
##  [8,]    0    1    1
##  [9,]    0    1    1
## [10,]    0    1    1
## [11,]    0    1    0
## [12,]    0    1    1
## [13,]    0    0    1
## [14,]    0    1    0
## [15,]    0    1    1
## [16,]    1    0    1
## [17,]    1    0    1
## [18,]    1    0    0
## [19,]    0    0    0
## [20,]    1    0    1
## [21,]    1    0    1
## [22,]    0    0    1
## [23,]    1    0    0
## [24,]    0    0    1
## [25,]    1    0    1
## [26,]    1    0    1
## [27,]    1    0    1
## [28,]    1    0    1
## [29,]    1    0    1
## [30,]    1    0    1
```

Now given this component weight structure we can simulate data as follows,

```
variances <- makeVariance(varianceOfComps = c(100, 80, 90),
                          J = J, error = 0.05) #create realistic eigenvalues
plot(variances, xlab ="components",
     ylab ="Eigenvalues", main = "Scree plot of the Eigenvalues X")
```



```
dat <- makeDat(n = 100, comdis = comdis, variances = variances)
X <- dat$X
round(dat$P[, 1:ncomp], 3) # The data generating component weight structure
```

```
##         [,1]   [,2]   [,3]
##  [1,]  0.000  0.000  0.000
##  [2,]  0.000  0.000  0.072
##  [3,]  0.000 -0.082 -0.004
##  [4,]  0.000  0.517  0.149
##  [5,]  0.000  0.165  0.121
##  [6,]  0.000 -0.133 -0.226
##  [7,]  0.000 -0.245 -0.103
##  [8,]  0.000 -0.343  0.098
##  [9,]  0.000 -0.313  0.233
## [10,]  0.000 -0.460 -0.086
## [11,]  0.000  0.340  0.000
## [12,]  0.000  0.245 -0.197
## [13,]  0.000  0.000 -0.418
## [14,]  0.000  0.078  0.000
## [15,]  0.000 -0.111  0.334
## [16,]  0.054  0.000  0.208
## [17,]  0.326  0.000 -0.162
## [18,] -0.023  0.000  0.000
## [19,]  0.000  0.000  0.000
## [20,]  0.441  0.000  0.158
## [21,] -0.280  0.000  0.004
## [22,]  0.000  0.000  0.365
## [23,]  0.019  0.000  0.000
## [24,]  0.000  0.000  0.378
## [25,] -0.220  0.000 -0.188
## [26,] -0.176  0.000  0.055
## [27,] -0.264  0.000 -0.177
## [28,]  0.295  0.000  0.085
## [29,]  0.468  0.000 -0.105
## [30,]  0.403  0.000 -0.203
```

In the scree plot you can see the eigenvalues of the data generating covariance matrix and `round(dat$P[, 1:ncomp], 3)` prints the data generating component weights for the signal components.

Given this generate data set we can perform `scads` by first looking for the common and distinctive structure by trying all structures out and finding the best structure according to model selection, in this case we will use cross-validation. To generate all common and distinctive structures we implemented a function called `allCommonDistinctive` for more details see the documentation.

```
# Generate all possible common and distinctive structures
allstructures <- allCommonDistinctive(vars = c(15, 15),
                      ncomp = 3, allPermutations = TRUE, filterZeroSegments = TRUE)

#Use cross-validation to look for the data generating structure
index <- rep(NA, length(allstructures))
for (i in 1:length(allstructures)) {
    index[i] <- CVforPCAwithSparseWeights(X = X, nrFolds = 10, FUN = scads,
                         ncomp, ridge = 0, lasso = rep(0, ncomp),
                         constraints = allstructures[[i]], Wstart = matrix(0, J, ncomp),
                         itr = 100000, nStarts = 1, printLoss = FALSE, tol = 10^-5)$MSPE
}

winningStructure <- allstructures[[which.min(index)]]
allstructures[[which.min(index)]] # print the best common and distinctive structure
```

Given this common and distinctive structure we can tune the `lasso` parameter in order to get some sparsity inside the weights, for this we will use cross-validation with the one standard error rule. This entails cross validating the model a bunch of times for different values of the `lasso` parameter, from which we will select the model with the most weights at zero still within one standard error of the model with the lowest mean squared prediction error (MSPE). If there are no models within one standard error of the best model you should decrease the step size of the LASSO sequence.

