# Package 'PMA2' 

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## Description

A modified version of PMA. The CCA() and CCA.permute() functions can also compute the component-wise standard deviations of estimated U and V through
permutations in addition to standardize them. Furthermore, it computes
the non-parametric p-values for each components.
Performs Penalized Multivariate Analysis: a penalized matrix decomposition, sparse principal components analysis, and sparse canonical correlation analysis, described in Ali Mahzarnia, Alexander Badea (2022), ‘Joint Estimation of Vulnerable Brain Networks and Alzheimer's Disease Risk Via Novel Extension of Sparse Canonical Correlation" at bioRxiv.

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PMA-package Penalized Multivariate Analysis

## Description

This package is called PMA, for __P__enalized __M__ultivariate __A__nalysis. It implements three methods: A penalized matrix decomposition, sparse principal components analysis, and sparse canonical correlations analysis. All are described in the reference below. The main functions are: PMD, CCA and SPC.

## Details

The first, PMD, performs a penalized matrix decomposition. CCA performs sparse canonical correlation analysis. SPC performs sparse principal components analysis.
There also are cross-validation functions for tuning parameter selection for each of the above methods: SPC.cv, PMD.cv, CCA.permute. And PlotCGH produces nice plots for DNA copy number data.

## References

Ali Mahzarnia, Alexander Badea (2022), Joint Estimation of Vulnerable Brain Networks and Alzheimer's Disease Risk Via Novel Extension of Sparse Canonical Correlation at bioRxiv.

## breastdata Breast cancer gene expression + DNA copy number data set from Chin

 et. al. and used in Witten, et. al. See references below.
## Description

This data set consists of gene expression and DNA copy number measurements on a set of 89 samples. The data set can be used to perform integrative analysis of gene expression and DNA copy number data, as in. That is, we can look for sets of genes that are associated with regions of chromosomal gain/loss.
Must be downloaded from https://github.com/Ali-Mahzarnia/PMA2/ and put into the folder PMA/data

## Format

The format is a list containing the following elements: - dna: a 2149 x 89 matrix of CGH spots x Samples - rna: a 19672x89 matrix of Genes x Samples - chrom: a 2149-vector of chromosomal location of each CGH spot - nuc: a 2149 -vector of nucleotide position for each CGH spot - gene: a 19672-vector wiith an accession number for each gene - genenames: a 19672-vector with a name for each gene - genechr: a 19672-vector with a chromosomal location for each gene - genedesc: a 19672-vector with a description for each gene - genepos: a 19672-vector with a nucleotide position for each gene

## Details

Missing values were imputed using 5-nearest neighbors (see library pamr).

## References

Ali Mahzarnia, Alexander Badea (2022), Joint Estimation of Vulnerable Brain Networks and Alzheimer's Disease Risk Via Novel Extension of Sparse Canonical Correlation at bioRxiv.

## Examples

```
data(breastdata)
attach(breastdata)
PlotCGH(dna[,1], chrom=chrom, main="Sample 1", nuc=nuc)
detach(breastdata)
```

Perform sparse canonical correlation analysis using the penalized matrix decomposition.

## Description

This is a function of a modification version of the PMA package. Given matrices X and Z , which represent two sets of features on the same set of samples, find sparse $u$ and $v$ such that $u^{\prime} X^{\prime} Z v$ is large. For X and Z , the samples are on the rows and the features are on the columns. X and Z must have same number of rows, but may (and usually will) have different numbers of columns. The columns of X and/or Z can be unordered or ordered. If unordered, then a lasso penalty will be used to obtain the corresponding canonical vector. If ordered, then a fused lasso penalty will be used; this will result in smoothness. In addition, this function would report the component-wise estimated standard deviation of each U and V component and standardize them accordingly. The package also computes the non-parametric p-values of the components of $u$ and $v$ based on the permutations.

```
Usage
    CCA(
        x,
        z,
        typex = c("standard", "ordered"),
        typez = c("standard", "ordered"),
        penaltyx = NULL,
        penaltyz = NULL,
        K = 1,
        niter = 15,
        v = NULL,
        trace = TRUE,
        standardize = TRUE,
        xnames = NULL,
        znames = NULL,
        chromx = NULL,
        chromz = NULL,
        upos = FALSE,
        uneg = FALSE,
        vpos = FALSE,
        vneg = FALSE,
        outcome = NULL,
        y = NULL,
        cens = NULL,
        UVperms=NA,
        allpenaltyxs=NA
    )
```


## Arguments

x
z
typex Are the columns of $x$ unordered (type="standard") or ordered (type="ordered")? If "standard", then a lasso penalty is applied to $u$, to enforce sparsity. If "ordered" (generally used for CGH data), then a fused lasso penalty is applied, to enforce both sparsity and smoothness.
typez Are the columns of z unordered (type="standard") or ordered (type="ordered")? If "standard", then a lasso penalty is applied to v , to enforce sparsity. If "ordered" (generally used for CGH data), then a fused lasso penalty is applied, to enforce both sparsity and smoothness.
penaltyx The penalty to be applied to the matrix $x$, i.e. the penalty that results in the canonical vector $u$. If typex is "standard" then the L1 bound on $u$ is penaltyx*sqrt(ncol(x)). In this case penaltyx must be between 0 and 1 (larger L1 bound corresponds to less penalization). If "ordered" then it's the fused lasso

|  | penalty lambda, which must be non-negative (larger lambda corresponds to more penalization). |
| :---: | :---: |
| penaltyz | The penalty to be applied to the matrix z , i.e. the penalty that results in the canonical vector v . If typez is "standard" then the L1 bound on v is penaltyz*sqrt(ncol(z)). In this case penaltyz must be between 0 and 1 (larger L1 bound corresponds to less penalization). If "ordered" then it's the fused lasso penalty lambda, which must be non-negative (larger lambda corresponds to more penalization). |
| K | The number of u's and v's desired; that is, the number of canonical vectors to be obtained. |
| niter | How many iterations should be performed? Default is 15. |
| v | The first K columns of the v matrix of the SVD of X'Z. If NULL, then the SVD of $X^{\prime} Z$ will be computed inside the CCA function. However, if you plan to run this function multiple times, then save a copy of this argument so that it does not need to be re-computed (since that process can be time-consuming if X and Z both have high dimension). |
| trace | Print out progress? |
| standardize | Should the columns of $x$ and $z$ be centered (to have mean zero) and scaled (to have standard deviation 1)? Default is TRUE. |
| xnames | An optional vector of column names for $x$. |
| znames | An optional vector of column names for z . |
| chromx | Used only if typex is "ordered"; allows user to specify a vector of length ncol(x) giving the chromosomal location of each CGH spot. This is so that smoothness will be enforced within each chromosome, but not between chromosomes. |
| chromz | Used only if typez is "ordered"; allows user to specify a vector of length ncol(z) giving the chromosomal location of each CGH spot. This is so that smoothness will be enforced within each chromosome, but not between chromosomes. |
| upos | If TRUE, then require elements of $u$ to be positive. FALSE by default. Can only be used if type is "standard". |
| uneg | If TRUE, then require elements of $u$ to be negative. FALSE by default. Can only be used if type is "standard". |
| vpos | If TRUE, require elements of $v$ to be positive. FALSE by default. Can only be used if type is "standard". |
| vneg | If TRUE, require elements of $v$ to be negative. FALSE by default. Can only be used if type is "standard". |
| outcome | If you would like to incorporate a phenotype into CCA analysis - that is, you wish to find features that are correlated across the two data sets and also correlated with a phenotype - then use one of "survival", "multiclass", or "quantitative" to indicate outcome type. Default is NULL. |
| y | If outcome is not NULL, then this is a vector of phenotypes - one for each row of $x$ and $z$. If outcome is "survival" then these are survival times; must be nonnegative. If outcome is "multiclass" then these are class labels ( $1,2,3, \ldots$ ). Default NULL. |

cens If outcome is "survival" then these are censoring statuses for each observation. 1 is complete, 0 is censored. Default NULL.
UVperms A list of U and V generated by CCA.permute function. It must include all of the estimated Us and Vs for all of the regularization parameters and all of the permutations. Read the CCA.permute for the format of this list. Check the example below.
allpenaltyxs A vector of all of the $x$ regularization parameters generated by the CCA.permute function. Check the example below for more information.

