

# Package ‘nnTensor’

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**Title** Non-Negative Tensor Decomposition

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**Depends** R (>= 3.4.0)

**Imports** methods, MASS, fields, rTensor, plot3D, tagcloud, ggplot2

**Description** Some functions for performing non-negative matrix factorization, non-negative CANDECOMP/PARAFAC (CP) decomposition, non-negative Tucker decomposition, and generating toy model data. See Andrzej Cichock et al (2009) and the reference section of GitHub README.md <<https://github.com/rikenbit/nnTensor>>, for details of the methods.

**License** MIT + file LICENSE

**URL** <https://github.com/rikenbit/nnTensor>

**NeedsCompilation** no

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nnTensor-package	<i>Non-Negative Tensor Decomposition</i>
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## Description

Some functions for performing non-negative matrix factorization, non-negative CANDECOMP/PARAFAC (CP) decomposition, non-negative Tucker decomposition, and generating toy model data. See Andrzej Cichock et al (2009) and the reference section of GitHub README.md <<https://github.com/rikenbit/nnTensor>>, for details of the methods.

## Details

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URL:       https://github.com/rikenbit/nnTensor
Author:     Koki Tsuyuzaki [aut, cre], Manabu Ishii [aut], Itoshi Nikaido [aut]
Maintainer: Koki Tsuyuzaki <k.t.the-answer@hotmail.co.jp>
```

Index of help topics:

GabrielNMF	Gabriel-type Bi-Cross-Validation for Non-negative Matrix Factorization
NMF	Non-negative Matrix Factorization Algorithms (NMF)
NMTF	Non-negative Matrix Tri-Factorization Algorithms (NMTF)

NTD	Non-negative Tucker Decomposition Algorithms (NTD)
NTF	Non-negative CP Decomposition Algorithms (NTF)
jNMF	Joint Non-negative Matrix Factorization Algorithms (jNMF)
kFoldMaskTensor	Mask tensors generator to perform k-fold cross validation
nnTensor-package	Non-Negative Tensor Decomposition
plot.NMF	Plot function of the result of NMF function
plotTensor2D	Plot function for visualization of matrix data structure
plotTensor3D	Plot function for visualization of tensor data structure
recTensor	Tensor Reconstruction from core tensor (S) and factor matrices (A)
siNMF	Simultaneous Non-negative Matrix Factorization Algorithms (siNMF)
toyModel	Toy model data for using NMF, NTF, and NTD

**Author(s)**

NA

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**References**

- Andrzej CICHOCK, et. al., (2009). Nonnegative Matrix and Tensor Factorizations. *John Wiley & Sons, Ltd*
- Keigo Kimura, (2017). A Study on Efficient Algorithms for Nonnegative Matrix/Tensor Factorization. *Hokkaido University Collection of Scholarly and Academic Papers*
- Andrzej CICHOCKI et. al., (2007). Non-negative Tensor Factorization using Alpha and Beta Divergence. *IEEE ICASSP 2007*
- Anh Huy PHAN et. al., (2008). Multi-way Nonnegative Tensor Factorization Using Fast Hierarchical Alternating Least Squares Algorithm (HALS). *NOLTA2008*
- Andrzej CICHOCKI et. al., (2008). Fast Local Algorithms for Large Scale Nonnegative Matrix and Tensor Factorizations. *IEICE Transactions on Fundamentals of Electronics, Communications and Computer Sciences*
- Yong-Deok Kim et. al., (2007). Nonnegative Tucker Decomposition. *IEEE Conference on Computer Vision and Pattern Recognition*
- Yong-Deok Kim et. al., (2008). Nonnegative Tucker Decomposition With Alpha-Divergence. *IEEE International Conference on Acoustics, Speech and Signal Processing*
- Anh Huy Phan, (2008). Fast and efficient algorithms for nonnegative Tucker decomposition. *Advances in Neural Networks - ISNN2008*
- Anh Hyu Phan et. al. (2011). Extended HALS algorithm for nonnegative Tucker decomposition and its applications for multiway analysis and classification. *Neurocomputing*

Jean-Philippe Brunet. et. al., (2004). Metagenes and molecular pattern discovery using matrix factorization. *PNAS*

Xiaoxu Han. (2007). CANCER MOLECULAR PATTERN DISCOVERY BY SUBSPACE CONSENSUS KERNEL CLASSIFICATION

Attila Frigyesi. et. al., (2008). Non-Negative Matrix Factorization for the Analysis of Complex Gene Expression Data: Identification of Clinically Relevant Tumor Subtypes. *Cancer Informatics*

Haesun Park. et. al., (2019). Lecture 3: Nonnegative Matrix Factorization: Algorithms and Applications. *SIAM Gene Golub Summer School, Aussois France, June 18, 2019*

Chunxuan Shao. et. al., (2017). Robust classification of single-cell transcriptome data by nonnegative matrix factorization. *Bioinformatics*

Paul Fogel (2013). Permuted NMF: A Simple Algorithm Intended to Minimize the Volume of the Score Matrix

Philip M. Kim. et. al., (2003). Subsystem Identification Through Dimensionality Reduction of Large-Scale Gene Expression Data. *Genome Research*

Lucie N. Hutchins. et. al., (2008). Position-dependent motif characterization using non-negative matrix factorization. *Bioinformatics*

Patrik O. Hoyer (2004). Non-negative Matrix Factorization with Sparseness Constraints. *Journal of Machine Learning* 5

N. Fujita et al., (2018) Biomarker discovery by integrated joint non-negative matrix factorization and pathway signature analyses, *Scientific Report*

Art B. Owen et. al., (2009). Bi-Cross-Validation of the SVD and the Nonnegative Matrix Factorization. *The Annals of Applied Statistics*

### See Also

[toyModel,NMF,NTF,NTD,recTensor,plotTensor3D](#)

### Examples