```
# Generate candidate lasso values on the log-scale
lasso <- exp(seq(log(0.0000001), log(1), length.out = 100))
MSPE <- rep(NA, length(lasso))
MSPEstdError <- rep(NA, length(lasso))
```

```r
nNonZeroCoef <- rep(NA, length(lasso))

for (i in 1:length(lasso)) {
    res <- CVforPCAwithSparseWeights(X = X, nrFolds = 10, FUN = scads,
                                     ncomp, ridge = 0, lasso = rep(lasso[i], ncomp),
                                     constraints = winningStructure, Wstart = matrix(0, J, ncomp),
                                     itr = 100000, nStarts = 1, printLoss = FALSE, tol = 10^-5)
    MSPE[i] <- res$MSPE # Store MSPE for each lasso value
    MSPEstdError[i] <- res$MSPEstdError # Store the standard error of the MSPE
    nNonZeroCoef[i] <- res$nNonZeroCoef # Store the number of non-zero weights
}

x <- 1:length(lasso)
plot(x , MSPE, xlab = "lasso", ylab = "MSPE",
     main = "MSPE with one standard error for different lasso values")

# Add error bars to the plot
arrows(x, MSPE - MSPEstdError, x , MSPE + MSPEstdError, length = 0.05, angle = 90, code = 3)

# Select all models within one standard error of the best model
eligibleModels <- MSPE < MSPE[which.min(MSPE)] + MSPEstdError[which.min(MSPE)]

# Selected from those models the models with the lowest number of non-zero weights
best <- which.min(nNonZeroCoef[eligibleModels])

# Do the analysis with the "winning" structure and best lasso
results <- scads(X = X, ncomp = ncomp,
                ridge = 0, lasso = rep(lasso[best], ncomp),
                constraints = allstructures[[which.min(index)]],
                Wstart = matrix(0, J, ncomp),
                itr = 100000, nStarts = 1, printLoss = FALSE , tol = 10^-5)

# Compare results from the analysis with the data generating model
compare <- cbind(dat$P[, 1:ncomp], results$W)
colnames(compare) <- c(paste("True W_", 1:3, sep = ""), paste("Est W_", 1:3, sep = ""))
rownames(compare) <- paste("Var", 1:30)
round(compare, 3)
```

This concludes the analysis of multi-block data with `scads`. This procedure offers lots of flexibility to the user at the cost of a little more complexity (i.e. the user has to know for-loops and some `R` basics). Note that the model selection procedures can be easily sped up making use of parallel versions of the for-loops.

Example of SCA with `mmsca`

We will now demonstrate data analysis of multi-block data using `mmsca`. In this example we will use the same data as in the `scads` example. We will demonstrate the use of `mmscaHyperCubeSelection` as already for this toy-example tuning an exhaustive grid with `mmscaModelSelection` takes too long. We use cross validation with the one standard error rule.

```r
# Tune the hyper parameters by looking at an adaptive grid that zooms in around plausible values
out <- mmscaHyperCubeSelection(X,
              ncomp = 3,
              ridgeSeq = 0, # No ridge
              lassoSeq = 0:10, # Lasso from 0 to 10
              grouplassoSeq = 0:10,  # Lasso from 0 to 10
              elitistlassoSeq = 0, # No elitist lasso
              stepsize = 3,
              logscale = FALSE,
              stopWhenRange = 0.01, # Stop when average range is < 0.01
              groups = c(15, 15),
              nStart = 1,
              itr = 100000,
              printProgress = FALSE,
              coorDes = FALSE,
              coorDesItr = 1,
              method = "CV1stdError",
              tol = 10e-5,
              nrFolds = 10)

