# Package 'PTAk'

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Title Principal Tensor Analysis on k modes
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Depends tensor
<b>Description</b> A multiway method to decompose a tensor (array) of any order, as a generalisation of SVD also supporting non-identity metrics and penalisations. 2-way SVD with these extensions is also available. The package includes also some other multiway methods: PCAn (Tucker-n) and PARAFAC/CANDECOMP with these extensions.
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APSOLU3 APSOLUk CANDPARA CauRuimet CONTRACTION COS2-CTR 1 datasets 1 FCA2 1 FCAk 1

APSOLU3

	CAmet	. 17
	owtoPTAk	. 18
	NITIA	. 19
	PCAn	. 20
	lot.PTAk	. 22
	reprocessings	. 24
	PROJOT	. 25
	TA3	. 27
	TAk	. 30
	TAk-internal	. 33
	REBUILD	. 34
	SINGVA	. 35
	ummary.PTAk	. 37
	VDgen	. 39
	ENSELE	. 42
Index		44
muex		44
4.000		

APS0LU3

Associated 3-modes Principal Tensors of a 3-modes Principal Tensor

# Description

Computes all the 2-modes solutions associated to the given Principal Tensor of the given tensor.

# Usage

# **Arguments**

X	a tensor (as an array) of order $3$ , if non-identity metrics are used X is a list with data as the array and met a list of metrics
solu	a PTAk object
pt3	a number identifying in solu the Principal Tensor to use or the last (if NULL)
nbPT2	integer, if 1 all solutions will be computed otherwise at maximum $nbPT2$ solutions
smoothing	see SVDgen
smoo	see PTA3
verbose	control printing
file	output printed at the prompt if NULL, or printed in the given 'file'
	any other arguments passed to SVDGen or other functions

APSOLUk 3

### **Details**

For each component of the identified Principal Tensor given in solu, an SVD of the contracted product of X and the component is done. This gives all the associated Principal Tensors which updates solu supposed to contain Principal Tensors of X.

#### Value

an updated PTAk object

#### Note

Usually (i.e. as in PTA3 and PTAk) the principal tensor used is the first Principal Tensor of X (and is the last updated in solu). If it is another Principal Tensor, the obtained associated solutions do not *stricto sensu* refer to the SVD-kmodes decomposition (because the orthogonality is defined in the whole tensor space not necessarily on each component space) but are still meaningful.

# Author(s)

Didier Leibovici <c3s2i@free.fr>

### References

Leibovici D and Sabatier R (1998) A Singular Value Decomposition of a k-ways array for a Principal Component Analysis of multi-way data, the PTA-k. Linear Algebra and its Applications, 269:307-329

# See Also

PTA3, APSOLUk

**APSOLUk** 

Associated k-modes Principal Tensors of a k-modes Principal Tensor

### **Description**

Computes all the (k-1)-modes associated solutions to the given Principal Tensor of the given tensor. Calls recursively PTAk.

# Usage

4 APSOLUk

### **Arguments**

X a tensor (as an array) of order k, if non-identity metrics are used X is a list with

data as the array and met a list of metrics

solu a PTAk object

nbPT a number or a vector of dimension (k-2)

nbPT2 integer, if 0 no 2-modes solutions will be computed, 1 means all, >1 otherwise

smoothing see SVDgen smoo see PTA3

minpct numerical 0-100 to control of computation of future solutions at this level and

below

ptk a number identifying in solutions the Principal Tensor to use or the last (if NULL)

verbose control printing

file output printed at the prompt if NULL, or printed in the given 'file' modesnam character vector of the names of the modes, if NULL "mo 1" ... "mo k"

any other arguments passed to PTAk or other functions

#### **Details**

For each component of the identified Principal Tensor given in solutions, a PTA-(k-1)modes of the contracted product of X and the component is done. This gives all the associated Principal Tensors which updates solutions supposed to contain a Principal Tensors of X at the first place. For full description of arguments see PTAk.

### Value

an updated PTAk object

#### Note

Usually (*i.e.* as in PTA3 and PTAk) the principal tensor used is the first Principal Tensor of X (and is the last updated in solutions). If it is another Principal Tensor, the obtained associated solutions do not *stricto sensu* refer to the SVD-*k*modes decomposition (because the orthogonality is defined in the whole tensor space not necessarily on each component space) but are still meaningful. This function is usually called by PTAk but can be used on its own to carry on a PTAk analysis if X is the projected (of the original data) on the orthogonal of all the *k*modes Principal Tensor. In other words the ptk rank-one tensor in solutions should be the first best rank-one tensor approximating X for this decomposition analysis to be called PTA-*k*modes.

# Author(s)

Didier Leibovici <c3s2i@free.fr>

# References

Leibovici D and Sabatier R (1998) A Singular Value Decomposition of a k-ways array for a Principal Component Analysis of multi-way data, the PTA-k. Linear Algebra and its Applications, 269:307-329.

CANDPARA 5

### See Also

**PTAk** 

**CANDPARA** 

CANonical DECOMPosition analysis and PARAllel FACtor analysis

# **Description**

Performs the identical models known as PARAFAC or CANDECOMP model.

# Usage

### **Arguments**

X a tensor (as an array) of order k, if non-identity metrics are used X is a list with

data as the array and met a list of metrics.

dim a number specifying the number of rank-one tensors

test control of convergence

Maxiter maximum number of iterations allowed for convergence

smoothing see SVDgen smoo see PTA3

verbose control printing

file output printed at the prompt if NULL, or printed in the given 'file' modesnam character vector of the names of the modes, if NULL "mo 1" ... "mo k"

addedcomment character string printed after the title of the analysis

# **Details**

Looking for the best rank-one tensor approximation (LS) the three methods described in the package are equivalent. If the number of tensors looked for is greater then one the methods differs: PTA-kmodes will look for best approximation according to the *orthogonal rank* (*i.e.* the rank-one tensors are orthogonal), PCA-kmodes will look for best approximation according to the *space ranks* (*i.e.* the ranks of all (simple) bilinear forms, that is the number of components in each space), PARAFAC/CANDECOMP will look for best approximation according to the *rank* (*i.e.* the rank-one tensors are not necessarily orthogonal). For sake of comparisons the PARAFAC/CANDECOMP method and the PCA-nmodes are also in the package but complete functionnality of the use these methods and more complete packages may be checked at the www site quoted below.

6 CauRuimet

#### Value

a CANDPARA (inherits from PTAk) object

#### Note

The use of metrics (diagonal or not) and smoothing extends flexibility of analysis. This program runs slow! A PARAFAC orthogonal can be done with PTAk looking only for k-modes Principal Tensors *i.e.* with the options nbPT=c(rep(0,k-2),dim), nbPT2=0. It is identical to look in any PTAk decomposition only for the k-modes solution but obviously with unecessary computations.

### Author(s)

Didier Leibovici <c3s2i@free.fr>

#### References

Caroll J.D and Chang J.J (1970) Analysis of individual differences in multidimensional scaling via n-way generalization of 'Eckart-Young' decomposition. Psychometrika 35,283-319.

Harshman R.A (1970) Foundations of the PARAFAC procedure: models and conditions for 'an explanatory' multi-mode factor analysis. UCLA Working Papers in Phonetics, 16,1-84.

Kroonenberg P (1983) *Three-mode Principal Component Analysis: Theory and Applications*. DSWO press. Leiden.(related references in <a href="http://three-mode.leidenuniv.nl">http://three-mode.leidenuniv.nl</a>)

Leibovici D and Sabatier R (1998) A Singular Value Decomposition of a k-ways array for a Principal Component Analysis of multi-way data, the PTA-k. Linear Algebra and its Applications, 269:307-329.

CauRuimet

Robust estimation of within group varinace-covariance

# **Description**

Gives a robust estimate of an unknown within group covariance, aiming either to look for dense groups or to sparse groups (outliers) according to *local variance and weighting function* choice.

# Usage

CauRuimet 7

# Arguments

Z	matrix
ker	either numerical or a function: if numerical the weighting function is $e^{(-ker\;t)}$ , otherwise ker=function(t){return(expression)} is a positive decreasing function.
mO	is a graph of neighbourhood or another proximity matrix, the hadamard product of the proximities will be operated
withingroup	logical,if TRUE the aim is to give a robust estimate for dense groups, if FALSE the aim is to give a robust estimate for outliers $\frac{1}{2}$
loc	a vector of locations or a function using mean, median, to give an estimate of it
matrixmethod	if TRUE (only with withing roup) uses some matrix computation rather than double looping as suggests the formula below
Nrandom	if Nrandom $< \dim(Z)[1]$ ) uses only a Nrandom sample from rows of Z and m0 if applicable.

# **Details**

When withingroup is TRUE, local(defined by the weighting) variance formula is returned, aiming at finding dense groups:

$$W_{l} = \frac{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} m0_{ij} ker(d_{S^{-}}^{2}(Z_{i}, Z_{j}))(Z_{i} - Z_{j})'(Z_{i} - Z_{j})}{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} m0_{ij} ker(d_{S^{-}}^{2}(Z_{i}, Z_{j}))}$$

where  $d_{S^-}^2(.,.)$  is the squared euclidian distance with  $S^-$  the inverse of a robust sample covariance (i.e. using loc instead of the mean); if FALSE robust Total weighted variance or if m0 not 1 Global weighted variance, is returned:

$$W_o = \frac{\sum_{i=1}^{n} ker(d_{S^-}^2(Z_i, \tilde{Z}))(Z_i - \tilde{Z})'(Z_i - \tilde{Z})}{\sum_{i=1}^{n} ker(d_{S^-}^2(Z_i, \tilde{Z}))}$$

$$W_g = \frac{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} m0_{ij}.ker(d_{S^-}^2(Z_i, Z_j))(Z_i - \tilde{Z})'(Z_j - \tilde{Z})}{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} m0_{ij}ker(d_{S^-}^2(Z_i, Z_j))}$$

where  $\tilde{Z}$  is the vector loc.