## Details

This function is useful for performing an integrative analysis of two sets of measurements taken on the same set of samples: for instance, gene expression and CGH measurements on the same set of patients. It takes in two data sets, called $x$ and $z$, each of which have (the same set of) samples on the rows. If z is a matrix of CGH data with ordered CGH spots on the columns, then use typez="ordered". If z consists of unordered columns, then use typez="standard". Similarly for typex.
This function performs the penalized matrix decomposition on the data matrix $\$ X^{\prime} \mathrm{Z} \$$. Therefore, the results should be the same as running the PMD function on $t(x) \backslash$ using the CCA function is much faster because it avoids computation of $\$ X^{\prime} \mathbf{Z} \$$.

The CCA criterion is as follows: find unit vectors $\$ u \$$ and $\$ v \$$ such that $\$ u^{\prime} X^{\prime} Z v \$$ is maximized subject to constraints on $\$ \mathbf{u} \$$ and $\$ v \$$. If typex="standard" and typez="standard" then the constraints on $\$ \mathrm{u} \$$ and $\$ \mathrm{v} \$$ are lasso ( $\$ \mathrm{~L} \_1 \$$ ). If typex="ordered" then the constraint on $\$ \mathrm{u} \$$ is a fused lasso penalty (promoting sparsity and smoothness). Similarly if typez="ordered".

When typex is "ordered": penaltyx controls the amount of sparsity and smoothness in $u$, via the fused lasso penalty: \$lambda sum_j lu_jl + lambda sum_j lu_j - $u_{-} \_(j-1) \mid \$$. If NULL, then it will be chosen adaptively from the data.

## Value

$u \quad u$ is output. If you asked for multiple factors then each column of $u$ is a factor. $u$ has dimension $n x K$ if you asked for K factors.
$v \quad v$ is output. If you asked for multiple factors then each column of $v$ is a factor. $v$ has dimension pxK if you asked for K factors.
d A vector of length $K$, which can alternatively be computed as the diagonal of the matrix $\$ u^{\prime} \mathrm{X}^{\prime} \mathrm{Zv} \$$.
$v$.init The first $K$ factors of the $v$ matrix of the SVD of $x$ ' $z$. This is saved in case this function will be re-run later.
SDu Standard deviations of the components of $U$ through the permutations for the given joint regularization parameter penaltyx and penaltyz.
SDv Similar to SDu.
standardu Standardized U using the estimated U and the component-wise standard deviation of U through permutations, SDu . There would be the following message if Inf values are created: The "Inf" in standardized U or V i.e. "standardu" or "standardv" indicates that the estimated U or V for that component
is nonzero and that its estimated standard deviation through all permutations is zero.Therefore, that component is the most significant among all. If a component of U or V is estimated zero, the associated "standardu" or "standardv" component is zero.
standardv Similar to SDv.
pvalsu No-paramteric p-values associated to the components of $u$ for the hypothesis testing with the null that each component is zero. If the estimated component is positive, the alternative would be that the true component is positive. Note that under the null hypothesis the permutation is zero, so in this scenario, the nonparamteric p -value is the proportion that the permutations resulted in a greater value than that of the component of $u$. If you need the $p$-value of the opposite direction of simply subtract this value from 1 .
pvalsv Similar to pvalsu.

## References

Ali Mahzarnia, Alexander Badea (2022), Joint Estimation of Vulnerable Brain Networks and Alzheimer's Disease Risk Via Novel Extension of Sparse Canonical Correlation at bioRxiv.

## See Also

PMD,CCA.permute

## Examples

```
set.seed(3128) # for replicating the result
n=100 # sample size
q=20 # base size
S=100*matrix(rnorm(100),n,q) # base matrix
u=c(rep(0,5),rep(1,3),rep(0,2) ) # True u
v=c(rep(1,5),rep(0,5),rep(1,5) ) # True v
p1=length(u) # length of true u
p2=length(v) #length of true v
U=matrix(rep(u, q),p1,q) # coefficients of base matrix for constructing X
V=matrix(rep(v, q),p2,q) # coefficients of base matrix for constructing Z
x=S%*%t(U) # constructing U
x=x+matrix(rnorm(dim(x)[1]*dim(x)[2]), dim(x)[1],dim(x)[2]); # adding noise
z=S%*%t(V) # constructing V
z=z+matrix(rnorm(dim(z)[1]*dim(z)[2]),dim(z)[1],dim(z)[2]); # adding noise
library(PMA2)
#for beter estimations try with more permutations,
# such as nperms=1000
perm.out <- CCA.permute(x,z,typex="standard",typez="standard",
                                    nperms=10, SD=TRUE, upos = TRUE, vpos = TRUE)
# by SD=TRUE we estimate SD of U and V components too.
# by upos and vpos we restrict the estimations to only
# positive values but this isn't necessary generally
print(perm.out)
```

```
out <- CCA(x,z,typex="standard",typez="standard",K=1,
    penaltyx=perm.out$bestpenaltyx,penaltyz=perm.out$bestpenaltyz,
    v=perm.out$v.init, UVperms = perm.out$UVperms,
    allpenaltyxs = perm.out$penaltyxs , upos = TRUE, vpos = TRUE)
print(out)
# results of projection for u
# respectively:True U, Estimated U, Standard deviations, Zscores, nonparametric-Pvalues
utable=base::cbind(u,out$u, out$SDu, out$standardu, out$pvalsu)
colnames(utable)=c("True U", "Estimated U", "SDs", "Zscores", "nonpar-Pvals")
utable
# results of projection for v
# respectively:True V, Estimated V, Standard deviations, Zscores, nonparametric-Pvalues
vtable=base::cbind(v,out$v, out$SDv, out$standardv, out$pvalsv)
colnames(vtable)=c("True V", "Estimated V", "SDs", "Zscores", "nonpar-Pvals")
vtable
```


## Description

This is a function of a modification version of the PMA package. This function can be used to automatically select tuning parameters for sparse CCA using the penalized matrix decompostion. For each data set x and z , two types are possible: (1) type "standard", which does not assume any ordering of the columns of the data set, and (2) type "ordered", which assumes that columns of the data set are ordered and thus that corresponding canonical vector should be both sparse and smooth (e.g. CGH data). In addition, this function would report the stored Us and Vs for all lambdas through all permutations for standard deviation estimations.