# Inspect the chosen hyper parameters
out

# Run the analysis with the chosen hyper parameters
results <- mmsca(X = X,
            ncomp = ncomp,
            ridge = out$ridge,
            lasso = out$lasso,
            grouplasso = out$grouplasso,
            elitistlasso = out$elitistlasso,
            groups = c(15, 15),
            constraints = matrix(1, J, ncomp),
            itr = 1000000,
            Wstart = matrix(0, J, ncomp),
            nStarts = 1,
            printLoss = FALSE)

# Compare results from the analysis with the data generating model
compare <- cbind(dat$P[, 1:ncomp], results$W)
colnames(compare) <- c(paste("True W_", 1:3, sep = ""), paste("Est W_", 1:3, sep = ""))
rownames(compare) <- paste("Var", 1:30)
round(compare, 3)
```

This conclude the demonstration. We now demonstrate another interesting use case for `mmsca` where a researcher wants to identifying common and distinctive components and where an exhaustive approach might fail because there are too many data blocks and components. We use multi-block data with 5 blocks and 5 variables per block and 5 components.

```
# Generate the data
set.seed(1)
ncomp <- 5
J <- 30
comdis <- matrix(0, J, ncomp) # Component weight structure
comdis[1:5, 1] <- 1
comdis[6:10, 2] <- 1
comdis[25:30, 3] <- 1
comdis[11:15, 4] <- 1
comdis[0:10, 5] <- 1
comdis[16:30, 5] <- 1
```

```r
# check the generated component weight structure
comdis

# Generate data according to that structure
variances <- makeVariance(varianceOfComps = c(100, 80, 90, 50, 60),
                          J = J, error = 0.05) #create realistic eigenvalues

dat <- makeDat(n = 100, comdis = comdis, variances = variances)
X <- dat$X

# Tune the group lasso parameter
out <- mmscaHyperCubeSelection(X,
              ncomp = ncomp,
              ridgeSeq = 0, # No ridge
              lassoSeq = 0, # No lasso
              grouplassoSeq = 0:10,  # Lasso from 0 to 10
              elitistlassoSeq = 0, # No elitist lasso
              stepsize = 3,
              logscale = FALSE,
              stopWhenRange = 0.01, # Stop when average range is < 0.01
              groups = c(5, 5, 5, 5, 5, 5),
              nStart = 1,
              itr = 100000,
              printProgress = FALSE, # When doing analysis set this to TRUE
              coorDes = FALSE,
              coorDesItr = 1,
              method = "CV1stdError",
              tol = 10e-5,
              nrFolds = 10)

# Inspect the chosen group lasso
out$grouplasso

# Run the analysis
results <- mmsca(X = X,
                ncomp = ncomp,
                ridge = out$ridge,
                lasso = out$lasso,
                grouplasso = out$grouplasso,
                elitistlasso = out$elitistlasso,
                groups = c(5, 5, 5, 5, 5, 5),
                constraints = matrix(1, J, ncomp),
                itr = 1000000,
                Wstart = matrix(0, J, ncomp),
                nStarts = 1,
                printLoss = FALSE)


# Check results from the analysis
colnames(results$W) <- paste("Est W_", 1:5, sep = "")
rownames(results$W) <- paste("Var", 1:30)
round(results$W, 3)
```

```r
# You can compare them to the data generating structure
round(dat$P[, 1:ncomp], 3)
```

The data generating structure has been estimated back fairly well. Note not all segments have been recovered. If a segments does not really contribute or only contributes marginally to the signal variance, it can be put to zero by the group lasso. You can also notice some small coefficients still being estimated, if you increase the `grouplasso` these small coefficients will be put to zero.

Example of PCA with `ccpca`

Here we will demonstrate data analysis using `ccpca`. In this example we will have just 1 data blocks each with 30 variables and 3 components. Here we demonstrate the use case for `ccpca` where the underlying model is rather sparse, and we already assume the model is sparse and we ball park the sparsity.