```
ls("package:nnTensor")
```

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GabrielNMF

*Gabriel-type Bi-Cross-Validation for Non-negative Matrix Factorization*

---

### Description

The input data is assumed to be non-negative matrix. GabrielNMF divides the input file into four matrices (A, B, C, and D) and perform cross validation by the prediction of A from the matrices B, C, and D.

### Usage

```
GabrielNMF(X, J = 3, nx = 5, ny = 5, ...)
```

**Arguments**

X	The input matrix which has N-rows and M-columns.
J	The number of low-dimension ( $J < N, M$ ).
nx	The number of hold-out in row-wise direction ( $2 < nx < N$ ).
ny	The number of hold-out in row-wise direction ( $2 < ny < M$ ).
...	Other parameters for NMF function.

**Value**

TestRecError : The reconstruction error calculated by Gabriel-style Bi-Cross Validation.

**Author(s)**

Koki Tsuyuzaki

**References**

Art B. Owen et. al., (2009). Bi-Cross-Validation of the SVD and the Nonnegative Matrix Factorization. *The Annals of Applied Statistics*

**Examples**

```
if(interactive()){
  # Test data
  matdata <- toyModel(model = "NMF")

  # Bi-Cross-Validation
  BCV <- rep(0, length=5)
  names(BCV) <- 2:6
  for(j in seq(BCV)){
    print(j+1)
    BCV[j] <- mean(GabrielNMF(matdata, J=j+1, nx=2, ny=2)$TestRecError)
  }
  proper.rank <- as.numeric(names(BCV)[which(BCV == min(BCV))])

  # NMF
  out <- NMF(matdata, J=proper.rank)
}
```

**Description**

The input data objects are assumed to be non-negative matrices. jNMF decompose the matrices to two low-dimensional factor matrices simultaneously.

**Usage**

```
jNMF(X, M=NULL, pseudocount=.Machine$double.eps,
     initW=NULL, initV=NULL, initH=NULL, fixW=FALSE, fixV=FALSE,
     fixH=FALSE,
     L1_W=1e-10, L1_V=1e-10, L1_H=1e-10,
     L2_W=1e-10, L2_V=1e-10, L2_H=1e-10,
     J = 3, w=NULL, algorithm = c("Frobenius", "KL", "IS", "PLTF"),
     p=1, thr = 1e-10, num.iter = 100, viz = FALSE,
     figdir = NULL, verbose = FALSE)
```

**Arguments**

X	A list containing input matrices ( $X_k$ , $\langle N \times M_k \rangle$ , $k=1..K$ ).
M	A list containing the mask matrices ( $X_k$ , $\langle N \times M_k \rangle$ , $k=1..K$ ). If the input matrix has missing values, specify the element as 0 (otherwise 1).
pseudocount	The pseudo count to avoid zero division, when the element is zero (Default: Machine Epsilon).
initW	The initial values of factor matrix W, which has N-rows and J-columns (Default: NULL).
initV	A list containing the initial values of multiple factor matrices ( $V_k$ , $\langle N \times J \rangle$ , $k=1..K$ , Default: NULL).
initH	A list containing the initial values of multiple factor matrices ( $H_k$ , $\langle M_k \times J \rangle$ , $k=1..K$ , Default: NULL).
fixW	Whether the factor matrix W is updated in each iteration step (Default: FALSE).
fixV	Whether the factor matrices $V_k$ are updated in each iteration step (Default: FALSE).
fixH	Whether the factor matrices $H_k$ are updated in each iteration step (Default: FALSE).
L1_W	Parameter for L1 regularization (Default: 1e-10). This also works as small positive constant to prevent division by zero, so should be set as 0.
L1_V	Parameter for L1 regularization (Default: 1e-10). This also works as small positive constant to prevent division by zero, so should be set as 0.
L1_H	Parameter for L1 regularization (Default: 1e-10). This also works as small positive constant to prevent division by zero, so should be set as 0.
L2_W	Parameter for L2 regularization (Default: 1e-10).
L2_V	Parameter for L2 regularization (Default: 1e-10).
L2_H	Parameter for L2 regularization (Default: 1e-10).
J	Number of low-dimension ( $J < N, M_k$ ).
w	Weight vector (Default: NULL)
algorithm	Divergence between X and $\bar{X}$ . "Frobenius", "KL", and "IS" are available (Default: "KL").
p	The parameter of Probabilistic Latent Tensor Factorization ( $p=0$ : Frobenius, $p=1$ : KL, $p=2$ : IS)

thr	When error change rate is lower than thr, the iteration is terminated (Default: 1E-10).
num.iter	The number of iteration step (Default: 100).
viz	If viz == TRUE, internal reconstructed matrix can be visualized.
figdir	the directory for saving the figure, when viz == TRUE.
verbose	If verbose == TRUE, Error change rate is generated in console windos.

### Value

W : A matrix which has N-rows and J-columns ( $J < N$ , Mk). V : A list which has multiple elements containing N-rows and J-columns ( $J < N$ , Mk). H : A list which has multiple elements containing Mk-rows and J-columns matrix ( $J < N$ , Mk). RecError : The reconstruction error between data matrix and reconstructed matrix from W and H. TrainRecError : The reconstruction error calculated by training set (observed values specified by M). TestRecError : The reconstruction error calculated by test set (missing values specified by M). RelChange : The relative change of the error.

### Author(s)

Koki Tsuyuzaki

### References

- Liviu Badea, (2008) Extracting Gene Expression Profiles Common to Colon and Pancreatic Adenocarcinoma using Simultaneous nonnegative matrix factorization. *Pacific Symposium on Biocomputing* 13:279-290
- Shihua Zhang, et al. (2012) Discovery of multi-dimensional modules by integrative analysis of cancer genomic data. *Nucleic Acids Research* 40(19), 9379-9391
- Zi Yang, et al. (2016) A non-negative matrix factorization method for detecting modules in heterogeneous omics multi-modal data, *Bioinformatics* 32(1), 1-8
- Y. Kenan Yilmaz et al., (2010) Probabilistic Latent Tensor Factorization, *International Conference on Latent Variable Analysis and Signal Separation* 346-353
- N. Fujita et al., (2018) Biomarker discovery by integrated joint non-negative matrix factorization and pathway signature analyses, *Scientific Report*

### Examples