If m0 is a graph of neighbourhood and ker is the function returning 1 (no proximity due to distance is used) the function will return (when withingroup=TRUE) the *local variance-covariance* matrix as define in Lebart(1969).

#### Value

a matrix

8 CauRuimet

### Note

As mentioned by Caussinus and Ruiz a good strategy to reveal dense groups with generalised PCA would be to reveal outliers first using the metric  $W_o^{-1}$  and remove them before using the metric  $W_l^{-1}$ . Based on theoretical considerations they recommand for the choice of ker, with the decreasing function  $e^{(-ker\ t)}$ : a lower bound of 1 if withingroup and something fairly small say in the interval [0.05;0.3] otherwise.

### Author(s)

Didier Leibovici <c3s2i@free.fr>

### References

Caussinus, H and Ruiz, A (1990) Interesting Projections of Multidimensional Data by Means of Generalized Principal Components Analysis. COMPSTAT90, Physica-Verlag, Heidelberg, 121-126.

Faraj, A (1994) *Interpretation tools for Generalized Discriminant Analysis*. In: New Approches in Classification and Data Analysis, Springer-Verlag, 286-291, Heidelberg.

Lebart, L (1969) *Analyse statistique de la contiguit*<*e9*>*e*.Publication de l'Institut de Statistiques Universitaire de Paris, XVIII,81-112.

Leibovici D (2008) Spatio-temporal Multiway Decomposition using Principal Tensor Analysis on k-modes: the R package PTAk. to be submitted soon at Journal of Statistical Software.

#### See Also

**SVDgen** 

### **Examples**

```
data(iris)
  iris2 <- as.matrix(iris[,1:4])
  dimnames(iris2)[[1]] <- as.character(iris[,5])

D2 <- CauRuimet(iris2,ker=1,withingroup=TRUE)
D2 <- Powmat(D2,(-1))
  iris2 <- sweep(iris2,2,apply(iris2,2,mean))
  res <- SVDgen(iris2,D2=D2,D1=1)
  plot(res,nb1=1,nb2=2,cex=0.5)
  summary(res,testvar=0)

# the same in a demo function
  # source(paste(R.home(),"/library/PTAk/demo/CauRuimet.R",sep=""))
# demo.CauRuimet(ker=4,withingroup=TRUE,openX11s=FALSE)
# demo.Cauruimet(ker=0.15,withingroup=FALSE,openX11s=FALSE)</pre>
```

CONTRACTION 9

CONTRACTION Contraction of two tensors
--

### **Description**

Computes the contraction product of two tensors as a generalisation of matrix product.

### Usage

```
\label{local_contraction} CONTRACTION(X,z, \ Xwiz=NULL,zwiX=NULL,rezwiX=FALSE,usetensor=TRUE) \\ CONTRACTION.list(X,zlist,moins=1,zwiX=NULL,usetensor=TRUE,withapply=FALSE) \\
```

# Arguments

Χ	a tensor(as an array) of any order
Z	another tensor (with at least one space in common)
zlist	a list of lists like a solution.PTAk at least with v for every list(here v can be any array)
Xwiz	Xwiz is to specify the entries of X to contract with entries of z specified by zwiX, if Xwiz NULL $\dim(z)[zwiX]$ matching $\dim(X)$ will do without ambiguity (taking all z dimensions if zwiX is NULL). In CONTRACTION.list it is not set as one supposes the contractions in the list to operate follow the dimensions of X
zwiX	idem as Xwiz. If both Xwiz and zwiX are NULL zwiXis replaced by full possibilities (1:length(dimz)) then Xwiz is looked for. In CONTRACTION.list it is the vector for dimensions in the v to contract with X. Only 1-way dimension for each v.
moins	the elements in zlist to skip (see also TENSELE)
rezwiX	logical if TRUE (and zwiX is NULL) rematches the dimensions in for zwiX: useful only if the dimensions of z were not following the Xwiz order and are not equals.
usetensor	if TRUE uses tensor (add-on package)
withapply	if TRUE (only for vectors in zlist uses apply

# **Details**

Like two matrices *contract* according to the appropriate dimensions (columns matching rows) when one performs a matrix product, this operation does pretty much the same thing for tensors(array) and specified contraction dimensions given by Xwiz and zwiX which should match. The function is actually written like: transforms both tensors as matrices with the "matching tensor product" of their contraction dimensions in columns (for higher order tensor) and rows (the other one), performs the matrix product and rebuild the result as a tensor(array). Without using tensor, if Xwiz and/or zwiX are not specified the functions tries to match all z dimensions onto the dimensions of X where X is the higher order tensor (if it is not the case in the arguments the function swaps them).

# Value

A tensor of dimension c(dim(X)[-Xwiz], dim(z)[-zwiX]) if X has got a bigger order than z.

10 CONTRACTION

### Note

This operation generalises the *matrix* product to the *contracted* product of any two tensors(arrays), and should theoretically perform the tensor product if no matching (no contraction) but has not been implemented. I recently put the option of using tensor which does exactly the same thing faster as well as it is from C. When using tensor if Xwiz or zwiX are NULL they are replaced by the full possibilities.

# Author(s)

Didier Leibovici <c3s2i@free.fr>

#### References

Leibovici D and Sabatier R (1998) A Singular Value Decomposition of a k-ways array for a Principal Component Analysis of multi-way data, the PTA-k. Linear Algebra and its Applications, 269:307-329.

Schwartz L (1975) Les Tenseurs. Herman, Paris.

#### See Also

PTAk, APSOLUk

# **Examples**

```
library(tensor)
  z \leftarrow array(1:12,c(2,3,2))
  X \leftarrow array(1:48,c(3,4,2,2))
  Xcz \leftarrow CONTRACTION(X,z,Xwiz=c(1,3,4),zwiX=c(2,3,1))
  dim(Xcz) # 4
  Xcz1 <- CONTRACTION(X,z,Xwiz=c(3,4),zwiX=c(1,3))</pre>
  dim(Xcz1) # 3,4,3
  Xcz2 \leftarrow CONTRACTION(X,z,Xwiz=c(3,4),zwiX=c(3,1))
  Xcz1[,,1]
  Xcz2[,,1]
  #######
  val0 \leftarrow list(list(v=c(1,2,3,4)), list(v=rep(1,3)), list(v=c(1,3)))
  tew <- array(1:24,c(4,3,2))
   CONTRACTION.list(tew,sval0,moins=1)
      #this is equivalent to the following which may be too expensive for big datasets
   CONTRACTION(tew, TENSELE(sval0, moins=1), Xwiz=c(2,3))
    CONTRACTION.list(tew,sval0,moins=c(1,2)) #must be equal to
    CONTRACTION(tew,sval0[[3]]$v,Xwiz=3)
```

COS2-CTR 11

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COS2-CTR	Interpretation summaries	

#### **Description**

After a FCA2, a SVDgen, a FCAk or a PTAk computes the traditional guides for interpretations used in PCA and correspondence analysis: COS2 or the percentage of variability rebuilt by the component and CTR or the amount of contribution towards that component.

### Usage

```
COS2(solu, mod=1, solnbs=2:4, FCA=FALSE)
CTR(solu, mod=1, solnbs=1:4)
```

# Arguments

solu	an object inheriting from class PTAk, representing a generalised singular value decomposition
mod	an integer representing the mode number entry, 1 is row, 2 columns,
solnbs	a vector of integers representing the tensor numbers in the listing summary
FCA	if TRUE substract the global independence to the data before computing the variability

# **Details**

Classical measures helping to interpret the plots in PCA, FCA and in PTAk as well. The sum of the COS2 across all the components ()needed to rebuild fully the tensor analysed) would make 1000 and the sum pf the CTR across the entry mode would be 1000.

# Value

a matrix whose columns are the COS2 or CTR as per thousands (%) for the mode considered

# Author(s)

```
Didier G. Leibovici <c3s2i@free.fr>
```

# References

Escoufier Y (1985) L'Analyse des correspondances : ses propriétés et ses extensions. ISI 45th session Amsterdam.

Leibovici D(1993) Facteurs à Mesures Répétées et Analyses Factorielles : applications à un suivi Epidémiologique. Université de Montpellier II. PhD Thesis in Mathématiques et Applications (Biostatistiques).

Leibovici DG (2010) Spatio-temporal Multiway Decomposition using Principal Tensor Analysis on k-modes:the R package PTAk. Journal of Statistical Software, 34(10), 1-34. http://www.jstatsoft.org/v34/i10/

12 datasets

### See Also

```
PTAk, FCA2, FCAk, summary.FCAk, plot.PTAk
```

# **Examples**

```
data(crimerate)
cri.FCA2 <- FCA2(crimerate)
summary(cri.FCA2)
plot(cri.FCA2, mod = c(1,2), nb1 = 2, nb2 = 3) # unscaled
plot(cri.FCA2, mod = c(1,2), nb1 = 2, nb2 = 3, coefi = list(rep(0.130787,50),rep(0.104359,7)) )# symmetric-m
CTR(cri.FCA2, mod = 1, solnbs = 2:4)
CTR(cri.FCA2, mod = 2, solnbs = 2:4)
COS2(cri.FCA2, mod = 2, solnbs = 2:4, FCA = TRUE)</pre>
```

datasets

data used for demo in SVDgen, PTA3

# **Description**

The crimerate dataset provides crime rates per 100,000 people in seven categories for each of the fifty states (USA) in 1977. The timage12 dataset is an image from fMRI analysis (one brain slice), it is a *t*-statistic image over 12 subjects of the activation (verbal) parameter. The Zone\_climTUN is an object of class Map representing montly (12) measurements in Tunisia of 10 climatic indicators. The grid of 2599 cells was stored previously as a shapefile and read using read.shape.

