

# Package ‘PMA’

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**Title** Penalized Multivariate Analysis

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**Description** Performs Penalized Multivariate Analysis: a penalized matrix decomposition, sparse principal components analysis, and sparse canonical correlation analysis, described in the following papers: (1) Witten, Tibshirani and Hastie (2009) A penalized matrix decomposition, with applications to sparse principal components and canonical correlation analysis. *Biostatistics* 10(3):515-534. (2) Witten and Tibshirani (2009) Extensions of sparse canonical correlation analysis, with applications to genomic data. *Statistical Applications in Genetics and Molecular Biology* 8(1): Article 28.

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PMA-package	<i>Penalized Multivariate Analysis</i>
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## Description

This package is called PMA, for "Penalized Multivariate Analysis". It implements three methods: A penalized matrix decomposition, sparse principal components analysis, and sparse canonical correlations analysis. All are described in the paper "A penalized matrix decomposition, with applications to sparse principal components and canonical correlation analysis", by D Witten, R Tibshirani, and T Hastie, and published in *Biostatistics* (2009).

The main functions are as follows: (1) PMD (2) CCA (3) SPC

The first function, 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 results in nice plots for DNA copy number data.

## Details

Package:	PMA
Type:	Package
Version:	1.0.8
Date:	2011-08-11
License:	GPL >= 2

## Author(s)

Daniela M. Witten and Robert Tibshirani and Sam Gross and Balasubramanian Narasimhan

## References

Witten, Tibshirani and Hastie (2009) A penalized matrix decomposition, with applications to sparse principal components and canonical correlation analysis. *Biostatistics* 10(3): 515-534.

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breastdata	<i>Breast cancer gene expression + DNA copy number data set from Chin et al (2006), Cancer Cell</i>
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### Description

This data set consists of gene expression and DNA copy number measurements on a set of 89 samples. This example is used in Witten, Tibshirani and Hastie (2008).

### Usage

```
data(breastdata)
```

### Format

The format is a list containing the following elements: - dna: a 2149x89 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 with 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

This data set can be used to perform integrative analysis of gene expression and DNA copy number data, as in e.g. Witten and Tibshirani and Hastie (2008). That is, we can look for sets of genes that are associated with regions of chromosomal gain/loss.

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

### Source

This data set was published in the following paper:

Chin, K., DeVries, S., Fridlyand, J., Spellman, P., Roydasgupta, R., Kuo, W.-L., Lapuk, A., Neve, R., Qian, Z., Ryder, T., Chen, F., Feiler, H., Tokuyasu, T., Kingsley, C., Dairkee, S., Meng, Z., Chew, K., Pinkel, D., Jain, A., Ljung, B., Esserman, L., Albertson, D., Waldman, F. & Gray, J. (2006), 'Genomic and transcriptional aberrations linked to breast cancer pathophysiologies', *Cancer Cell* 10, 529-541.

It is publicly available at <http://icbp.lbl.gov/breastcancer>.

### References

Chin, DeVries, Fridlyand, et al. (2006) *Cancer Cell* 10, 529-541.

Used as an example in Witten, Tibshirani and Hastie (2008) 'A penalized matrix decomposition, with applications to sparse principal components and canonical correlation analysis.'

**Examples**

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

---

 CCA

*Perform sparse canonical correlation analysis using the penalized matrix decomposition.*

---

**Description**

Given matrices  $X$  and  $Z$ , which represent two sets of features on the same set of samples, find sparse  $u$  and  $v$  such that  $u'X'Zv$  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.

**Usage**

```
CCA(x, z, typex=c("standard", "ordered"), typez=c("standard", "ordered"), penaltyx=NULL, penaltyz=NULL,
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)
```

**Arguments**

<code>x</code>	Data matrix; samples are rows and columns are features. Cannot contain missing values.
<code>z</code>	Data matrix; samples are rows and columns are features. Cannot contain missing values.
<code>typex</code>	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.
<code>typez</code>	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.
<code>penaltyx</code>	The penalty to be applied to the matrix $x$ , i.e. the penalty that results in the canonical vector $u$ . If <code>typex</code> is "standard" then the L1 bound on $u$ is <code>penaltyx*sqrt(ncol(x))</code> . In this case <code>penaltyx</code> 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'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 non-negative. If outcome is "multiclass" then these are class labels (1,2,3,...). Default NULL.
cens	If outcome is "survival" then these are censoring statuses for each observation. 1 is complete, 0 is censored. Default NULL.

