

TensorLABsp Documentation Release 0.1

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Project TensorLABsp

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Warning: This documentation is work-in-progress and unorganized.

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ONE

BASIS OF TENSOR ALGEBRA

1.1 Matrix Multiplication

Several special matrix products are important for representation of tensor factorizations and decompositions.

1.1.1 Hadamard product

Definition: The Hadamard product of two equal-sizematrices is the **elementwise product** denoted as ⊛ and defined as

$$A \circledast B = \begin{bmatrix} a_{11}b_{11} & a_{12}b_{12} & \cdots & a_{1n}b_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}b_{m1} & a_{m2}b_{m2} & \cdots & a_{mn}b_{mn} \end{bmatrix}$$

Matlab example:

```
>> A = [1,2;3,4]; B = [2,1;1,2];
>> A .* B

ans =

2  2
3  8
```

Python example:

1.1.2 Kroneker product

Definition: The Kronecker product of two matrices $A \in \mathbb{R}^{I \times J}$ and $B \in R^{T \otimes R}$ is a matrix denoted as $A \circledast B \in R^{IT \times JR}$ and defined as

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{11} \mathbf{B} & a_{12} \mathbf{B} & \cdots & a_{1J} \mathbf{B} \\ a_{21} \mathbf{B} & a_{22} \mathbf{B} & \cdots & a_{2J} \mathbf{B} \\ \vdots & \vdots & \ddots & \vdots \\ a_{I1} \mathbf{B} & a_{I2} \mathbf{B} & \cdots & a_{IJ} \mathbf{B} \end{bmatrix}$$

$$= [\mathbf{a}_1 \otimes \mathbf{b}_1 \ \mathbf{a}_1 \otimes \mathbf{b}_2 \ \mathbf{a}_1 \otimes \mathbf{b}_3 \ \cdots \ \mathbf{a}_J \otimes \mathbf{b}_{R-1} \ \mathbf{a}_J \otimes \mathbf{b}_R].$$

Python function:

numpy.kron	Kronecker product of two arrays.
scipy.linalg.kron	Kronecker product of a and b.

1.1.3 Khatri-Rao product

Definition: For two matrices $A = [a_1, a_2, \ldots, a_J] \in R^{I \times J}$ and $B = [b_1, b_2, \ldots, b_J] \in R^{T \times J}$ with the same number of columns J, their Khatri-Rao product, denoted by \odot , performs the following operation:

$$A \odot B = \begin{bmatrix} a_1 \otimes b_1 & a_2 \otimes b_2 & \cdots & a_J \otimes b_J \end{bmatrix}$$

= $\text{vec}(\boldsymbol{b}_1 \boldsymbol{a}_1^T) \text{ vec}(\boldsymbol{b}_2 \boldsymbol{a}_2^T) \cdots \text{ vec}(\boldsymbol{b}_J \boldsymbol{a}_J^T) \in \mathbb{R}^{IT \times J}$

Python function:

khatrirao(A, B)

Khatri-Rao product of a and b

Parameters A: array, shape (I, J)

B: array, shape (T, J)

Returns C : array, shape (I*T, J)

Examples

```
>>> from numpy import array
>>> from tensor import khatrirao
```

Implementation:

```
from scipy import kron, array, newaxis

C = array([kron(A[:,p][newaxis], B[:,p][newaxis]) for p in range(A.shape[1])])
return C[:,0,:].T
```

1.1.4 Matricized tensor times Khatri-Rao product

Python function:

```
\mathtt{mttkrp}(X, U, n)
```

Matricized tensor times Khatri-Rao product for tensor

Calculates the matrix product of the n-mode matricization of X with the Khatri-Rao product of all entries in U, a list of matrices, except the nth.

Parameters X : Tensor
U : list of matrices
n : ...
Returns C : ...

1.2 Tensor

tensor.tensor.ndims	The Tensor's number of dimensions
tensor.tensor.permute	returns a tensor permuted by the order specified.
tensor.tensor.ipermute	returns a tensor permuted by the inverse of the order specified.

1.2.1 Outer product

Definition: The outer product of the tensors $\mathbf{Y} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ and $\mathbf{X} \in \mathbb{R}^{J_1 \times J_2 \times \cdots \times J_M}$ is given by

$$\underline{\mathbf{Z}} = \underline{\mathbf{Y}} \circ \underline{\mathbf{X}} \in \mathbb{R}^{I_1 \times I_2 \times \dots \times I_N \times J_1 \times J_2 \times \dots \times J_M}$$

where

$$z_{i_1,i_2,\dots,i_N,j_1,j_2,\dots,j_M} = y_{i_1,i_2,\dots,i_N} x_{j_1,j_2,\dots,j_M}$$

seealso: numpy.outer Compute the outer product of two vectors.