### Usage

```
data(crimerate)
data(timage12)
data(Zone_climTUN)
```

#### **Format**

```
crimerate is a matrix of 50 \times 7 for the crimerate data. timage12 is a matrix 91 \times 109 for timage12 data.
```

#### Source

crimerate comes from SAS. The timage12 comes from FMRIB center, University of Oxford. The Zone\_climTUN comes from WorldCLIM database 2000 see references along with description of the indicators in Leibovici et al.(2007).

### References

Leibovici D, Quillevere G, Desconnets JC (2007). A Method to Classify Ecoclimatic Arid and Semi-Arid Zones in Circum-Saharan Africa Using Monthly Dynamics of Multiple Indicators. IEEE Transactions on Geoscience and Remote Sensing, 45(12), 4000-4007.

FCA2 13

FCA2

Correspondence Analysis for 2-way tables

# Description

Performs a particular SVDgen data as a ratio Observed/Expected under complete independence with metrics as margins of the contingency table (in frequencies).

### **Usage**

# **Arguments**

X a matrix table of positive values

nbdim a number of dimension to retain, if NULL the default value of maximum possible

number of dimensions is kept

minpct numerical 0-100 to control of computation of future solutions at this level and

below

smoothing see SVDgen
smoo see SVDgen
verbose control printing

file output printed at the prompt if NULL, or printed in the given 'file' modesnam character vector of the names of the modes, if NULL "mo 1" ... "mo k"

addedcomment character string printed if printt after the title of the analysis chi2 print the chi2 information when computing margins in FCAmet

E if not NULL is a matrix with the same dimensions as X with the same margins

... any other arguments passed to SVDGen or other functions

#### **Details**

Gives the SVD-2modes decomposition of the  $1 + \chi^2/N$  of the contingency table of full count  $N = \sum X_{ij}$ , i.e. complete independence + lack of independence (including marginal independences) as shown for example in Lancaster(1951)(see reference in Leibovici(1993 or 2000)). Noting P = X/N, a SVD of the (3)-uple is done, that is:

$$((D_I^{-1} \otimes D_J^{-1})..P, \quad D_I, \quad D_J)$$

where the metrics are diagonals of the corresponding margins. For full description of arguments see PTAk. If E is not NULL an FCAk-modes relatively to a model is done (see Escoufier(1985) and therin

14 FCA2

reference Escofier(1984) for a 2-way derivation), e.g. for a three way contingency table k=3 the 4-tuple data and metrics is:

$$((D_I^{-1} \otimes D_J^{-1} \otimes D_K^{-1})(P - E), D_I, D_J, D_K)$$

If E was the complete independence (product of the margins) then this would give an AFCk but without looking at the marginal dependencies (i.e. for a three way table no two-ways lack of independence are looked for).

#### Value

```
a FCA2 (inherits FCAk and PTAk) object
```

#### Author(s)

Didier G. Leibovici <c3s2i@free.fr>

#### References

Escoufier Y (1985) L'Analyse des correspondances : ses propriétés et ses extensions. ISI 45th session Amsterdam.

Leibovici D(1993) Facteurs à Mesures Répétées et Analyses Factorielles : applications à un suivi Epidémiologique. Université de Montpellier II. PhD Thesis in Mathématiques et Applications (Biostatistiques).

Leibovici D (2000) *Multiway Multidimensional Analysis for Pharmaco-EEG Studies*.http://www.fmrib.ox.ac.uk/analysis/techrep/tr00dl2/tr00dl2.pdf

Leibovici DG (2010) Spatio-temporal Multiway Decomposition using Principal Tensor Analysis on k-modes:the R package PTAk. Journal of Statistical Software, 34(10), 1-34. http://www.jstatsoft.org/v34/i10/

# See Also

```
PTAk, FCAmet, summary. FCAk
```

# **Examples**

```
data(crimerate)
cri.FCA2 <- FCA2(crimerate)
summary(cri.FCA2)
plot(cri.FCA2, mod = c(1,2), nb1 = 2, nb2 = 3) # unscaled
plot(cri.FCA2, mod = c(1,2), nb1 = 2, nb2 = 3, coefi = list(rep(0.130787,50),rep(0.104359,7)) )# symmetric-m
CTR(cri.FCA2, mod = 1, solnbs = 2:4)
CTR(cri.FCA2, mod = 2, solnbs = 2:4)
COS2(cri.FCA2, mod = 2, solnbs = 2:4, FCA = TRUE)</pre>
```

FCAk 15

**FCAk** 

Generalisation of Correspondence Analysis for k-way tables

# **Description**

Performs a particular PTAk data as a ratio Observed/Expected under complete independence with metrics as margins of the multiple contingency table (in frequencies).

### Usage

### **Arguments**

Χ a multiple contingency table (array) of order k a number or a vector of dimension (k-2)nbPT nbPT2 if 0 no 2-modes solutions will be computed, 1 = all, >1 otherwise minpct numerical 0-100 to control of computation of future solutions at this level and below see SVDgen smoothing smoo see SVDgen verbose control printing file output printed at the prompt if NULL, or printed in the given 'file' character vector of the names of the modes, if NULL "mo 1" ... "mo k" modesnam addedcomment character string printed if printt after the title of the analysis chi2 print the chi2 information when computing margins in FCAmet Ε if not NULL is an array with the same dimensions as X

### **Details**

Gives the SVD-kmodes decomposition of the  $1+\chi^2/N$  of the multiple contingency table of full count  $N=\sum X_{ijk...}$ , i.e. complete independence + lack of independence (including marginal independences) as shown for example in Lancaster(1951)(see reference in Leibovici(2000)). Noting P=X/N, a PTAk of the (k+1)-uple is done, e.g. for a three way contingency table k=3 the 4-uple data and metrics is:

any other arguments passed to SVDGen or other functions

$$((D_I^{-1} \otimes D_I^{-1} \otimes D_K^{-1})P, \quad D_I, \quad D_J, \quad D_K)$$

16 FCAk

where the metrics are diagonals of the corresponding margins. For full description of arguments see PTAk. If E is not NULL an FCAk-modes relatively to a model is done (see Escoufier(1985) and therin reference Escofier(1984) for a 2-way derivation), e.g. for a three way contingency table k=3 the 4-tuple data and metrics is:

$$((D_I^{-1}\otimes D_J^{-1}\otimes D_K^{-1})(P-E),\quad D_I,\quad D_J,\quad D_K)$$

If E was the complete independence (product of the margins) then this would give an AFCk but without looking at the marginal dependencies (i.e. for a three way table no two-ways lack of independence are looked for).

### Value

a FCAk (inherits PTAk) object

#### Author(s)

Didier Leibovici <c3s2i@free.fr>

#### References

Escoufier Y (1985) L'Analyse des correspondances : ses propri<e9>t<e9>s et ses extensions. ISI 45th session Amsterdam.

Leibovici D(1993) Facteurs <e0> Mesures R<e9>p<e9>t<e9>es et Analyses Factorielles : applications <e0> un suivi <e9>pid<e9>miologique. Universit<e9> de Montpellier II. PhD Thesis in Math<e9>matiques et Applications (Biostatistiques).

Leibovici D (2000) *Multiway Multidimensional Analysis for Pharmaco-EEG Studies*.http://www.fmrib.ox.ac.uk/analysis/techrep/tr00dl2/tr00dl2.pdf

Leibovici D (2008) Spatio-temporal Multiway Decomposition using Principal Tensor Analysis on k-modes:the R package PTAk. to be submitted soon at Journal of Statisticcal Software.

### See Also

PTAk, FCAmet, summary.FCAk

# **Examples**

```
# try the demo
# demo.FCAk()
```

FCAmet 17

FCAmet	Tool used in Generalisation of Correspondence Analysis for k-way ta- bles

# **Description**

Computes the ratio Observed/Expected under complete independence with margins of the multiple contingency table (in frequencies) and gives chi2 statistic of lack of complete independence.

# Usage

```
FCAmet(X,chi2=FALSE,E=NULL,No0margins=TRUE)
```

# **Arguments**

X a multiple contingency table (array) of order *k* chi2 if TRUE prints the chi2 statistic information

E if not NULL represent a model which would be used for an FCAk relatively to a

model

No0margins if TRUE, prevents zero margins in replacing cells involved by the min of the

non-zero margins /nb of zero cells

### Value

a list with

data an array (X/count (-E))/Indepen where Indepen is the array obtained from

he products of the margins

met a list wherein each entry is the vector of the corresponding margins i.e. apply(X,i,sum)/count

count is the total sum sum(X).

#### Note

The statistics and metrics do not depend on E. The statistic given measure only the lack of independence.

# Author(s)

Didier Leibovici <c3s2i@free.fr>

### See Also

FCAk

18 howtoPTAk

howtoPTAk

howto for Principal Tensors Analysis of a k-modes Tensor

# **Description**

A mini guide to handle PTAk model decomposittion

### Usage

howtoPTAk()

#### **Details**

The PTAk decomposition aims at building an approximation of a given multiway data, represented as a tensor, based on a variance criterion. This approximation is given by a set of rank one tensors, orthogonals to each other, in a nested algorithm process and so controlling the level of approximation by the amount of variability extracted and represented by the sum of squares of the singular values (associated to the rank one tensors). In that respect it offers a way of generalising PCA to tensors of order greater than 2.

The reference in JSS provides details about preparing a dataset and running a general PTAk and particularlities for spatio-temporal data.

The license is GPL-3, support can be provided via http://c3s2i.free.fr, donations via Paypal to c3s2i@free.fr are welcome.