## 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  $X'Z$ . Therefore, the results should be the same as running the PMD function on `t(x)%%z`. However, when `ncol(x)>nrow(x)` and `ncol(z)>nrow(z)` then using the CCA function is much faster because it avoids computation of  $X'Z$ .

The CCA criterion is as follows: find unit vectors  $u$  and  $v$  such that  $u'X'Zv$  is maximized subject to constraints on  $u$  and  $v$ . If `typex="standard"` and `typez="standard"` then the constraints on  $u$  and  $v$  are lasso ( $L_1$ ). If `typex="ordered"` then the constraint on  $u$  is a fused lasso penalty (promoting sparsity and smoothness). Similarly if `typez="ordered"`.

When `type x` is "standard": the  $L_1$  bound of  $u$  is `penaltyx*sqrt(ncol(x))`.

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

## Value

<code>u</code>	$u$ is output. If you asked for multiple factors then each column of $u$ is a factor. $u$ has dimension $n \times K$ if you asked for $K$ factors.
<code>v</code>	$v$ is output. If you asked for multiple factors then each column of $v$ is a factor. $v$ has dimension $p \times K$ if you asked for $K$ factors.
<code>d</code>	A vector of length $K$ , which can alternatively be computed as the diagonal of the matrix $u'X'Zv$ .
<code>v.init</code>	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.

## Author(s)

Daniela M. Witten and Robert Tibshirani

## References

Witten, DM and Tibshirani, R and T Hastie (2008) A penalized matrix decomposition, with applications to sparse principal components and canonical correlation analysis. Submitted. <<http://www-stat.stanford.edu/~dwitten>>

## See Also

[PMD,CCA,permute](#)

## Examples

```

# first, do CCA with type="standard"
# A simple simulated example
u <- matrix(c(rep(1,25),rep(0,75)),ncol=1)
v1 <- matrix(c(rep(1,50),rep(0,450)),ncol=1)
v2 <- matrix(c(rep(0,50),rep(1,50),rep(0,900)),ncol=1)
x <- u%*%t(v1) + matrix(rnorm(100*500),ncol=500)
z <- u%*%t(v2) + matrix(rnorm(100*1000),ncol=1000)
# Can run CCA with default settings, and can get e.g. 3 components
out <- CCA(x,z,typex="standard",typez="standard",K=3)
print(out,verbose=TRUE) # To get less output, just print(out)
# Or can use CCA.permute to choose optimal parameter values
perm.out <- CCA.permute(x,z,typex="standard",typez="standard",nperms=7)
print(perm.out)
plot(perm.out)
out <- CCA(x,z,typex="standard",typez="standard",K=1,penaltyx=perm.out$bestpenaltyx,penaltyz=perm.out$bestpenaltyz)
print(out)

##### The remaining examples are commented out, but uncomment to run: #####

# Not run, to save time:
## Now try CCA with a constraint that elements of u must be negative and
## elements of v must be positive:
#perm.out <- CCA.permute(x,z,typex="standard",typez="standard",nperms=7,
#penaltyxs=seq(.1,.7,len=10), penaltyzs=seq(.1,.7,len=10), uneg=TRUE, vpos=TRUE)
#print(perm.out)
#plot(perm.out)
#out <- CCA(x,z,typex="standard",typez="standard",K=1,penaltyx=perm.out$bestpenaltyx,penaltyz=perm.out$bestpenaltyz)
#v=perm.out$v.init, uneg=TRUE, vpos=TRUE)
#print(out)
#
#
## Suppose we also have a quantitative outcome, y, and we want to find
## features in x and z that are correlated with each other and with the
## outcome:
#y <- rnorm(nrow(x))
#perm.out <- CCA.permute(x,z,typex="standard",typez="standard",outcome="quantitative",y=y, nperms=6)
#print(perm.out)
#out<-CCA(x,z,typex="standard",typez="standard",outcome="quantitative",y=y,penaltyx=perm.out$bestpenaltyx,penaltyz=perm.out$bestpenaltyz)
#print(out)
#
## now, do CCA with type="ordered"
## Example involving the breast cancer data: gene expression + CGH
#set.seed(22)
#data(breastdata)
#attach(breastdata)
#dna <- t(dna)
#rna <- t(rna)
#perm.out <- CCA.permute(x=rna,z=dna[,chrom==1],typex="standard", typez="ordered",nperms=5,penaltyxs=seq(.02,.7),penaltyzs=seq(.02,.7))
## We run CCA using all gene exp. data, but CGH data on chrom 1 only.
#print(perm.out)