```
matdata <- toyModel(model = "siNMF_Hard")
out <- jNMF(matdata, J=2, num.iter=2)
```

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kFoldMaskTensor	<i>Mask tensors generator to perform k-fold cross validation</i>
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### Description

The output multiple mask tensors can be immediately specified as the argument M for NTF() or NTD().

### Usage

```
kFoldMaskTensor(X, k=5, avoid.zero=TRUE, seeds=123)
```

### Arguments

X	An rTensor object.
k	Number of split for k-fold cross validation.
avoid.zero	If TRUE, only non-zero elements are splitted (Default: TRUE).
seeds	Random seed to use for set.seed().

### Author(s)

Koki Tsuyuzaki

### Examples

```
tensordata <- toyModel(model = "CP")  
Ms <- kFoldMaskTensor(tensordata, k=5, avoid.zero=TRUE, seeds=123)
```

---

NMF	<i>Non-negative Matrix Factorization Algorithms (NMF)</i>
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### Description

The input data is assumed to be non-negative matrix. NMF decompose the matrix to two low-dimensional factor matrices. This function is also used as initialization step of tensor decomposition (see also NTF and NTD).



**Usage**

```

NMF(X, M=NULL, pseudocount=.Machine$double.eps, initU=NULL, initV=NULL,
    fixU=FALSE, fixV=FALSE,
    L1_U=1e-10, L1_V=1e-10, L2_U=1e-10, L2_V=1e-10, J = 3,
    rank.method=c("all", "ccc", "dispersion", "rss", "evar", "residuals",
    "sparseness.basis", "sparseness.coef", "sparseness2.basis",
    "sparseness2.coef", "norm.info.gain.basis", "norm.info.gain.coef",
    "singular", "volume", "condition"), runtime=30,
    algorithm = c("Frobenius", "KL", "IS", "Pearson", "Hellinger", "Neyman",
    "Alpha", "Beta", "ALS", "PGD", "HALS", "GCD", "Projected", "NHR", "DTPP",
    "Orthogonal", "OrthReg"), Alpha = 1, Beta = 2,
    eta = 1e-04, thr1 = 1e-10, thr2 = 1e-10, tol = 1e-04,
    num.iter = 100, viz = FALSE, figdir = NULL, verbose = FALSE)

```

**Arguments**

X	The input matrix which has N-rows and M-columns.
M	The mask matrix which has N-rows and M-columns. If the input matrix has missing values, specify the element as 0 (otherwise 1).
pseudocount	The pseudo count to avoid zero division, when the element is zero (Default: Machine Epsilon).
initU	The initial values of factor matrix U, which has N-rows and J-columns (Default: NULL).
initV	The initial values of factor matrix V, which has M-rows and J-columns (Default: NULL).
fixU	Whether the factor matrix U is updated in each iteration step (Default: FALSE).
fixV	Whether the factor matrix V is updated in each iteration step (Default: FALSE).
L1_U	Parameter for L1 regularization (Default: 1e-10). This also works as small positive constant to prevent division by zero, so should be set as 0.
L1_V	Parameter for L1 regularization (Default: 1e-10). This also works as small positive constant to prevent division by zero, so should be set as 0.
L2_U	Parameter for L2 regularization (Default: 1e-10).
L2_V	Parameter for L2 regularization (Default: 1e-10).
J	The number of low-dimension ( $J < N, M$ ). If a numerical vector is specified (e.g. 2:6), the appropriate rank is estimated.
rank.method	The rank estimation method (Default: "all"). Only if the J option is specified as a numerical vector longer than two, this option will be active.
runtime	The number of trials to estimate rank (Default: 10).
algorithm	NMF algorithms. "Frobenius", "KL", "IS", "Pearson", "Hellinger", "Neyman", "Alpha", "Beta", "ALS", "PGD", "HALS", "GCD", "Projected", "NHR", "DTPP", "Orthogonal", and "OrthReg" are available (Default: "Frobenius").
Alpha	The parameter of Alpha-divergence.
Beta	The parameter of Beta-divergence.

eta	The stepsize for PGD algorithm (Default: 0.0001).
thr1	When error change rate is lower than thr1, the iteration is terminated (Default: 1E-10).
thr2	If the minus-value is generated, replaced as thr2 (Default: 1E-10). This value is used within the internal function .positive().
tol	The tolerance parameter used in GCD algorithm.
num.iter	The number of iteration step (Default: 100).
viz	If viz == TRUE, internal reconstructed matrix can be visualized.
figdir	The directory for saving the figure, when viz == TRUE.
verbose	If verbose == TRUE, Error change rate is generated in console window.