## Usage

```
CCA.permute(
    x,
    z,
    typex = c("standard", "ordered"),
    typez = c("standard", "ordered"),
    penaltyxs = NULL,
    penaltyzs = NULL,
    niter = 3,
    v = NULL,
    trace = TRUE,
    nperms = 25,
    standardize = TRUE,
    chromx = NULL,
    chromz = NULL,
    upos = FALSE,
```

```
    uneg = FALSE,
    vpos = FALSE,
    vneg = FALSE,
    outcome = NULL,
    y = NULL,
    cens = NULL,
    SD=FALSE
)
```


## Arguments

X
Z
typex Are the columns of x unordered (type="standard") or ordered (type="ordered")? If "standard", then a lasso penalty is applied to $v$, to enforce sparsity. If "ordered" (generally used for CGH data), then a fused lasso penalty is applied, to enforce both sparsity and smoothness.
typez Are the columns of z unordered (type="standard") or ordered (type="ordered")? If "standard", then a lasso penalty is applied to v , to enforce sparsity. If "ordered" (generally used for CGH data), then a fused lasso penalty is applied, to enforce both sparsity and smoothness.
penaltyxs The set of $x$ penalties to be considered. If typex="standard", then the L1 bound on $u$ is penaltyxs*sqrt(ncol(x)). If "ordered", then it's the lambda for the fused lasso penalty. The user can specify a single value or a vector of values. If penaltyxs is a vector and penaltyzs is a vector, then the vectors must have the same length. If NULL, then the software will automatically choose a single lambda value if type is "ordered", or a grid of (L1 bounds)/sqrt(ncol(x)) if type is "standard".
penaltyzs The set of z penalties to be considered. If typez="standard", then the L1 bound on $v$ is penaltyzs*sqrt(ncol(z)). If "ordered", then it's the lambda for the fused lasso penalty. The user can specify a single value or a vector of values. If penaltyzs is a vector and penaltyzs is a vector, then the vectors must have the same length. If NULL, then the software will automatically choose a single lambda value if type is "ordered", or a grid of (L1 bounds)/sqrt(ncol(z)) if type is "standard".
niter How many iterations should be performed each time CCA is called? Default is 3 , since an approximate estimate of $u$ and $v$ is acceptable in this case, and otherwise this function can be quite time-consuming.
$v \quad$ The first K columns of the $v$ matrix of the SVD of X'Z. If NULL, then the SVD of $X^{\prime} Z$ will be computed inside this function. However, if you plan to run this function multiple times, then save a copy of this argument so that it does not need to be re-computed (since that process can be time-consuming if X and Z both have high dimension).
trace Print out progress?

| nperms | How many times should the data be permuted? Default is 25 . A large value of <br> nperms is very important here, since the formula for computing the z-statistics <br> requires a standard deviation estimate for the correlations obtained via permuta- <br> tion, which will not be accurate if nperms is very small. |
| :--- | :--- |
| standardize |  |
| Should the columns of X and Z be centered (to have mean zero) and scaled (to |  |
| have standard deviation 1)? Default is TRUE. |  |
| chromx |  |
| Used only if typex="ordered"; a vector of length ncol(x) that allows you to spec- |  |
| ify which chromosome each CGH spot is on. If NULL, then it is assumed that |  |
| all CGH spots are on same chromosome. |  |
| Used only if typex="ordered"; a vector of length ncol(z) that allows you to spec- |  |
| ify which chromosome each CGH spot is on. If NULL, then it is assumed that |  |
| all CGH spots are on same chromosome. |  |

## Details

For X and Z , the samples are on the rows and the features are on the columns.
The tuning parameters are selected using a permutation scheme. For each candidate tuning parameter value, the following is performed: (1) The samples in $X$ are randomly permuted nperms times, to obtain matrices $\$ X^{*} \_1, X^{*} \_2, \ldots \$$. (2) Sparse CCA is run on each permuted data set $\$\left(X^{*} \_i, Z\right) \$$ to obtain factors $\$\left(u^{*} \_i, v^{*} \_i\right) \$$. (3) Sparse CCA is run on the original data (X,Z) to obtain factors $u$ and v. (4) Compute $\$ c^{*} \_i=\operatorname{cor}\left(X^{*} \_i u^{*} \_i, Z v^{*} \_i\right) \$$ and $\$ c=\operatorname{cor}(X u, Z v) \$$. (5) Use Fisher's transformation to convert these correlations into random variables that are approximately normally distributed. Let Fisher(c) denote the Fisher transformation of c. (6) Compute a z-statistic for Fisher(c),
using $\$\left(\operatorname{Fisher}(\mathrm{c})-\operatorname{mean}\left(\operatorname{Fisher}\left(\mathrm{c}^{*}\right)\right)\right) /$ sd $\left(\operatorname{Fisher}\left(\mathrm{c}^{*}\right)\right) \$$. The larger the z -statistic, the "better" the corresponding tuning parameter value.
This function also gives the p -value for each pair of canonical variates ( $\mathrm{u}, \mathrm{v}$ ) resulting from a given tuning parameter value. This p-value is computed as the fraction of $\$ c^{*} \_i \$$ 's that exceed c (using the notation of the previous paragraph).
Using this function, only the first left and right canonical variates are considered in selection of the tuning parameter.

Note that x and z must have same number of rows. This function performs just a one-dimensional search in tuning parameter space, even if penaltyxs and penaltyzs both are vectors: the pairs (penaltyxs[1], penaltyzs[1]), (penaltyxs[2], penaltyzs[2]),.... are considered.

## Value

zstat The vector of z-statistics, one per element of sumabss.
pvals The vector of p-values, one per element of sumabss.
bestpenaltyx The $x$ penalty that resulted in the highest $z$-statistic.
bestpenaltyz The z penalty that resulted in the highest z -statistic.
cors The value of $\operatorname{cor}(\mathrm{Xu}, \mathrm{Zv})$ obtained for each value of sumabss.
corperms The nperms values of $\operatorname{cor}\left(\mathrm{X} u, \mathrm{Zv}^{*}\right)$ obtained for each value of sumabss, where $X^{*}$ indicates the $X$ matrix with permuted rows, and $u^{*}$ and $v^{*}$ are the output of CCA using data ( $X^{*}, Z$ ).
ft .cors $\quad$ The result of applying Fisher transformation to cors.
ft.corperms The result of applying Fisher transformation to corperms.
nnonzerous Number of non-zero u's resulting from applying CCA to data (X,Z) for each value of sumabss.
nnonzerouv Number of non-zero v's resulting from applying CCA to data (X,Z) for each value of sumabss.
v.init The first factor of the $v$ matrix of the SVD of $x$ ' $z$. This is saved in case this function (or the CCA function) will be re-run later.
UVperms A list of nperms i.e. number of permutations. Each object of this list is a list with the size of penaltyxs i.e. number of joint regularized parameters used in all permutations. Each of these lists is itself a list of two matrices, that are Us and Vs associated with the permutation and the joint regularized parameters.

## References

Ali Mahzarnia, Alexander Badea (2022), Joint Estimation of Vulnerable Brain Networks and Alzheimer's Disease Risk Via Novel Extension of Sparse Canonical Correlation at bioRxiv.

## See Also

PMD,CCA

## Examples

\# See examples in CCA function

MultiCCA Perform sparse multiple canonical correlation analysis.

## Description

Given matrices $\$ \mathrm{X} 1, \ldots, \mathrm{XK} \$$, which represent K sets of features on the same set of samples, find sparse $\$ \mathrm{w} 1, \ldots, \mathrm{wK} \$$ such that $\$$ sum_( $\mathrm{i}<\mathrm{j}$ ) (wi' $\left.\mathrm{Xi}{ }^{\prime} \mathrm{Xj} \mathrm{wj}\right) \$$ is large. If the columns of Xk are ordered (and type="ordered") then wk will also be smooth. For \$X1, $\ldots, \mathrm{XK} \$$, the samples are on the rows and the features are on the columns. \$X1,...,XK\$ must have same number of rows, but may (and usually will) have different numbers of columns.