```

```

#plot(perm.out)
#out <- CCA(x=rna,z=dna[,chrom==1], typex="standard", typez="ordered",penaltyx=perm.out$bestpenaltyx,
#v=perm.out$v.init, penaltyz=perm.out$bestpenaltyz, xnames=substr(genedesc,1,20),
#znames=paste("Pos", sep="", nuc[chrom==1])) # Save time by inputting lambda and v
#print(out) # could do print(out,verbose=TRUE)
#print(genechr[out$u!=0]) # Cool! The genes associated w/ gain or loss
## on chrom 1 are located on chrom 1!!
#par(mfrow=c(1,1))
#PlotCGH(out$v, nuc=nuc[chrom==1], chrom=chrom[chrom==1],
#main="Regions of gain/loss on Chrom 1 assoc'd with gene expression")
#detach(breastdata)

```

---

CCA.permute

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


---

## Description

This function can be used to automatically select tuning parameters for sparse CCA using the penalized matrix decomposition. 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).

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  $n$ perms times, to obtain matrices  $X^*_1, X^*_2, \dots$ . (2) Sparse CCA is run on each permuted data set  $(X^*_i, Z)$  to obtain factors  $(u^*_i, v^*_i)$ . (3) Sparse CCA is run on the original data  $(X, Z)$  to obtain factors  $u$  and  $v$ . (4) Compute  $c^*_i = \text{cor}(X^*_i, u^*_i, Z, v^*_i)$  and  $c = \text{cor}(Xu, Zv)$ . (5) Use Fisher's transformation to convert these correlations into random variables that are approximately normally distributed. Let  $\text{Fisher}(c)$  denote the Fisher transformation of  $c$ . (6) Compute a z-statistic for  $\text{Fisher}(c)$ , using  $(\text{Fisher}(c) - \text{mean}(\text{Fisher}(c^*))) / \text{sd}(\text{Fisher}(c^*))$ . 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  $(u, v)$  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.

## Usage

```

CCA.permute(x,z,typex=c("standard", "ordered"),typez=c("standard","ordered"),penaltyxs=NULL,penalt
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)

```

**Arguments**

x	Data matrix; samples are rows and columns are features.
z	Data matrix; samples are rows and columns are features. Note that x and z must have the same number of rows, but may (and generally will) have different numbers of columns.
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 penaltyxs 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	The first K columns of the v matrix of the SVD of X'Z. If NULL, then the SVD of X'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 nperms is very important here, since the formula for computing the z-statistics requires a standard deviation estimate for the correlations obtained via permutation, 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 specify which chromosome each CGH spot is on. If NULL, then it is assumed that all CGH spots are on same chromosome.

chromz	Used only if <code>typex="ordered"</code> ; a vector of length <code>ncol(z)</code> that allows you to specify which chromosome each CGH spot is on. If <code>NULL</code> , then it is assumed that all CGH spots are on same chromosome.
upos	If <code>TRUE</code> , then require all elements of <code>u</code> to be positive in sign. Default is <code>FALSE</code> . Can only be used if type is standard.
uneg	If <code>TRUE</code> , then require all elements of <code>u</code> to be negative in sign. Default is <code>FALSE</code> . Can only be used if type is standard.
vpos	If <code>TRUE</code> , then require all elements of <code>v</code> to be positive in sign. Default is <code>FALSE</code> . Can only be used if type is standard.
vneg	If <code>TRUE</code> , then require all elements of <code>v</code> to be negative in sign. Default is <code>FALSE</code> . 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 <code>NULL</code> .
y	If outcome is not <code>NULL</code> , then this is a vector of phenotypes - one for each row of <code>x</code> and <code>z</code> . If outcome is "survival" then these are survival times; must be non-negative. If outcome is "multiclass" then these are class labels. Default <code>NULL</code> .
cens	If outcome is "survival" then these are censoring statuses for each observation. 1 is complete, 0 is censored. Default <code>NULL</code> .