### Value

U : A matrix which has N-rows and J-columns ( $J < N, M$ ). V : A matrix which has M-rows and J-columns ( $J < N, M$ ). J : The number of dimension ( $J < N, M$ ). RecError : The reconstruction error between data tensor and reconstructed tensor from U and V. TrainRecError : The reconstruction error calculated by training set (observed values specified by M). TestRecError : The reconstruction error calculated by test set (missing values specified by M). RelChange : The relative change of the error. Trial : All the results of the trials to estimate the rank. Runtime : The number of the trials to estimate the rank. RankMethod : The rank estimation method.

### Author(s)

Koki Tsuyuzaki

### References

Andrzej CICHOCK, et. al., (2009). Nonnegative Matrix and Tensor Factorizations. *John Wiley & Sons, Ltd*

Keigo Kimura, (2017). A Study on Efficient Algorithms for Nonnegative Matrix/ Tensor Factorization. *Hokkaido University Collection of Scholarly and Academic Papers*

### Examples

```
if(interactive()){
  # Test data
  matdata <- toyModel(model = "NMF")

  # Simple usage
  out <- NMF(matdata, J=5)

  # Rank estimation mode (single method)
  out2 <- NMF(matdata, J=2:10, rank.method="ccc", runtime=3)
  plot(out2)

  # Rank estimation mode (all method)
  out3 <- NMF(matdata, J=2:10, rank.method="all", runtime=10)
  plot(out3)
}
```

**Description**

The input data is assumed to be non-negative matrix. NMTF decompose the matrix to three low-dimensional factor matrices.

**Usage**

```
NMTF(X, pseudocount=.Machine$double.eps,
      initU=NULL, initS=NULL, initV=NULL,
      fixU=FALSE, fixS=FALSE, fixV=FALSE,
      L1_U=1e-10, L1_S=1e-10, L1_V=1e-10,
      L2_U=1e-10, L2_S=1e-10, L2_V=1e-10,
      orthU=FALSE, orthV=FALSE,
      rank = c(3, 4),
      algorithm = c("Frobenius", "KL", "IS", "ALS", "PG", "COD", "Beta"),
      Beta = 2, root = FALSE, thr = 1e-10, num.iter = 100,
      viz = FALSE, figdir = NULL, verbose = FALSE)
```

**Arguments**

X	The input matrix which has N-rows and M-columns.
pseudocount	The pseudo count to avoid zero division, when the element is zero (Default: Machine Epsilon).
initU	The initial values of factor matrix U, which has N-rows and J1-columns (Default: NULL).
initS	The initial values of factor matrix S, which has J1-rows and J2-columns (Default: NULL).
initV	The initial values of factor matrix V, which has M-rows and J2-columns (Default: NULL).
fixU	Whether the factor matrix U is updated in each iteration step (Default: FALSE).
fixS	Whether the factor matrix S is updated in each iteration step (Default: FALSE).
fixV	Whether the factor matrix V is updated in each iteration step (Default: FALSE).
L1_U	Paramter for L1 regularitation (Default: 1e-10).
L1_S	Paramter for L1 regularitation (Default: 1e-10).
L1_V	Paramter for L1 regularitation (Default: 1e-10).
L2_U	Paramter for L2 regularitation (Default: 1e-10).
L2_S	Paramter for L2 regularitation (Default: 1e-10).
L2_V	Paramter for L2 regularitation (Default: 1e-10).
orthU	Whether the column vectors of matrix U are orthogonalized (Default: FALSE).

orthV	Whether the column vectors of matrix V are orthogonalized (Default: FALSE).
rank	The number of low-dimension (J1 (< N) and J2 (< M)) (Default: c(3,4)).
algorithm	NMTF algorithms. "Frobenius", "KL", "IS", "ALS", "PG", "COD", and "Beta" are available (Default: "Frobenius").
Beta	The parameter of Beta-divergence (Default: 2, which means "Frobenius").
root	Whether square root is calculated in each iteration (Default: FALSE).
thr	When error change rate is lower than thr, the iteration is terminated (Default: 1E-10).
num.iter	The number of iteration step (Default: 100).
viz	If viz == TRUE, internal reconstructed matrix can be visualized.
figdir	The directory for saving the figure, when viz == TRUE.
verbose	If verbose == TRUE, Error change rate is generated in console window.

### Value

U : A matrix which has N-rows and J1-columns (J1 < N). S : A matrix which has J1-rows and J2-columns. V : A matrix which has M-rows and J2-columns (J2 < M). RecError : The reconstruction error between data tensor and reconstructed tensor from U and V. RelChange : The relative change of the error. algorithm: algorithm specified.

### Author(s)

Koki Tsuyuzaki

### References

Fast Optimization of Non-Negative Matrix Tri-Factorization: Supporting Information, Andrej Copar, et. al., *PLOS ONE*, 14(6), e0217994, 2019

Co-clustering by Block Value Decomposition, Bo Long et al., *SIGKDD'05*, 2005

Orthogonal Nonnegative Matrix Tri-Factorizations for Clustering, Chris Ding et. al., *12th ACM SIGKDD*, 2006

### Examples