1.2.2 Contracted Tensor Product — Tensor times Tensor

Definition: The contracted product}of two tensors $\underline{\mathbf{A}} \in \mathbb{R}^{I_1 \times \cdots \times I_M \times J_1 \times \cdots \times J_N}$ and $\underline{\mathbf{B}} \in \mathbb{R}^{I_1 \times \cdots \times I_M \times K_1 \times \cdots \times K_P}$ along the first M modes is a tensor of size $J_1 \times \cdots \times J_N \times K_1 \times \cdots \times K_P$, given by

$$\langle \underline{\mathbf{A}}, \underline{\mathbf{B}} \rangle_{1,\dots,M;1,\dots,M} (j_1,\dots,j_N,k_1,\dots,k_P) = \sum_{i_1=1}^{I_1} \cdots \sum_{i_M=1}^{I_M} a_{i_1,\dots,i_M,j_1,\dots,j_N} b_{i_1,\dots,i_M,k_1,\dots,k_P}.$$

seealso: numpy.tensordot Compute tensor dot product along specified axes for arrays >= 1-D.

1.2.3 mode-n Tensor-Matrix product — Tensor times Matrix

Definition: The mode-n product $\underline{\mathbf{Y}} = \underline{\mathbf{G}} \times_n \mathbf{A}$ of a tensor $\underline{\mathbf{G}} \in \mathbb{R}^{J_1 \times J_2 \times \cdots \times J_N}$ and a matrix $\mathbf{A} \in \mathbb{R}^{I_n \times J_n}$ is a tensor $\underline{\mathbf{Y}} \in \mathbb{R}^{J_1 \times \cdots \times J_{n-1} \times I_n \times J_{n+1} \times \cdots \times J_N}$, with elements

$$y_{j_1,j_2,\dots,j_{n-1},i_n,j_{n+1},\dots,j_N} = \sum_{j_n=1}^{J_n} g_{j_1,j_2,\dots,J_N} \ a_{i_n,j_n}$$

Python function:

ttm (mat, dims=None, transpose=False, excludedim=False) mode-n tensor-matrix product

Parameters self: Tensor

mat: ndarray

Single matrix or a list of matrices to be sequentially multiplied along all dimensions.

dims: specifies the dimension (or mode) of X along which mat should be multiplied

option: if 't', performs the same computations as above except the matrices are transposed

excludedim: if True, multiply along all mode but those specified in the dims parameter

Returns a: ndarray

The filled array.

Implementation:

```
1
 N = self.ndims();
  shp = self.shape;
  order = [dims]+range(0, dims)+range(dims+1, N)
  newdata = self.permute(order)
  newdata = newdata.data.reshape(shp[dims], self.data.size/shp[dims])
  if transpose:
           newdata = numpy.dot(mat.transpose(), newdata)
10
           p = mat.shape[1]
11
  else:
12
          newdata = numpy.dot(mat, newdata)
13
           p = mat.shape[0]
15
  newshp = [p] + list(shp[0:dims]) + list(shp[dims+1:N])
16
17
  Y = tensor(newdata, newshp)
18
  Y = Y.ipermute(order)
  return Y
```

1.2.4 mode-n Tensor-Vector product — Tensor times Vector

Definition: The mode-n multiplication of a tensor $\underline{\mathbf{Y}} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ by a vector $\boldsymbol{a} \in \mathbb{R}^{I_n}$ is denoted by 1

$$\mathbf{Y} \stackrel{\cdot}{\times}_n \mathbf{a}$$

and has dimension $I_1 \times \cdots \times I_{n-1} \times I_{n+1} \times \cdots \times I_N$, that is,

$$\underline{\mathbf{Z}} = \underline{\mathbf{Y}} \stackrel{\cdot}{\times}_n \boldsymbol{a} \in \mathbb{R}^{I_1 \times \cdots \times I_{n-1} \times I_{n+1} \times \cdots \times I_N},$$

Element-wise, we have

$$z_{i_1,i_2,\dots,i_{n-1},i_{n+1},\dots,i_N} = \sum_{i_n=1}^{I_n} y_{i_1,i_2,\dots,i_N} \ a_{i_n}$$

 $^{^{1}}$ A bar over the operator \times indicates a contracted product.