### Details

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

<code>zstat</code>	The vector of z-statistics, one per element of <code>sumabss</code> .
<code>pvals</code>	The vector of p-values, one per element of <code>sumabss</code> .
<code>bestpenaltyx</code>	The x penalty that resulted in the highest z-statistic.
<code>bestpenaltyz</code>	The z penalty that resulted in the highest z-statistic.
<code>cors</code>	The value of <code>cor(Xu,Zv)</code> obtained for each value of <code>sumabss</code> .
<code>corperms</code>	The <code>nperms</code> values of <code>cor(X*u*,Zv*)</code> obtained for each value of <code>sumabss</code> , where <code>X*</code> indicates the <code>X</code> matrix with permuted rows, and <code>u*</code> and <code>v*</code> are the output of CCA using data <code>(X*,Z)</code> .
<code>ft.cors</code>	The result of applying Fisher transformation to <code>cors</code> .
<code>ft.corperms</code>	The result of applying Fisher transformation to <code>corperms</code> .
<code>nnonzerous</code>	Number of non-zero <code>u</code> 's resulting from applying CCA to data <code>(X,Z)</code> for each value of <code>sumabss</code> .
<code>nnonzerouv</code>	Number of non-zero <code>v</code> 's resulting from applying CCA to data <code>(X,Z)</code> for each value of <code>sumabss</code> .
<code>v.init</code>	The first factor of the <code>v</code> matrix of the SVD of <code>x'z</code> . This is saved in case this function (or the CCA function) will be re-run later.

**Author(s)**

Daniela M. Witten, Robert Tibshirani

**References**

Witten, DM and Tibshirani, R and T Hastie (2008) A penalized matrix decomposition, with applications to sparse principal components and canonical correlation analysis. Submitted. <<http://www-stat.stanford.edu/~dwitten>>

**See Also**

[PMD,CCA](#)

**Examples**

```
# See examples in CCA function
```

---

MultiCCA

*Perform sparse multiple canonical correlation analysis.*

---

**Description**

Given matrices  $X_1, \dots, X_K$ , which represent  $K$  sets of features on the same set of samples, find sparse  $w_1, \dots, w_K$  such that  $\sum_{(i,j)} (w_i' X_i' X_j w_j)$  is large. If the columns of  $X_k$  are ordered (and `type="ordered"`) then  $w_k$  will also be smooth. For  $X_1, \dots, X_K$ , the samples are on the rows and the features are on the columns.  $X_1, \dots, X_K$  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**

<code>xlist</code>	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 $n \times p_k$ where $p_k$ is the number of features in data set $k$ .
<code>penalty</code>	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 <code>type="standard"</code> then this is an L1 bound on $w_k$ , and it must be between 1 and $\sqrt{p_k}$ ( $p_k$ is the number of features in matrix $X_k$ ). If <code>type="ordered"</code> then this is the parameter for the fused lasso penalty on $w_k$ .

type	Are the columns of $X_1, \dots, X_K$ 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. This argument can be a vector of length $K$ (if different data sets are of different types) or it can be a single value "ordered"/"standard" (if all data sets are of the same type).
ncomponents	How many factors do you want? Default is 1.
niter	How many iterations should be performed? Default is 25.
ws	A list of length $K$ . The $k$ th element contains the first $ncomponents$ columns of the $v$ matrix of the SVD of $X_k$ . If NULL, then the SVD of $X_1, \dots, X_K$ 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.
trace	Print out progress?
standardize	Should the columns of $X_1, \dots, X_K$ be centered (to have mean zero) and scaled (to have standard deviation 1)? Default is TRUE.

**Value**

ws	A list of length $K$ , containing the sparse canonical variates found (element $k$ is a $p_k \times ncomponents$ 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 $X_k$ .