## Usage

MultiCCA(
xlist,
penalty = NULL,
ws = NULL,
niter = 25,
type = "standard",
ncomponents = 1,
trace = TRUE,
standardize = TRUE
)

## Arguments

xlist A list of length K , where K is the number of data sets on which to perform sparse multiple CCA. Data set $k$ should be a matrix of dimension $\$ \mathrm{n} x \mathrm{p} \_\mathrm{k} \$$ where $\$ p \_k \$$ is the number of features in data set $k$.
penalty The penalty terms to be used. Can be a single value (if the same penalty term is to be applied to each data set) or a K-vector, indicating a different penalty term for each data set. There are 2 possible interpretations for the penalty terms: If type="standard" then this is an L1 bound on wk, and it must be between 1 and $\$ \operatorname{sqrt}\left(p_{-} k\right) \$\left(\$ p \_k \$\right.$ is the number of features in matrix Xk). If type="ordered" then this is the parameter for the fused lasso penalty on wk.
ws A list of length K. The kth element contains the first ncomponents columns of the $v$ matrix of the SVD of Xk. If NULL, then the SVD of $\$ \mathrm{X} 1, \ldots, \mathrm{XK} \$$ will be computed inside the MultiCCA function. However, if you plan to run this function multiple times, then save a copy of this argument so that it does not need to be re-computed.
niter How many iterations should be performed? Default is 25 .

| type | Are the columns of $\$ x 1, \ldots, \mathrm{xK} \$$ unordered (type="standard") or ordered (type="ordered")? |
| :--- | :--- |
| If "standard", then a lasso penalty is applied to v, to enforce sparsity. If "or- |  |
| dered" (generally used for CGH data), then a fused lasso penalty is applied, to |  |
| enforce both sparsity and smoothness. This argument can be a vector of length |  |
|  | K (if different data sets are of different types) or it can be a single value "or- |
| dered"/"standard" (if all data sets are of the same type). |  |

## Value

ws $\quad$ A list of length K , containg the sparse canonical variates found (element k is a \$p_k x ncomponents\$ matrix).
ws.init A list of length K containing the initial values of ws used, by default these are the v vector of the svd of matrix Xk .

## References

Ali Mahzarnia, Alexander Badea (2022), Joint Estimation of Vulnerable Brain Networks and Alzheimer's Disease Risk Via Novel Extension of Sparse Canonical Correlation at bioRxiv.

## See Also

MultiCCA.permute,CCA, CCA.permute

## Examples

```
# Generate 3 data sets so that first 25 features are correlated across
# the data sets...
set.seed(123)
u <- matrix(rnorm(50),ncol=1)
v1 <- matrix(c(rep(.5,25),rep(0,75)),ncol=1)
v2 <- matrix(c(rep(1,25),rep(0,25)),ncol=1)
v3 <- matrix(c(rep(.5,25),rep(0,175)),ncol=1)
x1 <- u%*%t(v1) + matrix(rnorm(50*100),ncol=100)
x2 <- u%*%t(v2) + matrix(rnorm(50*50),ncol=50)
x3 <- u%*%t(v3) + matrix(rnorm(50*200),ncol=200)
xlist <- list(x1, x2, x3)
# Run MultiCCA.permute w/o specifying values of tuning parameters to
# try.
# The function will choose the lambda for the ordered data set.
# Then permutations will be used to select optimal sum(abs(w)) for
# standard data sets.
```

```
# We assume that x1 is standard, x2 is ordered, x3 is standard:
perm.out <- MultiCCA.permute(xlist, type=c("standard", "ordered",
"standard"))
print(perm.out)
plot(perm.out)
out <- MultiCCA(xlist, type=c("standard", "ordered", "standard"),
penalty=perm.out$bestpenalties, ncomponents=2, ws=perm.out$ws.init)
print(out)
# Or if you want to specify tuning parameters by hand:
# this time, assume all data sets are standard:
perm.out <- MultiCCA.permute(xlist, type="standard",
penalties=cbind(c(1.1,1.1,1.1),c(2,3,4),c(5,7,10)), ws=perm.out$ws.init)
print(perm.out)
oldpar <- par(mfrow = c(1,1))
plot(perm.out)
# Making use of the fact that the features are ordered:
out <- MultiCCA(xlist, type="ordered", penalty=.6)
par(mfrow=c(3,1))
PlotCGH(out$ws[[1]], chrom=rep(1,ncol(x1)))
PlotCGH(out$ws[[2]], chrom=rep(2,ncol(x2)))
PlotCGH(out$ws[[3]], chrom=rep(3,ncol(x3)))
par(oldpar)
```

Select tuning parameters for sparse multiple canonical correlation analysis using the penalized matrix decomposition.

## Description

This function can be used to automatically select tuning parameters for sparse multiple CCA. This is the analog of sparse CCA, when $>2$ data sets are available. Each data set may have features of type="standard" or type="ordered" (e.g. CGH data). Assume that there are K data sets, called \$X1,.., XK\$.

## Usage

```
    MultiCCA.permute(
        xlist,
        penalties = NULL,
    ws = NULL,
    type = "standard",
    nperms = 10,
    niter = 3,
    trace = TRUE,
    standardize = TRUE
)
```


## Arguments

xlist
penalties The penalty terms to be considered in the cross-validation. If the same penalty term is desired for each data set, then this should be a vector of length equal to the number of penalty terms to be considered. If different penalty terms are desired for each data set, then this should be a matrix with rows equal to the number of data sets, and columns equal to the number of penalty terms to be considered. For a given data set Xk , if type is "standard" then the penalty term should be a number between 1 and $\$$ sqrt(p_k) $\$$ (the number of features in data set k ); it is a L1 bound on wk. If type is "ordered", on the other hand, the penalty term is of the form lambda in the fused lasso penalty. Therefore, the interpretation of the argument depends on whether type is "ordered" or "standard" for this data set.

A list of length K ; the kth element contanis the first ncomponents columns of the $v$ matrix of the SVD of Xk. If NULL, then the SVD of Xk will be computed inside this function. However, if you plan to run this function multiple times, then save a copy of this argument so that it does not need to be re-computed.
type
niter How many iterations should be performed each time CCA is called? Default is 3 , since an approximate estimate of $u$ and $v$ is acceptable in this case, and otherwise this function can be quite time-consuming.
trace Print out progress?
standardize Should the columns of X and Z be centered (to have mean zero) and scaled (to have standard deviation 1)? Default is TRUE.

## Details

The tuning parameters are selected using a permutation scheme. For each candidate tuning parameter value, the following is performed: (1) Repeat the following $n$ times, for $n$ large: (a) The samples in $\$(\mathrm{X} 1, \ldots, \mathrm{XK}) \$$ are randomly permuted to obtain data sets $\$\left(\mathrm{X} 1^{*}, \ldots, \mathrm{XK}{ }^{*}\right) \$$. (b) Sparse multiple CCA is run on the permuted data sets $\$\left(\mathrm{X} 1^{*}, \ldots, \mathrm{XK}^{*}\right) \$$ to get canonical variates $\$\left(\mathrm{w} 1^{*}, \ldots, \mathrm{wK}\right) \$$. (c) Record $\$ t^{*}=\operatorname{sum} \_(i<j) \operatorname{Cor}\left(\mathrm{Xi}^{*} w i^{*}, X j^{*} w j^{*}\right) \$$. (2) Sparse CCA is run on the original data $\$(\mathrm{X} 1, \ldots, \mathrm{XK}) \$$ to obtain canonical variates $\$(\mathrm{w} 1, \ldots, \mathrm{wK}) \$$. (3) Record $\$ \mathrm{t}=$ sum_(i<j) Cor(Xi wi, $\mathrm{Xj} \mathrm{wj}) \$$. (4) The resulting p-value is given by $\$ \operatorname{mean}\left(\mathrm{t}^{*}>\mathrm{t}\right) \$$; that is, the fraction of permuted
totals that exceed the total on the real data. Then, choose the tuning parameter value that gives the smallest value in Step 4.
This function only selets tuning parameters for the FIRST sparse multiple CCA factors.
Note that $\$ \mathrm{x} 1, \ldots, \mathrm{xK} \$$ must have same number of rows. This function performs just a one-dimensional search in tuning parameter space.