```
if(interactive()){
  # Test data
  matdata <- toyModel(model = "NMF")

  # Simple usage
  out <- NMTF(matdata, rank=c(4,4))
}
```

NTD

*Non-negative Tucker Decomposition Algorithms (NTD)***Description**

The input data is assumed to be non-negative tensor. NTD decompose the tensor to the dense core tensor (S) and low-dimensional factor matrices (A).

**Usage**

```
NTD(X, M=NULL, pseudocount=.Machine$double.eps, initS=NULL, initA=NULL,
    fixS=FALSE, fixA=FALSE, L1_A=1e-10, L2_A=1e-10, rank = c(3, 3, 3),
    modes = 1:3,
    algorithm = c("Frobenius", "KL", "IS", "Pearson", "Hellinger", "Neyman",
        "HALS", "Alpha", "Beta", "NMF"), init = c("NMF", "ALS", "Random"),
    nmf.algorithm = c("Frobenius", "KL", "IS", "Pearson", "Hellinger", "Neyman",
        "Alpha", "Beta", "ALS", "PGD", "HALS", "GCD", "Projected", "NHR", "DTPP",
        "Orthogonal", "OrthReg"),
    Alpha = 1,
    Beta = 2, thr = 1e-10, num.iter = 100, num.iter2 = 10, viz = FALSE,
    figdir = NULL, verbose = FALSE)
```

**Arguments**

X	The input tensor which has I1, I2, and I3 dimensions.
M	The mask tensor which has I1, I2, and I3 dimensions. If the mask tensor has missing values, specify the element as 0 (otherwise 1).
pseudocount	The pseudo count to avoid zero division, when the element is zero (Default: Machine Epsilon).
initS	The initial values of core tensor which has J1, J2, and J3 dimensions (Default: NULL).
initA	A list containing the initial values of multiple factor matrices (A_k, <Ik*Jk>, k=1..K, Default: NULL).
fixS	Whether the core tensor S is updated in each iteration step (Default: FALSE).
fixA	Whether the factor matrices Ak are updated in each iteration step (Default: FALSE).
L1_A	Paramter for L1 regularitation (Default: 1e-10). This also works as small positive constant to prevent division by zero, so should be set as 0.
L2_A	Paramter for L2 regularitation (Default: 1e-10).
rank	The number of low-dimension in each mode (J1, J2, J3, J1<I1, J2<I2, J3 < I3) (Default: c(3,3,3)).
modes	The vector of the modes on whih to perform the decomposition (Default: 1:3 <all modes>).

algorithm	NTD algorithms. "Frobenius", "KL", "IS", "Pearson", "Hellinger", "Neyman", "HALS", "Alpha", "Beta", "NMF" are available (Default: "Frobenius").
nmf.algorithm	NMF algorithms, when the algorithm is "NMF". "Frobenius", "KL", "IS", "Pearson", "Hellinger", "Neyman", "Alpha", "Beta", "ALS", "PGD", "HALS", "GCD", "Projected", "NHR", "DTPP", "Orthogonal", and "OrthReg" are available (Default: "Frobenius").
init	The initialization algorithms. "NMF", "ALS", and "Random" are available (Default: "NMF").
Alpha	The parameter of Alpha-divergence.
Beta	The parameter of Beta-divergence.
thr	When error change rate is lower than thr1, the iteration is terminated (Default: 1E-10).
num.iter	The number of iteration step (Default: 100).
num.iter2	The number of NMF iteration step, when the algorithm is "NMF" (Default: 10).
viz	If viz == TRUE, internal reconstructed tensor can be visualized.
figdir	the directory for saving the figure, when viz == TRUE (Default: NULL).
verbose	If verbose == TRUE, Error change rate is generated in console windos.

### Value

S : Tensor object, which is defined as S4 class of rTensor package. A : A list containing three factor matrices. RecError : The reconstruction error between data tensor and reconstructed tensor from S and A. TrainRecError : The reconstruction error calculated by training set (observed values specified by M). TestRecError : The reconstruction error calculated by test set (missing values specified by M). RelChange : The relative change of the error.

### Author(s)

Koki Tsuyuzaki

### References

- Yong-Deok Kim et. al., (2007). Nonnegative Tucker Decomposition. *IEEE Conference on Computer Vision and Pattern Recognition*
- Yong-Deok Kim et. al., (2008). Nonnegative Tucker Decomposition With Alpha-Divergence. *IEEE International Conference on Acoustics, Speech and Signal Processing*
- Anh Huy Phan, (2008). Fast and efficient algorithms for nonnegative Tucker decomposition. *Advances in Neural Networks - ISNN2008*
- Anh Hyu Phan et. al. (2011). Extended HALS algorithm for nonnegative Tucker decomposition and its applications for multiway analysis and classification. *Neurocomputing*

### See Also

[plotTensor3D](#)

## Examples