**Author(s)**

Daniela M. Witten and Robert Tibshirani

**References**

Witten, DM and Tibshirani, R and T Hastie (2008) A penalized matrix decomposition, with applications to sparse principal components and canonical correlation analysis. Submitted. <<http://www-stat.stanford.edu/~dwitten>>

**See Also**

[MultiCCA.permute](#), [CCA](#), [CCA.permute](#)

**Examples**

```
# Generate 3 data sets so that first 25 features are correlated across
# the data sets...
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)
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)))

```

---

MultiCCA.permute

*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  $X_1, \dots, X_K$ .

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  $(X_1, \dots, X_K)$  are randomly permuted to obtain data sets  $(X_1^*, \dots, X_K^*)$ . (b) Sparse multiple CCA is run on the permuted data sets  $(X_1^*, \dots, X_K^*)$  to get canonical variates  $(w_1^*, \dots, w_K^*)$ . (c) Record  $t^* = \sum_{(i < j)} \text{Cor}(X_i^* w_i^*, X_j^* w_j^*)$ . (2) Sparse CCA is run on the original data  $(X_1, \dots, X_K)$  to obtain canonical variates  $(w_1, \dots, w_K)$ . (3) Record  $t = \sum_{(i < j)} \text{Cor}(X_i w_i, X_j w_j)$ . (4) The resulting p-value is given by  $\text{mean}(t^* > t)$ ; 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 selects tuning parameters for the FIRST sparse multiple CCA factors.

### Usage

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

### Arguments

<code>xlist</code>	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 $n \times p_k$ where $p_k$ is the number of features in data set $k$ .
<code>penalties</code>	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 $X_k$ , 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 $w_k$ . 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.
<code>type</code>	A $K$ -vector containing elements "standard" or "ordered" - or a single value. If a single value, then it is assumed that all elements are the same (either "standard" or "ordered"). If columns of $v$ are ordered (e.g. CGH spots ordered along the chromosome) then "ordered", otherwise use "standard". "standard" will result in a lasso ( $L_1$ ) penalty on $v$ , which will result in smoothness. "ordered" will result in a fused lasso penalty on $v$ , yielding both sparsity and smoothness.
<code>niter</code>	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.
<code>ws</code>	A list of length $K$ ; the $k$ th element contains the first $n$ components columns of the $v$ matrix of the SVD of $X_k$ . If NULL, then the SVD of $X_k$ 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.
<code>trace</code>	Print out progress?
<code>nperms</code>	How many times should the data be permuted? Default is 25. A large value of <code>nperms</code> is very important here, since the formula for computing the z-statistics requires a standard deviation estimate for the correlations obtained via permutation, which will not be accurate if <code>nperms</code> is very small.
<code>standardize</code>	Should the columns of $X$ and $Z$ be centered (to have mean zero) and scaled (to have standard deviation 1)? Default is TRUE.

**Details**

Note that  $x_1, \dots, x_K$  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 $\sum_{(j < k)} \text{cor}(X_k w_k, X_j w_j)$ obtained for each value of penalties.
corperms	The nperms values of $\sum_{(j < k)} \text{cor}(X_k^* w_k^*, X_j^* w_j^*)$ obtained for each value of penalties, where $X_k^*$ indicates the $X_k$ matrix with permuted rows, and $w_k^*$ is the canonical variate corresponding to the permuted data.
ws.init	Initial values used for ws in sparse multiple CCA algorithm.

**Author(s)**

Daniela M. Witten, Robert Tibshirani

**References**

Witten, DM and Tibshirani, R and T Hastie (2008) A penalized matrix decomposition, with applications to sparse principal components and canonical correlation analysis. Submitted. <<http://www-stat.stanford.edu/~dwitten>>

**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**

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

**Details**

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

**Author(s)**

Daniela M. Witten (adapted from Pei Wang and Rob Tibshirani's cghFLasso package)

**References**

Witten DM, Tibshirani R and T Hastie (2008) A penalized matrix decomposition with applications to sparse principal components and canonical correlation analysis. Submitted. <<http://www-stat.stanford.edu/~dwitten>>