### Author(s)

Didier Leibovici <c3s2i@free.fr>

### References

Leibovici D and Sabatier R (1998) A Singular Value Decomposition of a k-ways array for a Principal Component Analysis of multi-way data, the PTA-k. Linear Algebra and its Applications, 269:307-329 Leibovici D.G. (accepted in 2009) Spatio-temporal Multiway Decompositions using Principal Tensor Analysis on k-modes: the R-package PTAk. Journal of Statistical Software, vol x issue x, http://www.jstatsoft.org

### See Also

PTA3, PTAk, FCAk

INITIA 19

INITIA	Initialisation used in SINGVA	
INTITA	Intitutisation used in SIIVO VII	

### **Description**

Gives the first Tucker1 components of a given tensor.

# Usage

```
INITIA(X,modesnam=NULL,method="Presvd",dim=1,...)
```

### **Arguments**

a tensor (as an array) of order kmodesnam

a character vector of the names of the modes

method

uses either the inbuilt SVD method="svd" or a power algorithm giving only the first method="Presvd" or any other function given applying to the column space of a matrix and returning a list with v (in columns vectors as in svd) and d.

dim default 1 in each space otherwise specify the number of dimensions e.g. c(2,3..,2)

(with "Presvd" dim is obviously 1)

... extra arguments of the method method: the first argument is fixed (see details).

#### **Details**

Computes the first (or dim) right singular vector (or other summaries) for every representation of the tensor as a matrix with  $\dim(X)[i]$  columns, i=1...k.

#### Value

a list (of length k) of lists with arguments:

v the singular vectors in rows

modesnam a character object naming the mode, "m i" otherwise

n labels of mode i entries as given in dimnames of the data, can be NULL

d the corresponding first singular values

# Note

The collection these eigenvectors, is known as the Tucker1 solution or initialisation related to PCA-3modes or PCA-nmodes models. If a function is given it may include dim as argument.

# Author(s)

Didier Leibovici <c3s2i@free.fr>

20 **PCAn** 

### References

Kroonenberg P.M (1983) Three-mode Principal Component Analysis: Theory and Applications. DSWO Press, Leiden.

Leibovici D and Sabatier R (1998) A Singular Value Decomposition of a k-ways array for a Principal Component Analysis of multi-way data, the PTA-k. Linear Algebra and its Applications, 269:307-329.

### See Also

SINGVA, PTAk

**PCAn** 

Principal Component Analysis on n modes

# **Description**

Performs the Tuckern model using a space version of RPVSCC (SINGVA).

# Usage

```
PCAn(X, dim=c(2,2,2,3), test=1E-12, Maxiter=400,
             smoothing=FALSE,smoo=list(NA),
               verbose=getOption("verbose"),file=NULL,
                 modesnam=NULL,addedcomment="")
```

### **Arguments**

modesnam

Χ a tensor (as an array) of order k, if non-identity metrics are used X is a list with

data as the array and met a list of metrics

a vector of numbers specifying the dimensions in each space dim

test control of convergence

maximum number of iterations allowed for convergence Maxiter

smoothing see SVDgen see PTA3 smoo

verbose control printing

output printed at the prompt if NULL, or printed in the given 'file' file

character vector of the names of the modes, if NULL "mo  $\,$ 1" ... "mo  $\,$ k"

addedcomment character string printed after the title of the analysis

#### **Details**

Looking for the best rank-one tensor approximation (LS) the three methods described in the package are equivalent. If the number of tensors looked for is greater then one the methods differs: PTA-kmodes will "look" for "best" approximation according to the *orthogonal rank* (*i.e.* the rank-one tensors are orthogonal), PCA-kmodes will look for best approximation according to the *space ranks* (*i.e.* the rank of every bilinear form, that is the number of components in each space), PARAFAC/CANDECOMP will look for best approximation according to the *rank* (*i.e.* the rank-one tensors are not necessarily orthogonal). For the sake of comparisons the PARAFAC/CANDECOMP method and the PCA-nmodes are also in the package but complete functionnality of the use these methods and more complete packages may be fetched at the www site quoted below.

Recent work from Tamara G Kolda showed on an example that *orthogonal rank* decompositions are not necesseraly nested. This makes PTA-*k*modes a model with nested decompositions not giving the exact *orthogonal rank*. So PTA-*k*modes will look for best approximation according to orthogonal tensors in a nested approximmation process.

### Value

a PCAn (inherits PTAk) object

#### Note

The use of metrics (diagonal or not) and smoothing extend flexibility of analysis.

#### Author(s)

Didier Leibovici <c3s2i@free.fr>

### References

Caroll J.D and Chang J.J (1970) *Analysis of individual differences in multidimensional scaling via n-way generalization of "Eckart-Young" decomposition*. Psychometrika 35,283-319.

Harshman R.A (1970) Foundations of the PARAFAC procedure: models and conditions for "an explanatory" multi-mode factor analysis. UCLA Working Papers in Phonetics, 16,1-84.

Kroonenberg P (1983) *Three-mode Principal Component Analysis: Theory and Applications*. DSWO press. Leiden.(related references in http://three-mode.leidenuniv.nl/)

Leibovici D and Sabatier R (1998) A Singular Value Decomposition of a k-ways array for a Principal Component Analysis of multi-way data, the PTA-k. Linear Algebra and its Applications, 269:307-329.

Kolda T.G (2003) A Counterexample to the Possibility of an Extension of the Eckart-Young Low-Rank Approximation Theorem for the Orthogonal Rank Tensor Decomposition. SIAM J. Matrix Analysis, 24(2):763-767, Jan. 2003.

plot.PTAk

# Description

Screeplot of singular values or plot of superposed modes or not for one or two components.

# Usage

```
## S3 method for class 'PTAk'
plot(x, labels = TRUE, mod = 1, nb1 = 1, nb2 = NULL,
    coefi = list(NULL, NULL), xylab = TRUE, ppch = (1:length(solution)),
    lengthlabels = 2, scree = FALSE, ordered = TRUE,
    nbvs = 40, RiskJack = NULL, method = "",ZoomInOut=NULL, Zlabels=NULL, ...)
RiskJackplot(x, nbvs = 1:20, mod = NULL, max = NULL, rescaled=TRUE, ...)
```

# Arguments

Х	an object inheriting from class PTAk, representing a generalised singular value decomposition
labels	logical if TRUE plots the labels given in solution[[mod]]["n"]
mod	vectors of the modes numbers to be plotted
nb1	number identifying the Principal Tensor to display on the vertical axe, can be checked using $\operatorname{summary}.\operatorname{PTAk}$
nb2	as nb1 to be displayed on the horizontal axe, if NULL the horizontal axe will be used as Index (see plot.default)
coefi	coefficients to multiply components for rescaling or changing signs purposes; each element of the list correpond to nb1 and nb2 and are vectors of dimentions the tensor order
xylab	logical to display axes labels
ppch	a vector of length at least length(mod) used for pch=
lengthlabels	a number or a vector of numbers of characters in labels to be used for display
scree	logical to display a screeplot of squared singular values as percent of total variation
ordered	logical used when displaying the screeplot with sorted values (TRUE) or the order is given by output listing from $summary.PTAk$
nbvs	a maximum number of singular values to display on the screeplot or a vector of ranks
max	is the number of singular values to be considered as giving the perfect fit, NULL is the max possible in x
rescaled	boolean to rescale the y axis to 0-100

plot.PTAk 23

RiskJack if not NULL is a integer, scree is TRUE and ordered is TRUE, plots on top of the

scree plot a Risk plot with maximum dimension:

min(RiskJack+length(nbvs),length(solution[[k]][["d"]])). It is possible to use directly the function RiskJackplot: the default maximum dimen-

sion (argument max) is length(solution[[k]][["d"]]).

method default is "", a value "FCA" is to be used only if solution is after an FCA with

SVDgen

ZoomInOut used as xlim and ylim in xy-plots instead of max and min range

Zlabels used as labels instead of x[[mod]]\$n, it is a list with the same length as all

modes. For example on 3 modes changing the labels of the second mode only will have to set Zlabels=list(NULL,rep("a",length(x[[2]]\$n)), NULL)

... plot arguments can be passed (except xlim, ylim, ylab, pch, xaxt for compo-

nent plot, and xlab, ylab for screeplot)

### **Details**

Plot components of one or two Principal Tensors, modes are superposed if more than one is asked, or gives a screeplot. As it is using plot.default at some point some added features can be used in the ... part, especially xlab= may be useful when nb2=NULL. Plots are superposed as they correspond to the same Principal Tensor and so this gives insight to interpretation of it, but careful is recommended as only overall interpretation, once the Principal Tensor has been rebuilt mentally (*i.e.* product of signs ...) to work out oppositions or associations. The risk plot on top of a screeplot is an approximation of the Jacknife estimate of the MSE in the choice of number of dimensions (see Besse et al.(1997)).

# Note

This function is used all for FCAk, and CANDPARA, PCAn objjects notheless for this last object other interesting plots known as jointplots have not been implemented.

# Author(s)

Didier Leibovici <c3s2i@free.fr>

# References

Besse, P Cardot, H and Ferraty, F (1997) *Simultaneous non-parametric regressions of unbalanced longitudinal data*. Computational Statistics and Data Analysis, 24:255-270.

Leibovici D (2000) *Multiway Multidimensional Analysis for Pharmaco-EEG Studies*.(submitted) http://c3s2i.free.fr/cv/recentpub.html

# See Also

PTAk, PTA3, FCAk, SVDgen

24 preprocessings

# **Examples**

```
# see the demo function source(paste(R.home(),"/library/PTAk/demo/PTA3.R",sep=""));
# or source(paste(R.home(),"/library/PTAk/demo/PTAk.R",sep=""));
# demo.PTA3()
```

preprocessings

Few useful functions for preprocessing arrays

# Description

Choices of centering or detrending and scaling are important preprocessings for multiway analysis.