## Value

| zstat | The vector of z -statistics, one per element of penalties. |
| :---: | :---: |
| pvals | The vector of p -values, one per element of penalties. |
| bestpenalties | The best set of penalties (the one with the highest zstat). |
| cors | The value of \$sum_( $\mathrm{j}<\mathrm{k}$ ) cor $(\mathrm{Xk} w k, \mathrm{Xj} w \mathrm{j}) \$$ obtained for each value of penalties. |
| corperms | The nperms values of \$sum_(j<k) cor $\left(\mathrm{Xk}^{*} w \mathrm{k}^{*}, \mathrm{Xj}^{*} \mathrm{wj} \mathrm{j}^{*}\right) \$$ obtained for each value of penalties, where Xk * indicates the Xk matrix with permuted rows, and $\mathrm{wk} *$ is the canonical variate corresponding to the permuted data. |
| ws.init | Initial values used for ws in sparse multiple CCA algorithm. |

## References

Ali Mahzarnia, Alexander Badea (2022), Joint Estimation of Vulnerable Brain Networks and Alzheimer's Disease Risk Via Novel Extension of Sparse Canonical Correlation at bioRxiv.

## See Also

MultiCCA, CCA.permute, CCA

## Examples

\# See examples in MultiCCA function
PlotCGH Plot CGH data

## Description

Given a vector of gains/losses at CGH spots, this makes a plot of gain/loss on each chromosome.

## Usage

```
PlotCGH(array, chrom = NULL, nuc = NULL, main = "", scaleEachChrom = TRUE)
```


## Arguments

$$
\begin{array}{ll}
\text { array } \begin{array}{l}
\text { A vector containing the chromosomal location of each CGH spot. } \\
\text { chrom } \\
\text { A numeric vector of the same length as "array"; its values should indicate the } \\
\text { chromosome that each CGH spot is on (for instance, for human genomic data, } \\
\text { values of chrom should range from } 1 \text { to 24). If NULL, then it is assumed that } \\
\text { all elements of 'array' are on the same chromosome. } \\
\text { nuc } \\
\text { A numeric vector of same length as "array", indicating the nucleotide position } \\
\text { of each CGH spot. If NULL, then the function assumes that each CGH spot } \\
\text { corresponds to a consecutive position. E.g. if there are 200 CGH spots on } \\
\text { chromosome 1, then they are located at positions } 1,2, \ldots, 199,200 \text {. }
\end{array} \\
\text { main } & \text { Give your plot a title. } \\
\text { scaleEachChrom } & \begin{array}{l}
\text { Default is TRUE. This means that each chromosomes CGH spots are divided by } \\
\\
\\
\text { l.1 times the max of the CGH spots on that chromosome. This way, the CGH } \\
\text { spots on each chromosome of the plot are as big as possible (i.e. easy to see). } \\
\text { If FALSE, then all of the CGH spots are divided by } 1.1 \text { times the max of ALL } \\
\text { the CGH spots. This means that on some chromosomes CGH spots might be } \\
\text { hard to see, but has the advantage that now relative magnitudes of CGH spots } \\
\text { on different chromosomes can be seen from figure. }
\end{array}
\end{array}
$$

## Details

This function makes a plot of regions of genomic gain/loss.

## Value

No return value, called for plot

## References

Ali Mahzarnia, Alexander Badea (2022), Joint Estimation of Vulnerable Brain Networks and Alzheimer's Disease Risk Via Novel Extension of Sparse Canonical Correlation at bioRxiv.

## See Also

PMD, PMD.cv, CCA, CCA.permute

## Examples

```
# Use breast data
data(breastdata)
attach(breastdata)
# dna contains CGH data and chrom contains chromosome of each CGH spot;
# nuc contains position of each CGH spot.
dna <- t(dna)
PlotCGH(dna[1,],chrom=chrom,nuc=nuc,main="Sample 1: All Chromosomes")
```

```
PlotCGH(dna[1,chrom==1], chrom=chrom[chrom==1], nuc=nuc[chrom==1],
main= "Sample 1: Chrom 1")
PlotCGH(dna[1,chrom<=3], chrom=chrom[chrom<=3], nuc=nuc[chrom<=3],
    main="Sample 1: Chroms 1, 2, and 3")
detach(breastdata)
```


## PMD

Get a penalized matrix decomposition for a data matrix.

## Description

Performs a penalized matrix decomposition for a data matrix. Finds factors $u$ and $v$ that summarize the data matrix well. $u$ and $v$ will both be sparse, and $v$ can optionally also be smooth.

## Usage

PMD (
x ,
type = c("standard", "ordered"),
sumabs $=0.4$,
sumabsu = 5,
sumabsv = NULL,
lambda = NULL,
niter $=20$,
$\mathrm{K}=1$,
$v=$ NULL,
trace = TRUE,
center = TRUE,
chrom = NULL,
rnames = NULL,
cnames = NULL,
upos = FALSE,
uneg = FALSE,
vpos = FALSE,
vneg = FALSE
)

## Arguments

x

## type

Data matrix of dimension $\$ \mathrm{n} \mathrm{x} \mathrm{p} \$$, which can contain NA for missing values.
"standard" or "ordered": Do we want v to simply be sparse, or should it also be smooth? If the columns of $x$ are ordered (e.g. CGH spots along a chromosome) then choose "ordered". Default is "standard". If "standard", then the PMD function will make use of sumabs OR sumabsu\&sumabsv. If "ordered", then the function will make use of sumabsu and lambda.

| sumabs | Used only if type is "standard". A measure of sparsity for u and v vectors, be- <br> tween 0 and 1 . When sumabs is specified, and sumabsu and sumabsv are NULL, <br> then sumabsu is set to $\$$ sqrt(n)*sumabs $\$$ and sumabsv is set to $\$$ sqrt(p)*sumabs\$. <br> If sumabs is specified, then sumabsu and sumabsv should be NULL. Or if sum- <br> absu and sumabsv are specified, then sumabs should be NULL. <br> Used for types "ordered" AND "standard". How sparse do you want u to be? <br> This is the sum of absolute values of elements of u. It must be between 1 and <br> the square root of the number of rows in data matrix. The smaller it is, the <br> sparser u will be. |
| :--- | :--- |
| sumabsu |  |
| Used only if type is "standard". How sparse do you want v to be? This is the |  |
| sum of absolute values of elements of v. It must be between 1 and square root |  |
| of number of columns of data. The smaller it is, the sparser v will be. |  |

## Details

The criterion for the PMD is as follows: we seek vectors $\$ u \$$ and $\$ v \$$ such that $\$ u ’ \mathrm{Xv} \$$ is large, subject to $\$\|u\| l \_2=1,\|v\| \_2=1 \$$ and additional penalties on $\$ u \$$ and $\$ v \$$. These additional penalties
are as follows: If type is "standard", then lasso (\$L_1\$) penalties (promoting sparsity) are placed on $u$ and $v$. If type is "ordered", then lasso penalty is placed on $u$ and a fused lasso penalty (promoting sparsity and smoothness) is placed on $v$.
If type is "standard", then arguments sumabs OR sumabsu\&sumabsv are used. If type is "ordered", then sumabsu AND lambda are used. Sumabsu is the bound of absolute value of elements of $u$. Sumabsv is bound of absolute value of elements of $v$. If sumabs is given, then sumabsu is set to $\operatorname{sqrt}(\operatorname{nrow}(\mathrm{x})) *$ sumabs and sumabsv is set to $\operatorname{sqrt}(\mathrm{ncol}(\mathrm{x})) *$ sumabs. \$lambda\$ is the parameter for the fused lasso penalty on v when type is "ordered": \$lambda(\|v\|l + sum_j|v_j-v(j-1))\$. . .