```

tensordata <- toyModel(model = "Tucker")
out <- NTD(tensordata, rank=c(2,2,2), algorithm="Frobenius",
  init="Random", num.iter=2)

```

---

NTF

*Non-negative CP Decomposition Algorithms (NTF)*


---

## Description

The input data is assumed to be non-negative tensor. NTF decompose the tensor to the diagonal core tensor (S) and low-dimensional factor matrices (A).

## Usage

```

NTF(X, M=NULL, pseudocount=.Machine$double.eps, initA=NULL,
  fixA=FALSE, L1_A=1e-10, L2_A=1e-10, rank = 3,
  algorithm = c("Frobenius", "KL", "IS", "Pearson", "Hellinger", "Neyman",
    "HALS", "Alpha-HALS", "Beta-HALS", "Alpha", "Beta"),
  init = c("NMF", "ALS", "Random"), Alpha = 1,
  Beta = 2, thr = 1e-10, num.iter = 100, viz = FALSE,
  figdir = NULL, verbose = FALSE)

```

## Arguments

X	The input tensor which has I1, I2, and I3 dimensions.
M	The mask tensor which has I1, I2, and I3 dimensions. If the mask tensor has missing values, specify the element as 0 (otherwise 1).
pseudocount	The pseudo count to avoid zero division, when the element is zero (Default: Machine Epsilon).
initA	A list containing the initial values of multiple factor matrices (A <sub>k</sub> , <I <sub>k</sub> *J <sub>k</sub> >, k=1..K, Default: NULL).
fixA	Whether the factor matrices A <sub>k</sub> are updated in each iteration step (Default: FALSE).
L1_A	Parameter for L1 regularization (Default: 1e-10). This also works as small positive constant to prevent division by zero, so should be set as 0.
L2_A	Parameter for L2 regularization (Default: 1e-10).
rank	The number of low-dimension in each mode (J1=J2=J3, J1<I1, J2<I2, J3 < I3) (Default: 3).
algorithm	NTF algorithms. "Frobenius", "KL", "IS", "Pearson", "Hellinger", "Neyman", "HALS", "Alpha-HALS", "Beta-HALS", "Alpha", and "Beta" are available (Default: "Frobenius").
init	The initialization algorithms. "NMF", "ALS", and "Random" are available (Default: "NMF").

Alpha	The parameter of Alpha-divergence.
Beta	The parameter of Beta-divergence.
thr	When error change rate is lower than thr1, the iteration is terminated (Default: 1E-10).
num.iter	The number of iteration step (Default: 100).
viz	If viz == TRUE, internal reconstructed tensor can be visualized.
figdir	the directory for saving the figure, when viz == TRUE (Default: NULL).
verbose	If verbose == TRUE, Error change rate is generated in console windos.

### Value

S : Tensor object, which is defined as S4 class of rTensor package. A : A list containing three factor matrices. RecError : The reconstruction error between data tensor and reconstructed tensor from S and A. TrainRecError : The reconstruction error calculated by training set (observed values specified by M). TestRecError : The reconstruction error calculated by test set (missing values specified by M). RelChange : The relative change of the error.

### Author(s)

Koki Tsuyuzaki

### References

Andrzej CICHOCKI et. al., (2007). Non-negative Tensor Factorization using Alpha and Beta Divergence. *IEEE ICASSP 2007*

Anh Huy PHAN et. al., (2008). Multi-way Nonnegative Tensor Factorization Using Fast Hierarchical Alternating Least Squares Algorithm (HALS). *NOLTA2008*

Andrzej CICHOCKI et. al., (2008). Fast Local Algorithms for Large Scale Nonnegative Matrix and Tensor Factorizations. *IEICE Transactions on Fundamentals of Electronics, Communications and Computer Sciences*

### See Also

[plotTensor3D](#)

### Examples