# Usage

# **Arguments**

dat	array
bi	vector defining the "centering, bicentering or multi-centering" one wants to operate crossed with by
by	number or vector defining the entries used "with" in the other operations
centre	function used as FUN in applying "multi-centering"
centrebyBA	a bolean vector for "centering" with centre Before and After according to by
scalebyBA	idem as centrebyBA, for scaling operation
n	number of iterations between "centering" and scaling
Mm	margins to performs Detren or fFUN on
Vm	margins to scale
fFUN	function to use as FUN if usetren is FALSE
usetren	logical, to use Detren
tren	function to use in Detren

PROJOT 25

rsd	logical passed into Detren (only) to detrend or not
У	vector (length n)
Х	vector of same length, if NULL it is 1:n
sigmak	parameter related to kernel bandwidth with y values (default is 1/2*range
sigmat	parameter related to kernel bandwidth with x values (default value is $8*n^{-1/5}$ , with a minimum number of neigbours set as one apart)
ker	a list of two kernels list("t"=function "k"=function ) for each weightings (if only one given it is used for both)

### **Details**

Multcent performs in order "centering" by by; "multicentering" for every bi with by; then scale (standard deviation) to one by by.

IterMV performs an iterative "detrending" and scaling according to te margins defined (see Leibovici(2000) and references in it).

Detren detrends (or smooths if rsd is FALSE) the data accoding to th margins given.

Susan1D performs a non-linear kernel smoothing of y against x (both reordered in the function according to orders of x) with an usual kernel (t) as for kernel regression and a kernel (t) for the values of y (the product of the kernels constitutes the non-linear weightings. This function is adapted from SUSAN algorithm (see references).

# Author(s)

Didier Leibovici <c3s2i@free.fr>

# References

Smith S.M. and J.M. Brady (1997) SUSAN - a new approach to low level image processing. International Journal of Computer Vision, 23(1):45-78, May 1997.

PROJOT Orthogonal Tensor projection
-------------------------------------

# Description

Orthogonal-tensoriel projection of a tensor according to a rank-1 tensor, or a to bigger structure defined by kronecker product of matrices.

# Usage

PROJOT(X, solu, numo=1, bortho=TRUE, Ortho=TRUE, metrics=NULL)

26 PROJOT

### **Arguments**

X a tensor(as an array) of any order

solu an object like a solutions. PTAk object with at least v

numo a vector of numbers or a list of vectors (length the order of the tensor) identifying

for each space the structure to project onto, if NULL for a specific space then no

projection is done for this space

bortho list of logicals saying if the structures are othogonal or not.

Ortho list of logicals telling the projectors on each space to be on the structure or on

its orthogonal.

metrics NULL or list of metrics (either diagonal or not) for each entry of X

#### **Details**

This function computes the *tensorial orthogonal projection* of X onto the *tensorial structure* defined by solu and numo. For each space (involved in the tensorial product where from X belongs), one defined the projector onto solu[[i]]\$v[numo,] (or on its orthogonal if Ortho[[i]]==TRUE), then the result is the image of X by the tensorial product of the projectors, i.e.

$$(P_{S1} \otimes P_{S2} \otimes \ldots \otimes P_{Sk})(X)$$

•

#### Value

A tensor with dimensions as X

### Note

For PTA-kmodes the projection used is only on rank-one tensors (Principal Tensors), *i.e.* numo is a number. The code here can be used for any structure (on each spaces) and constitutes the projector onto a tensorial structure, and can define the PTAIV-kmodes (PTAk on Instrumental Variables Leibovici(1993). (see other references for tensorial product of linear operators in Leibovici(2000) *e.g.* Dauxois et al.(1994))

### Author(s)

Didier Leibovici <c3s2i@free.fr>

# References

Leibovici D(1993) Facteurs <e0> Mesures R<e9>p<e9>t<e9>es et Analyses Factorielles : applications <e0> un suivi <e9>pid<e9>miologique. Universit<e9> de Montpellier II. PhD Thesis in Math<e9>matiques et Applications (Biostatistiques).

# See Also

PTAk

PTA3 27

# **Examples**

PTA3

Principal Tensor Analysis on 3 modes

# **Description**

Performs a truncated SVD-3 modes analysis with or without specific metrics, penalised or not.

# Usage

# **Arguments**

X	a tensor (as an array) of order $3$ , if non-identity metrics are used $X$ is a list with data as the array and met a list of metrics	
nbPT	a number specifying the number of 3modes Principal Tensors requested	
nbPT2	if 0 no 2-modes solutions will be computed, 1 =all, >1 otherwise	
smoothing	logical to consider smoothing or not	
smoo	a list of length 3 with lists of functions operating on vectors component for the appropriate dimension (see details)	

28 PTA3

minpct numerical 0-100 to control of computation of future solutions at this level and

below

verbose control printing

file output printed at the prompt if NULL, or printed in the given 'file'

modesnam character vector of the names of the modes, if NULL "mo 1" ... "mo k"

addedcomment character string printed after the title of the analysis

... any other arguments passed to SVDGen or other functions

#### **Details**

According to the decomposition described in Leibovici(1993) and Leibovici and Sabatier(1998) the function gives a generalisation of the SVD (2 modes) to 3 modes. It is the same algorithm used for PTAk but simpler as the recursivity implied by the *k* modes analysis is reduced only to one level *i.e* for every 3-modes Principal Tensors, 3 SVD are performed for every contracted product with one the three components of the 3-modes Principal Tensors (see APSOLU3, PTAk).

Recent work from Tamara G Kolda showed on an example that *orthogonal rank* decompositions are not necesseraly nested. This makes PTA-3modes a model with nested decompositions not giving the exact *orthogonal rank*. So PTA-3modes will look for best approximation according to orthogonal tensors in a nested approximation process. PTA3 decompositions is "a" generalisation of SVD but not the ...

With the smoothing option smoo contain a list of (lists) of functions to apply on vectors of component (within the algorithm, see SVDgen). For a given dimension (1,2,or 3) a list of functions is given. If this list consists only of one function (no list needed) this function will be used at any level all the time: if one want to smooth only for the first Principal Tensor, put list(function, NA). Now you start to understand this list will have a maximum length of nbPT and the corresponding function will be used for the corresponding 3 mode Principal Tensor. To smooth differently the associated solutions one have to put another level of nested lists otherwise the function given at the 3 mode level will be used for all. These rules are te same for PTAk.

# Value

a PTAk object

#### Note

The use of metrics (diagonal or not) allows flexibility of analysis like in 2 modes *e.g.* correspondence analysis, discriminant analysis, robust analysis. Smoothing option extends the analysis towards functional data analysis, and or outliers "protection" is theoretically valid for tensors belonging to a tensor product of separable Hilbert spaces (*e.g.* Sobolev spaces) (see references in PTAK, SVDgen).

#### Author(s)

Didier Leibovici <c3s2i@free.fr>

PTA3 29

#### References

Leibovici D(1993) Facteurs <e0> Mesures R<e9>p<e9>t<e9>es et Analyses Factorielles : applications <e0> un suivi <e9>pid<e9>miologique. Universit<e9> de Montpellier II. PhD Thesis in Math<e9>matiques et Applications (Biostatistiques).

Leibovici D and Sabatier R (1998) A Singular Value Decomposition of a k-ways array for a Principal Component Analysis of multi-way data, the PTA-k. Linear Algebra and its Applications, 269:307-329.

Kolda T.G (2003) A Counterexample to the Possibility of an Extension of the Eckart-Young Low-Rank Approximation Theorem for the Orthogonal Rank Tensor Decomposition. SIAM J. Matrix Analysis, 24(2):763-767, Jan. 2003.

#### See Also

```
SVDgen, FCAk, PTAk, summary.PTAk
```

# **Examples**

```
# example using Zone_climTUN dataset
# library(maptools)
# library(RColorBrewer)
# Yl=brewer.pal(11,"PuOr")
# data(Zone_climTUN)
## in fact a modified version of plot.Map was used
# plot(Zone_climTUN,ol=NA,auxvar=Zone_climTUN$att.data$PREC_OCTO)
##indicators 84 +3 to repeat
# Zone_clim<-Zone_climTUN$att.data[,c(2:13,15:26,28:39,42:53,57:80,83:95,55:56)]
# Zot <-Zone_clim[,85:87] ;temp <-colnames(Zot)</pre>
# Zot <- as.matrix(Zot)%x%t(as.matrix(rep(1,12)))</pre>
# colnames(Zot) <-c(paste(rep(temp [1],12),1:12),paste(rep(temp [2],12),1:12), paste(rep(temp [3],12),1:12))
# Zone_clim <-cbind(Zone_clim[,1:84],Zot)</pre>
# Zone3w <- array(as.vector(as.matrix(Zone_clim)),c(2599,12,10))</pre>
## preprocessing
#Zone3w<-Multcent(dat=Zone3w,bi=NULL,by=3,centre=mean, centrebyBA=c(TRUE,FALSE),scalebyBA=c(TRUE,FALSE))
# Zone3w.PTA3<-PTA3(Zone3w,nbPT=3,nbPT2=3)
## summary and plot
# summary(Zone3w.PTA3)
#plot(Zone3w.PTA3,mod=c(2,3),nb1=1,nb2=11,lengthlabels=5,coefi=list(c(1,1,1),c(1,-1,-1)))
#plot(Zone_climTUN,ol=NA,auxvar=Zone3w.PTA3[[1]]$v[1,],nclass=30)
#plot(Zone_climTUN,ol=NA,auxvar=Zone3w.PTA3[[1]]$v[11,],nclass=30)
 ##############
 cat(" A little fun using iris3 and matching randomly 15 for each iris sample!","\n")
        then performing a PTA-3modes. If many draws are done, plots")
        show the stability of the first and third Principal Tensors.","\n")
cat("iris3 is centered and reduced beforehand for each original variables.","\n")
# demo function
# source(paste(R.home(),"/library/PTAk/demo/PTA3.R",sep=""))
# demo.PTA3(bootn=10, show=5, openX11s=FALSE)
```

30 PTAk

РΊ	ГΔ	k

Principal Tensor Analysis on k modes

# **Description**

Performs a truncated SVD-kmodes analysis with or without specific metrics, penalised or not.