## Value

$u \quad u$ is output. If you asked for multiple factors then each column of $u$ is a factor. $u$ has dimension $n x K$ if you asked for K factors.
$v \quad v$ is output. If you asked for multiple factors then each column of $v$ is a factor. $v$ has dimension pxK if you asked for K factors.
d d is output. Computationally, $\$ \mathrm{~d}=\mathrm{u}^{\prime} \mathrm{Xv} \$$ where $\$ \mathrm{u} \$$ and $\$ \mathrm{v} \$$ are the sparse factors output by the PMD function and $\$ \mathrm{X} \$$ is the data matrix input to the PMD function. When $K=1$, the residuals of the rank-1 PMD are given by $\$ \mathrm{X}$ - duv'\$.
v.init The first right singular vector(s) of the data; these are returned to save on computation time if PMD will be run again.
meanx Mean of $x$ that was subtracted out before PMD was performed.

## References

Ali Mahzarnia, Alexander Badea (2022), Joint Estimation of Vulnerable Brain Networks and Alzheimer's Disease Risk Via Novel Extension of Sparse Canonical Correlation at bioRxiv.

## See Also

PMD.cv, SPC

## Examples

```
# Try PMD with L1 penalty on rows and columns: type="standard"
# A simple simulated example
set.seed(1)
# Our data is a rank-one matrix, plus noise. The underlying components
# contain 50 and 75 non-zero elements, respectively.
u <- matrix(c(rnorm(50), rep(0,150)),
ncol=1)
v <- matrix(c(rnorm(75),rep(0,225)), ncol=1)
x <- u%*%t(v)+
matrix(rnorm(200*300),ncol=300)
# We can use cross-validation to try to find optimal value of sumabs
cv.out <- PMD.cv(x, type="standard", sumabss=seq(0.1, 0.6, len=20))
print(cv.out)
```

```
plot(cv.out)
# The optimal value of sumabs is 0.4157, but we can get within one
# standard error of that CV error using sumabs=0.337, which corresponds to
# an average of 45.8 and 71.8 non-zero elements in each component - pretty
# close to the true model.
# We can fit the model corresponding to the lowest cross-validation error:
out <- PMD(x, type="standard", sumabs=cv.out$bestsumabs, K=1, v=cv.out$v.init)
print(out)
oldpar <- par(mfrow = c(1,1))
par(mfrow=c(2,2))
par(mar=c(2,2,2,2))
plot(out$u[,1], main="Est. u")
plot(out$v[,1], main="Est. v")
plot(u, main="True u")
plot(v, main="True v")
# And if we want to control sumabsu and sumabsv separately, we can do
# that too. Let's get 2 components while we're at it:
out2 <- PMD(x, type="standard", K=2, sumabsu=6, sumabsv=8, v=out$v.init,
cnames=paste("v", sep=" ", 1:ncol(x)), rnames=paste("u", sep=" ", 1:nrow(x)))
print(out2)
# Now check out PMD with L1 penalty on rows and fused lasso penalty on
# columns: type="ordered". We'll use the Chin et al (2006) Cancer Cell
# data set; try "?breastdata" for more info.
data(breastdata)
attach(breastdata)
# dna contains CGH data and chrom contains chromosome of each CGH spot;
# nuc contains position of each CGH spot.
dna <- t(dna) # Need samples on rows and CGH spots on columns
# First, look for shared regions of gain/loss on chromosome 1.
# Use cross-validation to choose tuning parameter value
par(mar=c(2, 2, 2, 2))
cv.out <- PMD.cv(dna[,chrom==1], type="ordered", chrom=chrom[chrom==1],
nuc=nuc[chrom==1],
sumabsus=seq(1, sqrt(nrow(dna)), len=15))
print(cv.out)
plot(cv.out)
out <- PMD(dna[, chrom==1],type="ordered",
sumabsu=cv.out$bestsumabsu, chrom=chrom[chrom==1],K=1,v=cv.out$v.init,
cnames=paste("Pos", sep="",
nuc[chrom==1]), rnames=paste("Sample", sep=" ", 1:nrow(dna)))
print(out, verbose=TRUE)
# Which samples actually have that region of gain/loss?
par(mfrow=c(3,1))
par(mar=c(2,2,2,2))
PlotCGH(dna[which.min(out$u[,1]), chrom==1], chrom=chrom[chrom==1],
main=paste(paste(paste("Sample ", sep="", which.min(out$u[,1])),
sep="; u=", round(min(out$u[,1]),3))),nuc=nuc[chrom==1])
PlotCGH(dna[88, chrom==1], chrom=chrom[chrom==1],
main=paste("Sample 88; u=", sep="", round(out$u[88,1],3)),
nuc=nuc[chrom==1])
```

```
PlotCGH(out$v[,1], chrom=chrom[chrom==1], main="V", nuc=nuc[chrom==1])
detach(breastdata)
par(oldpar)
```


## Description

Performs cross-validation to select tuning parameters for rank-1 PMD, the penalized matrix decomposition for a data matrix.

## Usage

```
    PMD.cv(
        x,
        type = c("standard", "ordered"),
        sumabss = seq(0.1, 0.7, len = 10),
        sumabsus = NULL,
        lambda = NULL,
        nfolds = 5,
        niter = 5,
        v = NULL,
        chrom = NULL,
        nuc = NULL,
        trace = TRUE,
        center = TRUE,
        upos = FALSE,
        uneg = FALSE,
        vpos = FALSE,
        vneg = FALSE
    )
```


## Arguments

x
type

Data matrix of dimension $\$ n \times \mathrm{p} \$$, which can contain NA for missing values.
"standard" or "ordered": Do we want v to simply be sparse, or should it also be smooth? If the columns of $x$ are ordered (e.g. CGH spots along a chromosome) then choose "ordered". Default is "standard". If "standard", then the PMD function will make use of sumabs OR sumabsu\&sumabsv. If "ordered", then the function will make use of sumabsu and lambda.