**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=.4, sumabsu=5,
  sumabsv=NULL, lambda=NULL, niter=20, K=1, v=NULL, trace=TRUE,
  center=TRUE, chrom=NULL, rnames=NULL, cnames=NULL, upos=FALSE,
  uneg=FALSE, vpos=FALSE, vneg=FALSE)
```

## Arguments

<code>x</code>	Data matrix of dimension $n \times p$ , which can contain NA for missing values.
<code>type</code>	"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 <code>sumabs</code> OR <code>sumabsu</code> & <code>sumabsv</code> . If "ordered", then the function will make use of <code>sumabsu</code> and <code>lambda</code> .
<code>sumabs</code>	Used only if <code>type</code> is "standard". A measure of sparsity for $u$ and $v$ vectors, between 0 and 1. When <code>sumabs</code> is specified, and <code>sumabsu</code> and <code>sumabsv</code> are NULL, then <code>sumabsu</code> is set to $\sqrt{n} \times \text{sumabs}$ and <code>sumabsv</code> is set to $\sqrt{p} \times \text{sumabs}$ . If <code>sumabs</code> is specified, then <code>sumabsu</code> and <code>sumabsv</code> should be NULL. Or if <code>sumabsu</code> and <code>sumabsv</code> are specified, then <code>sumabs</code> should be NULL.
<code>sumabsu</code>	Used for types "ordered" AND "standard". How sparse do you want $u$ to be? This is the sum of absolute values of elements of $u$ . It must be between 1 and the square root of the number of rows in data matrix. The smaller it is, the sparser $u$ will be.
<code>sumabsv</code>	Used only if <code>type</code> 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.
<code>lambda</code>	Used only if <code>type</code> is "ordered". This is the tuning parameter for the fused lasso penalty on $v$ , which takes the form $\lambda \ v\ _1 + \lambda  v_j - v_{(j-1)} $ . <code>lambda</code> must be non-negative. If NULL, then it is chosen adaptively from the data.
<code>niter</code>	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.
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.
trace	Print out progress as iterations are performed? Default is TRUE.
center	Subtract out mean of x? Default is TRUE.
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 <i>within</i> each chromosome but not <i>between</i> 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.
rnames	An optional vector containing a name for each row of x.
cnames	An optional vector containing a name for each column of x.
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

The criterion for the PMD is as follows: we seek vectors  $u$  and  $v$  such that  $u'Xv$  is large, subject to  $\|u\|_2=1$ ,  $\|v\|_2=1$  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  $\sqrt{\text{nrow}(x)} \cdot \text{sumabs}$  and `sumabsv` is set to  $\sqrt{\text{ncol}(x)} \cdot \text{sumabs}$ . `lambda` is the parameter for the fused lasso penalty on  $v$  when type is "ordered":  $\lambda(\|v\|_1 + \sum_j |v_j - v_{(j-1)}|)$ .

### Value

u	u is output. If you asked for multiple factors then each column of u is a factor. u has dimension $n \times K$ if you asked for K factors.
v	v is output. If you asked for multiple factors then each column of v is a factor. v has dimension $p \times K$ if you asked for K factors.
d	d is output. Computationally, $d = u'Xv$ where $u$ and $v$ are the sparse factors output by the PMD function and $X$ is the data matrix input to the PMD function. When $K=1$ , the residuals of the rank-1 PMD are given by $X - duv'$ .

`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.

### Author(s)

Daniela M. Witten and Robert Tibshirani

### References

Witten, DM and Tibshirani, R and T Hastie (2008) A penalized matrix decomposition, with applications to sparse principal components and canonical correlation analysis. Submitted. <<http://www-stat.stanford.edu/~dwitten>>

### 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)
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)

```

## 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, nfold=5, niter=5, v=NULL, chrom=NULL, nuc=NULL,
trace=TRUE, center=TRUE, upos=FALSE, uneg=FALSE, vpos=FALSE, vneg=FALSE)
```

**Arguments**

x	Data matrix of dimension $n \times p$ , which can contain NA for missing values.
type	"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 $\sqrt{n} \times \text{sumabss}$ and sumabsvs is set at $\sqrt{p} \times \text{sumabss}$ . 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 $\sqrt{n}$ .
lambda	Used only if type is "ordered". This is the tuning parameter for the fused lasso penalty on v, which takes the form $\lambda \ v\ _1 + \lambda  v_j - v_{(j-1)} $ . $\lambda$ must be non-negative. If NULL, then it is chosen adaptively from the data.
nfold	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 sumabsu (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 partially-missing 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 is "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  $x - udv'$ .

### 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 sumabsu 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.

### Author(s)

Daniela M. Witten and Robert Tibshirani

### References

Witten, DM and Tibshirani, R and T Hastie (2008) A penalized matrix decomposition, with applications to sparse principal components and canonical correlation analysis. Submitted. <<http://www-stat.stanford.edu/~dwitten>>

**See Also**[PMD](#), [SPC](#)**Examples**