# Usage

# **Arguments**

Χ	tensor (as an array) of order k, if non-identity metrics are used X is a list with

data as the array and met a list of metrics

nbPT integer vector of length (k-2) specifying the maximum number of Principal Ten-

sors requested for the (3,...,k-1, k) modes levels (see details), if it is not a vector

every levels would have the same given nbPT value

nbPT2 if 0 no 2-modes solutions will be computed, 1 =all, >1 otherwise

minpct numerical 0-100 to control of computation of future solutions at this level and

below

smoothing see PTA3, SVDgen

smoo see PTA3

verbose control printing

file output printed at the prompt if NULL, or printed in the given 'file' modesnam character vector of the names of the modes, if NULL mo 1 ...mo k addedcomment character string printed if printt after the title of the analysis

... any other arguments passed to other functions

# **Details**

According to the decomposition described in Leibovici(1993) and Leibovici and Sabatier(1998) the function gives a generalisation of the SVD (2 modes) to k modes. The algorithm is recursive, calling APSOLUk which calls PTAk for (k-1). nbPT, nbPT2 and minpct control the number of Principal Tensors desired. For example nbPT=c(2,4,3) means a tensor of order 5 is analysed, the maximum number of 5-modes PT is set to 3, for each of them one sets a maximum of 4 associated 4-modes (for each of the five components), for each of these later a maximum of 2 associated 3-modes PT is asked (for each of the four components). Then nbPT2 complete for 2-modes associated or not. Overall minpct controls to carry on the algorithm at any level and lower, i.e. stops if  $100(vs^2/ssx) < minpct$  (where vs is the singular value, and ssx is the total sum of squares of the tensor X or the

PTAk 31

"metric transformed" X). Putting a 0 at a given level in nbPT obviously automatically puts 0 in nbPT at lower levels. Putting high values in nbPT allows control only on minpct helping to reach the full decomposition. All these controls allow to truncate the full decomposition in a level-controlled fashion. Notice the full decomposition always contains any possible choice of truncation, *i.e.* the solutions are not dependant on the truncation scheme (Generalised Eckart-Young Theorem).

Recent work from Tamara G Kolda showed on an example that *orthogonal rank* decompositions are not necesseraly nested. This makes PTA-*k*modes a model with nested decompositions not giving the exact *orthogonal rank*. So PTA-*k*modes will look for best approximation according to orthogonal tensors in a nested approximmation process.

#### Value

a PTAk object which consist of a list of lists. Each mode has a list in which is listed:

\$v matrix of components for the given mode

\$iter vector of iterations numbers where maximum was reach

\$test vector of test values at maximum

\$modesnam name of the mode

\$v matrix of components for the given mode

The last mode list has also some additional information on the analysis done:

\$d vector of singular values

\$pct percentage of sum of squares for each quared singular value

\$ssX vector of local sum of squares *i.e.* of the current tensor with the rescursive

algorithm

\$vsnam vector of names given to the singular value according to a recursive data depen-

dent scheme

\$datanam data reference

\$method call applied: could be PTAk or CANDPARA or PCAn or even SVDgen, with

parameters choices

\$addedcomment (repeated) given in the call

You will notice that methods other than PTAk may not have all list elements but the essential ones such as: \$v, \$d, \$ssX, and may also have additional ones like \$coremat for PCAn (the core array).

### Note

The use of metrics (diagonal or not) allows flexibility of analysis like in 2 modes *e.g.* correspondence analysis, discriminant analysis, robust analysis. Smoothing option extending the analysis towards functional data analysis is theoretically valid for Principal Tensors belonging to a tensor product of separable Hilbert spaces (*e.g.* Sobolev spaces) see Leibovici and El Maach (1997).

#### Author(s)

Didier Leibovici <c3s2i@free.fr>

32 PTAk

#### References

Leibovici D(1993) Facteurs <e0> Mesures R<e9>p<e9>t<e9>es et Analyses Factorielles : applications <e0> un suivi <e9>pid<e9>miologique. Universit<e9> de Montpellier II. PhD Thesis in Math<e9>matiques et Applications (Biostatistiques).

Leibovici D and El Maache H (1997) *Une d<e9>composition en Valeurs Singuli<e8>res d'un <e9>l<e9>ment d'un produit Tensoriel de k espaces de Hilbert S<e9>parables.* Compte Rendus de l'Acad<e9>mie des Sciences tome 325, s<e9>rie I, Statistiques (Statistics) & Probabilit<e9>s (Probability Theory): 779-782.

Leibovici D and Sabatier R (1998) A Singular Value Decomposition of a k-ways array for a Principal Component Analysis of multi-way data, the PTA-k. Linear Algebra and its Applications, 269:307-329.

Leibovici D (2008) Spatio-temporal Multiway Decomposition using Principal Tensor Analysis on k-modes:the R package PTAk. to be submitted soon at Journal of Statisticcal Software.

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#### See Also

```
REBUILD, FCAk, PTA3 summary.PTAk
```

# **Examples**

```
# don <- array((1:3)%x%rnorm(6*4)%x%(1:10),c(10,4,6,3))
don <- array(1:360,c(5,4,6,3))
don <- don + rnorm(360,1,2)
dimnames(don) <- list(paste("s",1:5,sep=""),paste("T",1:4,sep=""),</pre>
          paste("t",1:6,sep=""),c("young","normal","old"))
  # hypothetic data on learning curve at different age and period of year
ones <-list(list(v=rep(1,5)),list(v=rep(1,4)),list(v=rep(1,6)),list(v=rep(1,3)))
don <- PROJOT(don,ones)</pre>
don.sol <- PTAk(don,nbPT=1,nbPT2=2,minpct=0.01,</pre>
               verbose=TRUE,
                modesnam=c("Subjects", "Trimester", "Time", "Age"),
                 addedcomment="centered on each mode")
don.sol[[1]] # mode Subjects results and components
don.sol[[2]] # mode Trimester results and components
don.sol[[3]] # mode Time results and components
don.sol[[4]] # mode Age results and components with additional information on the call
summary(don.sol,testvar=2)
```

PTAk-internal 33

```
plot(don.sol,mod=c(1,2,3,4),nb1=1,nb2=NULL,
    xlab="Subjects/Trimester/Time/Age",main="Best rank-one approx" )
plot(don.sol,mod=c(1,2,3,4),nb1=4,nb2=NULL,
    xlab="Subjects/Trimester/Time/Age",main="Associated to Subject vs1111")
# demo function
# demo.PTAk()
```

PTAk-internal

Internal PTAk functions

# Description

Internal PTAk functions

# Usage

### **Arguments**

These functions are not supposed to be called directly.

a matrix

Xest a zero limit number

pena list of functions to be used as smoother

ini initialisation method over the dual dimension

vsmin zero limit for singular value
Maxiter limit number of iteration

A a matrix

pw power value number

eltw boolean to perform power elementwise or matrix power

34 REBUILD

B a matrix

solb an object inheriting from class PTAk sola an object inheriting from class PTAk solu an object inheriting from class PTAk

numass position number of the associated solution, NULL is equivalent to the last in

sola

verbose boolean playing a verbose role

file string pointing a destination of file output summary boolean to show the summary or not

testvar threshold control for minimum percent of variability explained with boolean expression to give a supplementary selection criterion

nomb integer giving the number of components to fit

smooth idem as pena li any list

... any other arguments passed to functions

### Author(s)

Didier Leibovici <c3s2i@free.fr>

### See Also

**PTAk** 

REBUILD	Build an approximation of the tensor of any order
KEBOIED	Butte an approximation of the tensor of any order

# **Description**

Gives the approximation of a previously analysed tensor using its given decomposition.

# Usage

REBUILD(solutions,nTens=1:2,testvar=1 ,redundancy=FALSE)

### **Arguments**

solutions a PTAk object

nTens a vector of identifying positions (numbers given in summary) for the choice of

Principal Tensors to use

testvar control within nTens used Principal Tensor with minimum percent of variability

explained

redundancy logical to take into account (within nTens) PT tested redundant during analysis

(see also RESUM) if TRUE.

SINGVA 35

#### **Details**

The function rebuilds the Principal Tensors, *i.e.* rank-one tensors of order the order of the tensor analysed, and add them up to build an approximation of the tensor analysed (according to the method used see method). This constitutes a best Least Squares (ordinary or "weighted" if metrics are used) approximation of datanam for a given orthogonal-rank r (number of principal tensors used), if and only if the singular values used are the r highest.

### Value

A tensor with dimensions as solutions[[k]][["datanam"]].

#### Note

This function can be called for PARAFAC/CANDECOMP and PCAn. A specific rebuilt is implemented for this last one.

#### Author(s)

Didier Leibovici <c3s2i@free.fr>

### See Also

**PTAk** 

SINGVA

Optimisation algorithm RPVSCC

# **Description**

Computes the best rank-one approximation using the RPVSCC algorithm.