| sumabss | Used only if type is "standard". A vector of sumabs values to be used. Sumabs is a measure of sparsity for $u$ and $v$ vectors, between 0 and |
| :---: | :---: |
|  | 1. When sumabss is specified, and sumabsus and sumabsvs are NULL, then sumabsus is set to $\$$ sqrt $(\mathrm{n}) *$ sumabss $\$$ and sumabsvs is set at $\$ \mathrm{sqrt}(\mathrm{p}) *$ sumabss\$. If sumabss is specified, then sumabsus and sumabsvs should be NULL. Or if sumabsus and sumabsvs are specified, then sumabss should be NULL. |
| sumabsus | Used only for type "ordered". A vector of sumabsu values to be used. Sumabsu measures sparseness of $u$ - it is the sum of absolute values of elements of $u$. Must be between 1 and $\operatorname{sqrt}(\mathrm{n})$. |
| lambda | Used only if type is "ordered". This is the tuning parameter for the fused lasso penalty on v , which takes the form \$lambda $\\|\mathrm{v}\\| 1+$ lambda $\left\|v_{j} j-v(\mathrm{j}-1)\right\| \$$. \$lambda\$ must be non-negative. If NULL, then it is chosen adaptively from the data. |
| nfolds | How many cross-validation folds should be performed? Default is 5 . |
| niter | How many iterations should be performed. For speed, only 5 are performed by default. |
| v | The first right singular vector(s) of the data. (If missing data is present, then the missing values are imputed before the singular vectors are calculated.) v is used as the initial value for the iterative PMD algorithm. If $x$ is large, then this step can be time-consuming; therefore, if PMD is to be run multiple times, then v should be computed once and saved. |
| chrom | If type is "ordered", then this gives the option to specify that some columns of x (corresponding to CGH spots) are on different chromosomes. Then v will be sparse, and smooth within each chromosome but not between chromosomes. Length of chrom should equal number of columns of $x$, and each entry in chrom should be a number corresponding to which chromosome the CGH spot is on. |
| nuc | If type is "ordered", can specify the nucleotide position of each CGH spot (column of $x$ ), to be used in plotting. If NULL, then it is assumed that CGH spots are equally spaced. |
| trace | Print out progress as iterations are performed? Default is TRUE. |
| center | Subtract out mean of $x$ ? Default is TRUE |
| upos | Constrain the elements of $u$ to be positive? TRUE or FALSE. |
| uneg | Constrain the elements of $u$ to be negative? TRUE or FALSE. |
| vpos | Constrain the elements of $v$ to be positive? TRUE or FALSE. Cannot be used if type is "ordered". |
| vneg | Constrain the elements of $v$ to be negative? TRUE or FALSE. Cannot be used if type is "ordered." |

## Details

If type is "standard", then lasso (\$L_1\$) penalties (promoting sparsity) are placed on $u$ and $v$. If type is "ordered", then lasso penalty is placed on $u$ and a fused lasso penalty (promoting sparsity and smoothness) is placed on $v$.

Cross-validation of the rank-1 PMD is performed over sumabss (if type is "standard") or over sumabsus (if type is "ordered"). If type is "ordered", then lambda is chosen from the data without cross-validation.
The cross-validation works as follows: Some percent of the elements of \$x\$ is removed at random from the data matrix. The PMD is performed for a range of tuning parameter values on this partiallymissing data matrix; then, missing values are imputed using the decomposition obtained. The value of the tuning parameter that results in the lowest sum of squared errors of the missing values if "best".

To do cross-validation on the rank-2 PMD, first the rank-1 PMD should be computed, and then this function should be performed on the residuals, given by $\$ x-u d v$ ' $\$$.

## Value

cv Average sum of squared errors obtained over cross-validation folds.
cv.error Standard error of average sum of squared errors obtained over cross-validation folds.
bestsumabs If type="standard", then value of sumabss resulting in smallest CV error is returned.
bestsumabsu If type="ordered", then value of sumabsus resulting in smallest CV error is returned.
$v$.init The first right singular vector(s) of the data; these are returned to save on computation time if PMD will be run again.

## References

Ali Mahzarnia, Alexander Badea (2022), Joint Estimation of Vulnerable Brain Networks and Alzheimer's Disease Risk Via Novel Extension of Sparse Canonical Correlation at bioRxiv.

## See Also

PMD, SPC

## Examples

\# See examples in PMD help file

## Description

Performs sparse principal components analysis by applying PMD to a data matrix with lasso (\$L_1\$) penalty on the columns and no penalty on the rows.

```
Usage
    SPC(
        X,
        sumabsv = 4,
        niter = 20,
        K = 1,
        orth = FALSE,
        trace = TRUE,
        v = NULL,
        center = TRUE,
        cnames = NULL,
        vpos = FALSE,
        vneg = FALSE,
        compute.pve = TRUE
    )
```


## Arguments

$x \quad$ Data matrix of dimension $\$ n \mathrm{xp}$, which can contain NA for missing values. We are interested in finding sparse principal components of dimension $\$ \mathrm{p} \$$.
sumabsv How sparse do you want $v$ to be? This is the sum of absolute values of elements of $v$. It must be between 1 and square root of number of columns of data. The smaller it is, the sparser $v$ will be.
niter How many iterations should be performed. It is best to run at least 20 of so. Default is 20.
K The number of factors in the PMD to be returned; default is 1 .
orth If TRUE, then use method of Section 3.2 of Witten, Tibshirani and Hastie (2008) to obtain multiple sparse principal components. Default is FALSE.
trace Print out progress as iterations are performed? Default is TRUE.
$v \quad$ The first right singular vector(s) of the data. (If missing data is present, then the missing values are imputed before the singular vectors are calculated.) v is used as the initial value for the iterative $\operatorname{PMD}\left(\$ L_{-} 1 \$, \$ L_{-} 1 \$\right)$ algorithm. If x is large, then this step can be time-consuming; therefore, if PMD is to be run multiple times, then v should be computed once and saved.
center Subtract out mean of $x$ ? Default is TRUE
cnames An optional vector containing a name for each column.
vpos Constrain the elements of $v$ to be positive? TRUE or FALSE.
vneg Constrain the elements of $v$ to be negative? TRUE or FALSE.
compute.pve Compute percent variance explained? Default TRUE. If not needed, then choose FALSE to save time.

## Details

$\operatorname{PMD}(x$, sumabsu=sqrt(nrow $(x))$, sumabsv=3, $K=1)$ and $\operatorname{SPC}(x, s u m a b s v=3, K=1)$ give the same result, since the SPC method is simply PMD with an L1 penalty on the columns and no penalty on the rows.

In Witten, Tibshirani, and Hastie (2008), two methods are presented for obtaining multiple factors for SPC. The methods are as follows:
(1) If one has already obtained factors $\$ \mathrm{k}-1 \$$ factors then oen can compute residuals by subtracting out these factors. Then $\$ \mathrm{u} \_\mathrm{k} \$$ and $\$ \mathrm{v} \_\mathrm{k} \$$ can be obtained by applying the SPC/PMD algorithm to the residuals.
(2) One can require that $\$ \mathrm{u} \_\mathrm{k} \$$ be orthogonal to $\$ \mathrm{u} \_i \$$ 's with $\$ \mathrm{i}<\mathrm{k} \$$; the method is slightly more complicated, and is explained in WT\&H(2008).
Method 1 is performed by running SPC with option orth=FALSE (the default) and Method 2 is performed using option orth=TRUE. Note that Methods 1 and 2 always give identical results for the first component, and often given quite similar results for later components.

## Value

$u \quad u$ is output. If you asked for multiple factors then each column of $u$ is a factor. $u$ has dimension $n x K$ if you asked for K factors.
$v \quad v$ is output. These are the sparse principal components. If you asked for multiple factors then each column of $v$ is a factor. $v$ has dimension $p x K$ if you asked for K factors.
d
d is output; it is the diagonal of the matrix $\$ \mathrm{D} \$$ in the penalized matrix decomposition. In the case of the rank-1 decomposition, it is given in the formulation \$\|X-duv’ll_F^2\$ subject to \$\|ull_1 <= sumabsu\$, \$\|v\|_1 <= sumabsv\$. Computationally, $\$ d=u$ ' $\mathrm{Xv} \$$ where $\$ \mathrm{u} \$$ and $\$ v \$$ are the sparse factors output by the PMD function and $\$ \mathrm{X} \$$ is the data matrix input to the PMD function.
prop.var.explained
A vector containing the proportion of variance explained by the first $1,2, \ldots, \mathrm{~K}$ sparse principal components obtaineds. Formula for proportion of variance explained is on page 20 of Shen \& Huang (2008), Journal of Multivariate Analysis 99: 1015-1034.
$v$.init The first right singular vector(s) of the data; these are returned to save on computation time if PMD will be run again.
meanx Mean of $x$ that was subtracted out before SPC was performed.