```
tensordata <- toyModel(model = "CP")
out <- NTF(tensordata, rank=3, algorithm="Beta-HALS", num.iter=2)
```



---

`plot.NMF`*Plot function of the result of NMF function*

---

**Description**

Only if J is specified as a vector longer than 1, this function will be active.

**Usage**

```
plot(x, ...)
```

**Arguments**

x	The result of NMF function (NMF class).
...	Optional parameter for plot.

**Value**

A ggplot will be generated.

**Author(s)**

Koki Tsuyuzaki

**References**

- Jean-Philippe Brunet. et. al., (2004). Metagenes and molecular pattern discovery using matrix factorization. *PNAS*
- Xiaoxu Han. (2007). CANCER MOLECULAR PATTERN DISCOVERY BY SUBSPACE CONSENSUS KERNEL CLASSIFICATION
- Attila Frigyesi. et. al., (2008). Non-Negative Matrix Factorization for the Analysis of Complex Gene Expression Data: Identification of Clinically Relevant Tumor Subtypes. *Cancer Informatics*
- Haesun Park. et. al., (2019). Lecture 3: Nonnegative Matrix Factorization: Algorithms and Applications. *SIAM Gene Golub Summer School, Aussois France, June 18, 2019*
- Chunxuan Shao. et. al., (2017). Robust classification of single-cell transcriptome data by nonnegative matrix factorization. *Bioinformatics*
- Paul Fogel (2013). Permuted NMF: A Simple Algorithm Intended to Minimize the Volume of the Score Matrix
- Philip M. Kim. et. al., (2003). Subsystem Identification Through Dimensionality Reduction of Large-Scale Gene Expression Data. *Genome Research*
- Lucie N. Hutchins. et. al., (2008). Position-dependent motif characterization using non-negative matrix factorization. *Bioinformatics*
- Patrik O. Hoyer (2004). Non-negative Matrix Factorization with Sparseness Constraints. *Journal of Machine Learning* 5

**Examples**

```
plot.NMF
```

---

```
plotTensor2D
```

---

*Plot function for visualization of matrix data structure*

---

**Description**

Combined with recTensor function and the result of NTF or NTD, the reconstructed tensor structure can be visullized.

**Usage**

```
plotTensor2D(X = NULL, method=c("sd", "mad"),
             sign=c("positive", "negative", "both"), thr=2)
```

**Arguments**

X	Matrix object.
method	Cutoff method to focus on large/small value in the tensor data (Default: "sd").
sign	Direction to cutoff the large/small value in the tensor data (Default: "positive").
thr	Threshold of cutoff method (Default: 2).

**Author(s)**

Koki Tsuyuzaki

**Examples**

```
tensordata <- toyModel(model = "CP")
out <- NTF(tensordata, rank=3, num.iter=2)
tmp <- tempdir()
png(filename=paste0(tmp, "/NTF.png"))
plotTensor2D(out$A[[1]])
dev.off()
```

---

plotTensor3D	<i>Plot function for visualization of tensor data structure</i>
--------------	---

---

**Description**

Combined with recTensor function and the result of NTF or NTD, the reconstructed tensor structure can be visullized.

**Usage**

```
plotTensor3D(X = NULL, method=c("sd", "mad"),
             sign=c("positive", "negative", "both"), thr=2)
```

**Arguments**

X	Tensor object, which is defined as S4 class of rTensor package.
method	Cutoff method to focus on large/small value in the tensor data (Default: "sd").
sign	Direction to cutoff the large/small value in the tensor data (Default: "positive").
thr	Threshold of cutoff method (Default: 2).

**Author(s)**

Koki Tsuyuzaki

**Examples**

```
tensordata <- toyModel(model = "CP")

out <- NTF(tensordata, rank=3, algorithm="Beta-HALS", num.iter=2)

tmp <- tempdir()

png(filename=paste0(tmp, "/NTF.png"))
plotTensor3D(recTensor(out$S, out$A))
dev.off()
```

---

recTensor	<i>Tensor Reconstruction from core tensor (S) and factor matrices (A)</i>
-----------	---

---

**Description**

Combined with plotTensor3D function and the result of NTF or NTD, the reconstructed tesor structure can be visullized.

**Usage**

```
recTensor(S = NULL, A = NULL, idx = 1:3, reverse = FALSE)
```

**Arguments**

S	Tensor object, which is defined as S4 class of rTensor package.
A	A list containing three factor matrices.
idx	The direction of mode-n multiplication (Default: 1:3). For example idx=1 is defined. $S \times_1 A$ is calculated ( $\times_1$ : mode-1 multiplication).
reverse	If reverse = TRUE, $t(A[[n]])$ is multiplied to S (Default: FALSE).

**Value**

Tensor object, which is defined as S4 class of rTensor package.

**Author(s)**

Koki Tsuyuzaki

**See Also**

[Tensor-class](#), [NTF](#), [NTD](#)

**Examples**

```
tensordata <- toyModel(model = "CP")
out <- NTF(tensordata, rank=3, algorithm="Beta-HALS", num.iter=2)
rec <- recTensor(out$S, out$A)
```

---

 siNMF

---

*Simultaneous Non-negative Matrix Factorization Algorithms (siNMF)*


---

**Description**

The input data objects are assumed to be non-negative matrices. siNMF decompose the matrices to two low-dimensional factor matrices simultaneously.

**Usage**