# Usage

### **Arguments**

)	X a	tensor (	(as an array	) of ore	der k,	if non	1-1dentity	metrics a	are used X	is a list with	

data as the array and met a list of metrics

test numerical value to stop optimisation

PTnam character giving the name of the *k*-modes Principal Tensor

Maxiter if iter > Maxiter prompts to carry on or not, then do it every other 200 itera-

tions

36 SINGVA

verbose control printing

file output printed at the prompt if NULL, or printed in the given 'file'

smoothing logical to use smooth functiosns or not (see SVDgen)

smoo list of functions returning smoothed vectors (see PTA3)

modesnam character vector of the names of the modes, if NULL "mo 1" ... "mo k"

Ini method used for initialisation of the algorithm (see INITIA)

sym description of the symmetry of the tensor e.g. c(1,1,3,4,1) means the second

mode and the fifth are identical to the first

#### **Details**

The algorithm termed *RPVSCC* in Leibovici(1993) is implemented to compute the first Principal Tensor (rank-one tensor with its singular value) of the given tensor X. According to the decomposition described in Leibovici(1993) and Leibovici and Sabatier(1998), the function gives a generalisation to *k* modes of the *best rank-one approximation* issued from SVD whith 2 modes. It is identical to the PCA-*k*modes if only 1 dimension is asked in each space, and to PARAFAC/CANDECOMP if the rank of the approximation is fixed to 1. Then the methods differs, PTA-*k*modes will look for best approximation according to the *orthogonal rank* (*i.e.* the rank-one tensors (of the decomposition) are orthogonal), PCA-*k*modes will look for best approximation according to the *space ranks* (*i.e.* ranks of every bilinear form deducted from the original tensor, that is the number of components in each space), PARAFAC/CANDECOMP will look for best approximation according to the *rank* (*i.e.* the rank-one tensors are not necessarily orthogonal).

Recent work from Tamara G Kolda showed on an example that *orthogonal rank* decompositions are not necesseraly nested. This makes PTA-*k*modes a model with nested decompositions not giving the exact *orthogonal rank*. So PTA-*k*modes will look for best approximation according to orthogonal tensors in a nested approximmation process.

#### Value

a PTAk object (without datanam method)

### Note

The algorithm was derived in generalising the *transition formulae* of SVD (Leibovici 1993), can also be understood as a generalisation of the *power method* (De Lathauwer et al. 2000). In this paper they also use a similar algorithm to build bases in each space, reminiscent of three-modes and *n*-modes PCA (Kroonenberg(1980)), *i.e.* defining what they called a rank-(R1,R2,...,Rn) approximation (called here *space ranks*, see PCAn). *RPVSCC* stands for *Recherche de la Premi*<e8>re *Valeur Singuli*<e8>re par *Contraction Compl*<ea>te.

# Author(s)

Didier Leibovici <c3s2i@free.fr>

summary.PTAk 37

### References

Kroonenberg P (1983) *Three-mode Principal Component Analysis: Theory and Applications*. DSWO press. Leiden.(related references in <a href="http://three-mode.leidenuniv.nl">http://three-mode.leidenuniv.nl</a>)

Leibovici D(1993) Facteurs <e0> Mesures R<e9>p<e9>t<e9>es et Analyses Factorielles : applications <e0> un suivi <e9>pid<e9>miologique. Universit<e9> de Montpellier II. PhD Thesis in Math<e9>matiques et Applications (Biostatistiques).

Leibovici D and Sabatier R (1998) A Singular Value Decomposition of a k-ways array for a Principal Component Analysis of multi-way data, the PTA-k. Linear Algebra and its Applications, 269:307-329.

De Lathauwer L, De Moor B and Vandewalle J (2000) *On the best rank-1 and rank-(R1,R2,...,Rn) approximation of higher-order tensors*. SIAM J. Matrix Anal. Appl. 21,4:1324-1342.

Kolda T.G (2003) A Counterexample to the Possibility of an Extension of the Eckart-Young Low-Rank Approximation Theorem for the Orthogonal Rank Tensor Decomposition. SIAM J. Matrix Analysis, 24(2):763-767, Jan. 2003.

### See Also

INITIA, PTAK, PCAn, CANDPARA

summary.PTAk

Summary of a PTA-k modes analysis

# Description

Print a summary listing of the decomposition obtained.

# Usage

```
## $3 method for class 'PTAk'
summary(object,testvar=1,dontshow="*", ...)
## $3 method for class 'FCAk'
summary(object,testvar=0.5,dontshow="*", ...)
```

# **Arguments**

object	an object inheriting from class PTAk, representing a generalised singular value decomposition
testvar	control within nTens used Principal Tensor with minimum percent of variability explained
dontshow	boolean criterion to remove Principal Tensors from the summary, or default is a character "*" equivalent to the criterion: !substr(solution[[length(solution)]][["vsnam"]],1,1)=="*"
	summary generic additional arguments not used here

38 summary.PTAk

### **Details**

The function prints a listing of the decomposition with historical order (instead of traditional singular value order). It is useful before any plots or reconstruction, a screeplot (using plot.PTAk) will be also useful. It is useful before any plots r reconstruction, a screeplot (using plot.PTAk) will be also useful. summary.FCAk is alike summary.PTAk but testvar operates on the variability of the lack of complete independence.

### Value

prints on the prompt

#### Note

At the moment can be used for PCAn, CANDPRA, better summaries will be in the next release.

#### Author(s)

Didier Leibovici <c3s2i@free.fr>

#### References

Leibovici D (2000) *Multiway Multidimensional Analysis for Pharmaco-EEG Studies*.(submitted) http://c3s2i.free.fr/cv/recentpub.html

#### See Also

```
plot.PTAk
```

### **Examples**

```
data(crimerate)
crimerate.mat <- sweep(crimerate,2,apply(crimerate,2,mean))</pre>
crimerate.mat <- sweep(crimerate.mat,2,sqrt(apply(crimerate,2,var)),FUN="/")</pre>
cri.svd <- SVDgen(crimerate.mat)</pre>
summary(cri.svd,testvar=0)
plot(cri.svd,scree=TRUE)
par(new=TRUE)
RiskJackplot(cri.svd,nbvs=1:7,mod=NULL,max=NULL,rescaled=TRUE,
       axes=FALSE, ann=FALSE)
par(new=FALSE)
# or equivalently
plot(cri.svd,scree=TRUE,type="b",lty=3,RiskJack=1) #set mod=NULL or c(1,2)
###
 data(crimerate)
 criafc <- FCAmet(crimerate,chi2=TRUE)</pre>
 cri.afc <- SVDgen(criafc$data,criafc$met[[2]],criafc$met[[1]])</pre>
  summary(cri.afc)
 plot(cri.afc,scree=TRUE)
 plot(cri.afc,scree=TRUE,type="b",lty=3,RiskJack=1,method="FCA")
```

SVDgen 39

SVDgen

SVD with metrics and smoothing approximation

# **Description**

Computes the generalised Singular Value Decomposition, *i.e.* with non-identity metrics. A smooth approximation can be asked to constraint the components (u and v) to be smooth.

### Usage

# **Arguments**

Υ	a matrix $n \times p$
D2	metric in $\mathbb{R}^p$ either a vector $(p \times 1)$ or a matrix $(p \times p)$
D1	metric in $\mathbb{R}^n$ either a vector $(n \times 1)$ or a matrix $(n \times n)$
smoothing	logical if TRUE the smoothing methods in smoo are used
nomb	numeric number of components to extract (typically when smoothing is used less components are used as the screeplot becomes flatter faster)
SMOO	list of lists of smoothing functions on a vector of the approriate dimension; if on one dimension it is NA no smoothing will be done for this one; if the length of a list is one the function is used for all components. If only one list in the list it will be used for both dimensions.

#### **Details**

The function computes the decomposition  $X = UL^{1/2}V'$  where  $U'D_1U = Id_p$  and  $V'D_2V = Id_p$  and the diagonal matrix L containing no zeros squared singular values. If smoothing a constraint on Least Squares solution is used, then the above decomposition becomes an approximation (unless X belongs to the space defined by the constraints). A Power Method algorithm to compute each principal tensor is used wherein Alternated Least Squares are always followed by a smoothed version of the updated vectors. If a Spline smoothing was used the algorithm would be equivalent to use the traditional penalised least squares at each iteration and could be called Penalised Power Method or Splined Alternated Least Squares Algorithm (SALSA is already an acronym used by Besse and Ferraty (1995) in where a similar idea is developped: but smoothing operates only on variables, and is model based as the Alternating operates on the whole approximation i.e. given the choice of the dimension reduction).

40 SVDgen

#### Value

a PTAk object

#### Note

SVDgen makes use of a non-identity version svd (inbuilt) or svdksmooth which outputs like the inbuilt svd. The smoothing option is also implemented in PTA-kmodes, FCA-kmodes, PCAn and CANDECOMP/PARAFAC. The use of metrics (diagonal or not) allows flexibility of analysis like *e.g.* correspondence analysis, discriminant analysis, robust analysis. Smoothing option extends the analysis towards functional data analysis, and or outliers protection.

This smoothing penalising approach is theoretically valid for Principal Tensors (here order 2) belonging to a tensor product of separable Hilbert spaces (*e.g.* Sobolev spaces) see Leibovici and El Maach (1997), and in fact only valid for projection onto this space: this includes polynomial fitting, spline basis fitting ... As you are penalysing the alternating optimisation criterion you also need the to get a *robust fit* at each iteration to be able to reach stationarity and declare optimisation done. If the smoother is not linear one looses orthogonality of the corresponding components but they are usually not too much correlated and preserving one mode to be unsmoothed insured orthogonality of the whole decomposition. Alternatively keepOrtho insures (as a third step optimisation for each iteration) orthogonality with the previous component (but then the solution is approximatively in the space of constraints).

The flexibility of this function smoothing constraint should be carefully used. The function offers also the choice to change of smoothing (method or parameters) as the number of components grows as in Ramsay and Silverman (1997).

# Author(s)

Didier Leibovici <c3s2i@free.fr>

### References

Leibovici D and El Maache H (1997) *Une décomposition en Valeurs Singulières d'un élément d'un produit Tensoriel de k espaces de Hilbert Séparables*. Compte Rendus de l'Académie des Sciences tome 325, série I, Statistiques (Statistics) & Probabilités (Probability Theory): 779-782.