## References

Ali Mahzarnia, Alexander Badea (2022), Joint Estimation of Vulnerable Brain Networks and Alzheimer's Disease Risk Via Novel Extension of Sparse Canonical Correlation at bioRxiv.

See Also<br>SPC.cv, PMD, PMD.cv

## Examples

```
#A simple simulated example
```

```
set.seed(1)
u <- matrix(c(rnorm(50), rep(0,150)),ncol=1)
v <- matrix(c(rnorm(75),rep(0,225)), ncol=1)
x <- u%*%t(v)+matrix(rnorm(200*300),ncol=300)
# Perform Sparse PCA - that is, decompose a matrix w/o penalty on rows
# and w/ L1 penalty on columns
# First, we perform sparse PCA and get 4 components, but we do not
# require subsequent components to be orthogonal to previous components
out <- SPC(x, sumabsv=3, K=4)
print(out,verbose=TRUE)
# We could have selected sumabsv by cross-validation, using function SPC.cv
# Now, we do sparse PCA using method in Section 3.2 of WT&H(2008) for getting
# multiple components - that is, we require components to be orthogonal
out.orth <- SPC(x,sumabsv=3, K=4, orth=TRUE)
print(out.orth,verbose=TRUE)
oldpar <- par(mfrow = c(1,1))
par(mfrow=c(1,1))
plot(out$u[,1], out.orth$u[,1], xlab="", ylab="")
# Note that the first components w/ and w/o orth option are identical,
# since the orth option only affects the way that subsequent components
# are found
print(round(t(out$u)%*%out$u,4)) # not orthogonal
print(round(t(out.orth$u)%*%out.orth$u,4)) # orthogonal
# Use SPC.cv to choose tuning parameters:
cv.out <- SPC.cv(x)
print(cv.out)
plot(cv.out)
out <- SPC(x, sumabsv=cv.out$bestsumabsv)
print(out)
# or we could do
out <- SPC(x, sumabsv=cv.out$bestsumabsv1se)
print(out)
par(oldpar)
```

SPC.cv

Perform cross-validation on sparse principal component analysis

## Description

Selects tuning parameter for the sparse principal component analysis method of Witten, Tibshirani, and Hastie (2008), which involves applying PMD to a data matrix with lasso (\$L_1\$) penalty on the columns and no penalty on the rows. The tuning parameter controls the sum of absolute values - or \$L_1\$ norm - of the elements of the sparse principal component.

## Usage

SPC.cv(

```
    X,
    sumabsvs = seq(1.2, 5, len = 10),
    nfolds = 5,
    niter = 5,
    v = NULL,
    trace = TRUE,
    orth = FALSE,
    center = TRUE,
    vpos = FALSE,
    vneg = FALSE
)
```


## Arguments

| x | Data matrix of dimension $\$ \mathrm{n} x \mathrm{p} \$$, which can contain NA for missing values. <br> We are interested in finding sparse principal components of dimension $\$ \mathrm{p} \$$. |
| :--- | :--- |
| sumabsvs | Range of sumabsv values to be considered in cross-validation. Sumabsv is the <br> sum of absolute values of elements of v . It must be between 1 and square root <br> of number of columns of data. The smaller it is, the sparser v will be. |
| nfolds | Number of cross-validation folds performed. |
| niter | How many iterations should be performed. By default, perform only 5 for speed <br> reasons. |
| v | The first right singular vector(s) of the data. (If missing data is present, then the <br> missing values are imputed before the singular vectors are calculated.) v is used <br> as the initial value for the iterative PMD (\$L_1\$, \$L_1\$) algorithm. If x is large, <br> then this step can be time-consuming; therefore, if PMD is to be run multiple |
| times, then v should be computed once and saved. |  |
| trace | Print out progress as iterations are performed? Default is TRUE. |
| orth | If TRUE, then use method of Section 3.2 of Witten, Tibshirani and Hastie (2008) <br> to obtain multiple sparse principal components. Default is FALSE. |
| center | Subtract out mean of $x ?$ Default is TRUE <br> vpos |
| Constrain elements of v to be positive? Default is FALSE. |  |

## Details

This method only performs cross-validation for the first sparse principal component. It does so by performing the following steps nfolds times: (1) replace a fraction of the data with missing values, (2) perform SPC on this new data matrix using a range of tuning parameter values, each time getting a rank-1 approximationg \$udv'\$ where $\$ \mathrm{v} \$$ is sparse, (3) measure the mean squared error of the rank-1 estimate of the missing values created in step 1.
Then, the selected tuning parameter value is that which resulted in the lowest average mean squared error in step 3.
In order to perform cross-validation for the second sparse principal component, apply this function to \$X-udv'\$ where \$udv'\$ are the output of running SPC on the raw data \$X\$.

## Value

| cv | Average sum of squared errors that results for each tuning parameter value. |
| :--- | :--- |
| cv.error | Standard error of the average sum of squared error that results for each tuning <br> parameter value. |
| bestsumabsv | Value of sumabsv that resulted in lowest CV error. |
| nonzerovs | Average number of non-zero elements of $v$ for each candidate value of sumab- <br> svs. |
| v.init | Initial value of $v$ that was passed in. Or, if that was NULL, then first right <br> singular vector of $X$. |
| bestsumabsv1se | The smallest value of sumabsv that is within 1 standard error of smallest CV <br> error. |

## References

Ali Mahzarnia, Alexander Badea (2022), Joint Estimation of Vulnerable Brain Networks and Alzheimer's Disease Risk Via Novel Extension of Sparse Canonical Correlation at bioRxiv.

## See Also

SPC, PMD, PMD.cv

## Examples

```
#A simple simulated example
set.seed(1)
u <- matrix(c(rnorm(50), rep(0,150)),ncol=1)
v <- matrix(c(rnorm(75),rep(0,225)), ncol=1)
x <- u%*%t(v)+matrix(rnorm(200*300),ncol=300)
# Perform Sparse PCA - that is, decompose a matrix w/o penalty on rows
# and w/ L1 penalty on columns
# First, we perform sparse PCA and get 4 components, but we do not
# require subsequent components to be orthogonal to previous components
out <- SPC(x, sumabsv=3, K=4)
print(out,verbose=TRUE)
# We could have selected sumabsv by cross-validation, using function SPC.cv
# Now, we do sparse PCA using method in Section 3.2 of WT&H(2008) for getting
# multiple components - that is, we require components to be orthogonal
out.orth <- SPC(x,sumabsv=3, K=4, orth=TRUE)
print(out.orth,verbose=TRUE)
oldpar <- par(mfrow = c(1,1))
par(mfrow=c(1,1))
plot(out$u[,1], out.orth$u[,1], xlab="", ylab="")
# Note that the first components w/ and w/o orth option are identical,
# since the orth option only affects the way that subsequent components
# are found
print(round(t(out$u)%*%out$u,4)) # not orthogonal
print(round(t(out.orth$u)%*%out.orth$u,4)) # orthogonal
```

```
# Use SPC.cv to choose tuning parameters:
cv.out <- SPC.cv(x)
print(cv.out)
plot(cv.out)
out <- SPC(x, sumabsv=cv.out$bestsumabsv)
print(out)
# or we could do
out <- SPC(x, sumabsv=cv.out$bestsumabsv1se)
print(out)
par(oldpar)
```


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