```
siNMF(X, M=NULL, pseudocount=.Machine$double.eps, initW=NULL, initH=NULL,
      fixW=FALSE, fixH=FALSE,
      L1_W=1e-10, L1_H=1e-10, L2_W=1e-10, L2_H=1e-10, J = 3,
      w=NULL, algorithm = c("Frobenius", "KL", "IS", "PLTF"), p=1,
      thr = 1e-10, num.iter = 100,
      viz = FALSE, figdir = NULL, verbose = FALSE)
```

**Arguments**

X	A list containing the input matrices ( $X_k$ , $\langle N \times M_k \rangle$ , $k=1..K$ ).
M	A list containing the mask matrices ( $X_k$ , $\langle N \times M_k \rangle$ , $k=1..K$ ). If the input matrix has missing values, specify the element as 0 (otherwise 1).
pseudocount	The pseudo count to avoid zero division, when the element is zero (Default: Machine Epsilon).
initW	The initial values of factor matrix W, which has N-rows and J-columns (Default: NULL).
initH	A list containing the initial values of multiple factor matrices ( $H_k$ , $\langle M_k \times J \rangle$ , $k=1..K$ , Default: NULL).
fixW	Whether the factor matrix W is updated in each iteration step (Default: FALSE).
fixH	Whether the factor matrices $H_k$ are updated in each iteration step (Default: FALSE).
L1_W	Parameter for L1 regularization (Default: 1e-10). This also works as small positive constant to prevent division by zero, so should be set as 0.
L1_H	Parameter for L1 regularization (Default: 1e-10). This also works as small positive constant to prevent division by zero, so should be set as 0.
L2_W	Parameter for L2 regularization (Default: 1e-10).
L2_H	Parameter for L2 regularization (Default: 1e-10).
J	Number of low-dimension ( $J < N, M_k$ ).
w	Weight vector (Default: NULL)
algorithm	Divergence between X and $X_{bar}$ . "Frobenius", "KL", and "IS" are available (Default: "KL").
p	The parameter of Probabilistic Latent Tensor Factorization (p=0: Frobenius, p=1: KL, p=2: IS)
thr	When error change rate is lower than thr, the iteration is terminated (Default: 1E-10).
num.iter	The number of iteration step (Default: 100).
viz	If viz == TRUE, internal reconstructed matrix can be visualized.
figdir	the directory for saving the figure, when viz == TRUE.
verbose	If verbose == TRUE, Error change rate is generated in console window.

**Value**

W : A matrix which has N-rows and J-columns ( $J < N, M_k$ ). H : A list which has multiple elements containing  $M_k$ -rows and J-columns matrix ( $J < N, M_k$ ). RecError : The reconstruction error between data matrix and reconstructed matrix from W and H. TrainRecError : The reconstruction error calculated by training set (observed values specified by M). TestRecError : The reconstruction error calculated by test set (missing values specified by M). RelChange : The relative change of the error.

**Author(s)**

Koki Tsuyuzaki

## References

- Liviu Badea, (2008) Extracting Gene Expression Profiles Common to Colon and Pancreatic Adenocarcinoma using Simultaneous nonnegative matrix factorization. *Pacific Symposium on Biocomputing* 13:279-290
- Shihua Zhang, et al. (2012) Discovery of multi-dimensional modules by integrative analysis of cancer genomic data. *Nucleic Acids Research* 40(19), 9379-9391
- Zi Yang, et al. (2016) A non-negative matrix factorization method for detecting modules in heterogeneous omics multi-modal data, *Bioinformatics* 32(1), 1-8
- Y. Kenan Yilmaz et al., (2010) Probabilistic Latent Tensor Factorization, *International Conference on Latent Variable Analysis and Signal Separation* 346-353
- N. Fujita et al., (2018) Biomarker discovery by integrated joint non-negative matrix factorization and pathway signature analyses, *Scientific Report*

## Examples

```
matdata <- toyModel(model = "siNMF_Easy")
out <- siNMF(matdata, J=2, num.iter=2)
```

---

toyModel

*Toy model data for using NMF, NTF, and NTD*

---

## Description

The data is used for confirming the algorithm are properly working.

## Usage

```
toyModel(model = "CP", seeds=123)
```

## Arguments

- |       |  |
|-------|--|
| model | Single character string is specified. "NMF", "CP", and "Tucker" are available (Default: "CP"). |
| seeds | Random number for setting set.seeds in the function (Default: 123).                            |

## Value

If model is specified as "NMF", a matrix is generated. Otherwise, a tensor is generated.

## Author(s)

Koki Tsuyuzaki

## See Also

[NMF](#), [NTF](#), [NTD](#)

**Examples**

```
matdata <- toyModel(model = "NMF", seeds=123)
tensordata1 <- toyModel(model = "CP", seeds=123)
tensordata2 <- toyModel(model = "Tucker", seeds=123)
```

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