Besse P and Ferraty F (1995) Curvilinear fixed effect model. Computational Statistics, 10:339-351.

Leibovici D (2008) A Simple Penalised algorithm for SVD and Multiway functional methods. (to be submitted)

Ramsay J.O. and Silverman B.W. (1997) Functional Data Analysis. Springer Series in Statistics.

#### See Also

PTAk, PCAn, CANDPARA

# Examples

```
#library(stats)
#library(tensor)
# on smoothing
```

SVDgen 41

```
data(longley)
 long <- as.matrix(longley[,1:7])</pre>
 long.svd <- SVDgen(long,smoothing=FALSE)</pre>
 summary.PTAk(long.svd,testvar=0)
  # X11(width=4,height=4)
 plot.PTAk(long.svd,scree=TRUE,RiskJack=0,type="b",lty=3)
 long.svdo <- SVDgen(long,smoothing=TRUE,</pre>
 smoo=list(function(u)ksmooth(1:length(u),
      u,kernel="normal",bandwidth=3,x.points=(1:length(u)))$y,NA))
 summary.PTAk(long.svdo,testvar=0)
 # X11(width=4,height=4)
 plot.PTAk(long.svdo,scree=TRUE,RiskJack=0,type="b",lty=3)
 ###using polynomial fitting
   polyfit <- function(u,deg=length(u)/5)</pre>
       {n <- length(u); time <- rep(1,n);</pre>
        for(e in 1:deg)time<-cbind(time,(1:n)^e);return(lm.fit(time,u)$fitted.values)}</pre>
bsfit<-function(u,deg=42)</pre>
       {n \leftarrow length(u); time \leftarrow rep(1,n);}
        return(lm.fit(bs(time,df=deg),u)$fitted.values)}
###
long.svdo2 <- SVDgen(long,nomb=4,smoothing=TRUE,smoo=list(polyfit,NA))</pre>
 long.svdo2[[1]]$v[1:3,]
long.svdo[[1]]$v[1:3,]
# orthogonality may be lost with non-projective smoother
     ####
comtoplot <- function(com=1,solua=long.svd,solub=long.svdo,openX11s=FALSE,...)</pre>
 if(openX11s)X11(width=4,height=4)
 yla <- c(round((100*(solua[[2]]$d[com])^2)/</pre>
     solua[[2]]$ssX[1],4),
     round((100*(solub[[2]]$d[com])^2)/solua[[2]]$ssX[1],4))
limi <- range(c(solua[[1]]$v[com,],solub[[1]]$v[com,]))</pre>
 plot(solua, nb1=com, mod=1, type="b", lty=3, lengthlabels=4, cex=0.4,
   ylimit=limi,ylab="",...)
mtext(paste("vs",com,":",yla[1],"%"),2,col=2,line=2)
par(new=TRUE)
 plot.PTAk(solub,nb1=com,mod=1,labels=FALSE,type="b",lty=1,
 lengthlabels=4,cex=0.6,ylimit=limi,ylab="",main=paste("smooth vs",com,":",yla[2],"%"),...)
 par(new=FALSE)
   ####
comtoplot(com=1)
```

# on using non-diagonal metrics

42 TENSELE

```
data(crimerate)
 crimerate.mat <- sweep(crimerate,2,apply(crimerate,2,mean))</pre>
 crimerate.mat <- sweep(crimerate.mat,2,sqrt(apply(crimerate.mat,2,var)),FUN="/")</pre>
  metW <- Powmat(CauRuimet(crimerate.mat),(-1))</pre>
  # inverse of the within "group" (to play a bit more you could set m0 relating
  # the neighbourhood of states (see CauRuimet)
 cri.svd <- SVDgen(crimerate.mat,D2=1,D1=1)</pre>
 summary(cri.svd,testvar=0)
  plot(cri.svd,scree=TRUE,RiskJack=0,type="b",lty=3)
 cri.svdo <- SVDgen(crimerate.mat,D2=metW,D1=1)</pre>
   summary(cri.svdo,testvar=0)
  plot(cri.svdo,scree=TRUE,RiskJack=0,type="b",lty=3)
 # X11(width=8,height=4)
 par(mfrow=c(1,2))
  plot(cri.svd,nb1=1,nb2=2,mod=1,lengthlabels=3)
 plot(cri.svd,nb1=1,nb2=2,mod=2,lengthlabels=4,main="canonical")
 # X11(width=8,height=4)
 par(mfrow=c(1,2))
 plot(cri.svdo,nb1=1,nb2=2,mod=1,lengthlabels=3)
 plot(cri.svdo,nb1=1,nb2=2,mod=2,lengthlabels=4,
       main=expression(paste("metric ",Wg^{-1})))
###########
# demo function
 # when ima is NULL it uses the dataset timage12 but you can put any array
 # demo.SVDgen(ima=NULL,snr=3,openX11s=TRUE)
```

**TENSELE** 

Elementary Tensor product

# **Description**

Computes the Tensor Product of a list of vectors (or matrices) according to a given order.

### Usage

```
TENSELE(T,moins=NULL, asarray=TRUE, order=NULL, id=NULL)
```

# Arguments

T	a list like a PTAk object and minimally just contains v
moins	if not NULL, vector of indexes (in the list T) to skip
asarray	logical to specify the output form TRUE gives an array, FALSE gives a vector
order	if not NULL vector of length length(T), NULL is equivalent to length(T):1 as the function makes indexes in order run slowest to fastest

TENSELE 43

id

when T is a list of matrices, can be either a vector of length(T) giving indexes of the vectors for each space (following order) or a list of vectors of indexes.

# **Details**

The tensor product of the vectors (or matrices) in the list T is computed, skipping or not the indexes in moins, the output tensor is either in tensor form or in vector form. The way the tensor product is done follows order.

# Value

According to asarray the value is either an array, or a vector representing the tensor product of the vectors (not in moins), the dimension in order[1] running the slowest.

# Author(s)

Didier Leibovici <c3s2i@free.fr>

# See Also

**REBUILD** 

# **Index**

*Topic algebra	PTAk-internal, 33
APSOLU3, 2	*Topic <b>models</b>
APSOLUK, 3	COS2-CTR, 11
CANDPARA, 5	FCA2, 13
CONTRACTION, 9	FCAk, 15
COS2-CTR, 11	FCAmet, 17
FCA2, 13	PCAn, 20
FCAK, 15	REBUILD, 34
howtoPTAk, 18	*Topic <b>multivariate</b>
INITIA, 19	APSOLU3, 2
PCAn, 20	APSOLUk, 3
PROJOT, 25	CANDPARA, 5
PTA3, 27	CauRuimet, 6
PTAK, 30	COS2-CTR, 11
SINGVA, 35	FCA2, 13
summary.PTAk, 37	FCAk, 15
TENSELE, 42	FCAmet, 17
*Topic array	howtoPTAk, 18
APSOLU3, 2	INITIA, 19
APSOLUK, 3	PCAn, 20
CANDPARA, 5	plot.PTAk, 22
CONTRACTION, 9	preprocessings, 24
COS2-CTR, 11	PROJOT, 25
FCA2, 13	PTA3, 27
FCAK, 15	PTAk, 30
howtoPTAk, 18	REBUILD, 34
INITIA, 19	SINGVA, 35
PCAn, 20	summary.PTAk,37
PROJOT, 25	SVDgen, 39
PTA3, 27	*Topic principal components analysis
PTAS, 27 PTAK, 30	COS2-CTR, 11
SINGVA, 35	*Topic <b>robust</b>
	CauRuimet, 6
summary.PTAk, 37	*Topic <b>smooth</b>
TENSELE, 42	preprocessings, 24
*Topic datasets	SINGVA, 35
datasets, 12	SVDgen, 39
*Topic <b>hplot</b>	ADCOLUB 2 20
plot.PTAk, 22	APSOLU3, 2, 28
*Topic <b>misc</b>	APSOLUK, <i>3</i> , <i>3</i> , <i>10</i>

INDEX 45

```
CANDPARA, 5, 37, 40
                                                   TENSELE, 9, 42
CauRuimet, 6
                                                   timage12 (datasets), 12
CONTRACTION, 9
                                                   toplist (PTAk-internal), 33
COS2 (COS2-CTR), 11
                                                   Zone_climTUN (datasets), 12
COS2-CTR, 11
crimerate (datasets), 12
CTR (COS2-CTR), 11
datasets, 12
Detren (preprocessings), 24
FCA2, 11, 12, 13
FCAk, 11, 12, 14, 15, 17, 18, 23, 29, 32
FCAmet, 13-16, 17
Ginv (PTAk-internal), 33
howtoPTAk, 18
INITIA, 19, 37
IterMV (preprocessings), 24
Multcent (preprocessings), 24
PCAn, 20, 37, 40
plot.default, 22
plot.PTAk, 12, 22, 38
Powmat (PTAk-internal), 33
PPMA (PTAk-internal), 33
preprocessings, 24
PROJOT, 25
PTA3, 2-5, 18, 20, 23, 27, 30, 32, 36
PTAk, 2-6, 10-14, 16, 18, 20, 21, 23, 26, 28,
         29, 30, 31, 34–37, 40
PTAk-internal, 33
RaoProd (PTAk-internal), 33
REBUILD, 32, 34, 43
REBUILDPCAn (PTAk-internal), 33
RESUM (PTAk-internal), 33
RiskJackplot (plot.PTAk), 22
SINGVA, 20, 35
summary.FCAk, 12, 14, 16
summary.FCAk (summary.PTAk), 37
summary.PTAk, 22, 29, 32, 37
Susan1D (preprocessings), 24
SVDgen, 2, 4, 5, 8, 11, 13, 15, 20, 23, 28–30,
         36, 39
svdsmooth (PTAk-internal), 33
```