```
# See examples in PMD help file
```

---

SPC	<i>Perform sparse principal component analysis</i>
-----	--

---

**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	Data matrix of dimension $n \times p$ , which can contain NA for missing values. We are interested in finding sparse principal components of dimension $p$ .
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.
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( $\$L_1$ , $\$L_1$ ) 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.
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) to obtain multiple sparse principal components. Default is FALSE.
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

$\text{PMD}(x, \text{sumabsu}=\sqrt{\text{nrow}(x)}, \text{sumabsv}=3, K=1)$  and  $\text{SPC}(x, \text{sumabsv}=3, K=1)$  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  $k-1$  factors then one can compute residuals by subtracting out these factors. Then  $u_k$  and  $v_k$  can be obtained by applying the SPC/PMD algorithm to the residuals.

(2) One can require that  $u_k$  be orthogonal to  $u_i$ 's with  $i < k$ ; 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

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

## Author(s)

Daniela M. Witten and Robert Tibshirani

## References

Witten, DM and Tibshirani, R and T Hastie (2008) A penalized matrix decomposition, with applications to sparse principal components and canonical correlation analysis. Submitted. <http://www-stat.stanford.edu/~dwitten>

**See Also**

[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)
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)
```

---

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), nolds=5, niter=5, v=NULL,
trace=TRUE, orth=FALSE, center=TRUE, vpos=FALSE, vneg=FALSE)
```

**Arguments**

x	Data matrix of dimension $n \times p$ , which can contain NA for missing values. We are interested in finding sparse principal components of dimension $p$ .
sumabsvs	Range of sumabsv values to be considered in cross-validation. Sumabsv 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.
nolds	Number of cross-validation folds performed.
niter	How many iterations should be performed. By default, perform only 5 for speed reasons.
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( $L_1$ , $L_1$ ) 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.
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) to obtain multiple sparse principal components. Default is FALSE.
center	Subtract out mean of $x$ ? Default is TRUE
vpos	Constrain elements of $v$ to be positive? Default is FALSE.
vneg	Constrain elements of $v$ to be negative? Default is FALSE.

**Details**

This method only performs cross-validation for the first sparse principal component. It does so by performing the following steps  $nolds$  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 approximation  $udv'$  where  $u$  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 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 $\text{sumabsvs}$ .
$v$ .init	Initial value of $v$ that was passed in. Or, if that was NULL, then first right singular vector of $X$ .
bestsumabsv1se	The smallest value of $\text{sumabsv}$ that is within 1 standard error of smallest CV error.

**Author(s)**

Daniela M. Witten and Robert Tibshirani

**References**

Witten, DM and Tibshirani, R and T Hastie (2008) A penalized matrix decomposition, with applications to sparse principal components and canonical correlation analysis. Submitted. <<http://www-stat.stanford.edu/~dwitten>>

**See Also**

[SPC](#), [PMD](#), [PMD.cv](#)

**Examples**

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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
cv.out <- SPC.cv(x, sumabsvs=seq(1.2, sqrt(ncol(x)), len=6))
print(cv.out)
plot(cv.out)
out <- SPC(x,sumabsv=cv.out$bestsumabs, K=4) # could use
# cv.out$bestsumabsv1se instead
print(out,verbose=TRUE)
# 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
cv.out <- SPC.cv(x, sumabsvs=seq(1.2, sqrt(ncol(x)), len=6), orth=TRUE)
print(cv.out)
plot(cv.out)
out.orth <- SPC(x,sumabsv=cv.out$bestsumabsv, K=4, orth=TRUE)
print(out.orth,verbose=TRUE)
par(mfrow=c(1,1))
plot(out$u[,1], out.orth$u[,1], xlab="", ylab="")
```

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