```r
set.seed(1)
ncomp <- 3
J <- 30
comdis <- matrix(1, J, ncomp) # Component weight structure
comdis <- sparsify(comdis, 0.8) #set 80 percent of the 1's to zero
comdis

variances <- makeVariance(varianceOfComps = c(100, 80, 90),
                          J = J, error = 0.05) #create realistic eigenvalues
dat <- makeDat(n = 100, comdis = comdis, variances = variances)
X <- dat$X
round(dat$P[, 1:ncomp], 3) # The data generating component weight structure

# We can ball park the number of zeros and can get pretty good results
results <- ccpca(X = X, ncomp = ncomp,  nzeros = c(20, 20, 20), itr = 10000000,
   Wstart = matrix(0, J, ncomp), nStarts = 1, tol = 10^-8, printLoss = FALSE)

# Compare the results
compare <- cbind(dat$P[, 1:ncomp], results$W)
colnames(compare) <- c(paste("True W_", 1:3, sep = ""), paste("Est W_", 1:3, sep = ""))
rownames(compare) <- paste("Var", 1:30)
round(compare, 3)
```

The estimation results are similar to the data generating model, this shows you do not have to know the number of zero weights before hand in order to get interpretable results. That being said, it should preferably in the ball park of what it should really be. In order to examine that in more detail we will now provide an example of model selection with `ccpca` also in this example we use cross-validation with the one standard error rule.

```r
# Cross validate the number of non-zero weights per component weight vector
# Note: we assume the sparsity within the columns of W to be the same
nzeros <- rep(15:29, each = ncomp)
nzeros <- split(nzeros, ceiling(seq_along(nzeros) / ncomp))

MSPE <- rep(NA, length(nzeros))
MSPEstdError <- rep(NA, length(nzeros))
nNonZeroCoef <- rep(NA, length(nzeros))

for (i in 1:length(nzeros)) {
    res <- CVforPCAwithSparseWeights(X = X, nrFolds = 10, FUN = ccpca,
                 ncomp = ncomp,  nzeros = nzeros[[i]], itr = 10000000,
                   Wstart = matrix(0, J, ncomp), nStarts = 1, tol = 10^-5, printLoss = FALSE)

    MSPE[i] <- res$MSPE # Store MSPE for each lasso value
    MSPEstdError[i] <- res$MSPEstdError # Store the standard error of the MSPE
    nNonZeroCoef[i] <- res$nNonZeroCoef # Store the number of non-zero weights
}


x <- 15:29
plot(x , MSPE, xlab = "number of zeros", ylab = "MSPE",
     main = "MSPE with one standard error for different lasso values")

# Add error bars to the plot
arrows(x, MSPE - MSPEstdError, x , MSPE + MSPEstdError, length = 0.05, angle = 90, code = 3)

# Select all models within one standard error of the best model
eligibleModels <- MSPE < MSPE[which.min(MSPE)] + MSPEstdError[which.min(MSPE)]
eligibleModels

# Selected from those models the models with the lowest number of non-zero weights
best <- which.min(nNonZeroCoef[eligibleModels])

# The number of zero weights per component that was "best"
nzeros[[best]]

results <- ccpca(X = X, ncomp = ncomp,  nzeros = nzeros[[best]], itr = 10000000,
   Wstart = matrix(0, J, ncomp), nStarts = 1, tol = 10^-8, printLoss = FALSE)


compare <- cbind(dat$P[, 1:ncomp], results$W)
colnames(compare) <- c(paste("True W_", 1:3, sep = ""), paste("Est W_", 1:3, sep = ""))
rownames(compare) <- paste("Var", 1:30)
round(compare, 3)
```

Doing the model selection procedure gives the user a pretty good idea what number of zero weights is plausible. The results of the estimation using cross-validation with the one standard error rule are very similar the to one where we ball parked the number of zero weights.

Conclusion

The `sparseWeightBasedPCA` provides flexible analysis tools to perform SCA and PCA on multi- or single block data with sparsity in the component weights. Model selection tools are provided to select the hyper-parameters of these models. Future research, should focus on selecting the regularization parameters together with the number of components. Although doable with this package it is still too computationally demanding for most practical use cases, the user is better of sticking to using a scree-plots or use `CVforPCAwithSparseWeights` to determine the number of components before tuning the other hyper parameters. Furthermore this package includes `mmscaHyperCubeSelection` a promising procedure of doing model selection because of its speed and ability to examine an enormous grid of potential candidate values for the hyper parameter, however it still needs to be properly examined using a simulation study in further research.

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