Python function:

```
ttv (vect, dims=, [])
mode-n tensor-vector product
```

Parameters self: Tensor, ndims: N

vect: sequence of vectors

dims: specifies the dimension (or mode) of X along which vect should be multiplied

Returns Y: Tensor, ndims: N-1

Implementation:

```
dims = range(len(vect))
  vidx = range(len(vect))
   """ Permute it so that the dimensions we're working with come last """
  remdims = numpy.setdiff1d(range(self.ndims()), dims)
  if self.ndims() > 1:
           c = self.permute(numpy.concatenate([remdims, numpy.array(dims)]))
           c = c.data
10
  n = self.ndims() - 1
11
  for i in range(len(dims) -1, -1, -1):
12
           if n == 0:
13
                   c = c.reshape( [1, self.shape[n]] )
14
           else:
                   c = c.reshape( [reduce(numpy.multiply, self.shape[0:n]), self.shape
16
           c = numpy.dot(c, vect[vidx[i]])
17
           n = 1
18
19
  return c
20
```

1.2.5 Frobenius norm

Definition:

$$|A|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n |a_{ij}|^2} = \sqrt{\operatorname{trace}(A^*A)} = \sqrt{\sum_{i=1}^{\min\{m, n\}} \sigma_i^2}$$

Python function:

```
norm()
```

Frobenius norm of a Tensor

seealso: scipy.linalg.norm Matrix or vector norm.

norm()

Frobenius norm for a K-Tensor

Implementation

```
def norm(self):
    """ Frobenius norm for a K-Tensor
    """

from numpy import sqrt, outer, dot

# Compute the matrix of correlation coefficients
coefMatrix = outer(self.mylambda, self.mylambda.T)

for i in range(self.ndims()):
    coefMatrix *= dot(self.u[i].T, self.u[i])

return sqrt(coefMatrix.sum())
```

1.2.6 Inner product — scalar product

Definition: The inner product of two tensors $\underline{\mathbf{A}}, \underline{\mathbf{B}} \in \mathbb{R}^{I_1 \times I_2, \times \cdots \times I_N}$ of the same order is denoted by $\langle \underline{\mathbf{A}}, \underline{\mathbf{B}} \rangle$ and is computed as a sum of element-wise products over all the indices, that is

$$c = \langle \underline{\mathbf{A}}, \underline{\mathbf{B}} \rangle = \sum_{i_1}^{I_1} \sum_{i_2}^{I_2} \cdots \sum_{i_N}^{I_N} b_{i_1, i_2, \dots, i_N} a_{i_1, i_2, \dots, i_N} \in \mathbb{R}$$

Python function:

innerprod(Y)

Inner product of a tensor and a K-tensor

Parameters A: K-Tensor

Y: Tensor

Returns scalar: double

Implementation:

```
def innerprod(self, Y):
    """ Inner product of a tensor and a K-tensor
    """
```

```
res = 0
for r in range(self.mylambda.size):
vect = [n[:,r] for n in self.u]
res += self.mylambda[r] * Y.ttv(vect)
return res
```

Implementation 2:

```
return sum([self.mylambda[r] * Y.ttv([n[:,r] for n in self.u]) for r in range(self.u)

seealso: numpy.inner Inner product of two arrays.
```

1.2.7 Vectorization

Definition: It is often convenient to represent tensors and matrices as vectors, whereby vectorization of matrix $\mathbf{Y} = [\boldsymbol{y}_1, \boldsymbol{y}_2, \dots, \boldsymbol{y}_T] \in \mathbb{R}^{I \times T}$ is defined as

$$oldsymbol{y} = \operatorname{vec}(\mathbf{Y}) = \left[oldsymbol{y}_1^T, oldsymbol{y}_2^T, \dots, oldsymbol{y}_T^T
ight]^T \in \mathbb{R}^{IT}.$$

The vec-operator applied on a matrix Y stacks its columns into a vector. The reshape is a reverse function to vectorization which converts a vector to a matrix.

Example

seealso: numpy.ndarray.flatten Return a copy of the array collapsed into one dimension.

See Also:

http://docs.scipy.org/doc/numpy/reference/routines.array-manipulation.html

1.2.8 Matricization — Unfolding

Definition: The mode-n unfolding of tensor $\underline{\mathbf{Y}} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$ is denoted by ${}^2\mathbf{Y}_{(n)}$ and arranges the mode-n fibers into columns of a matrix. More specifically, a tensor element (i_1, i_2, \dots, i_N)

² We use the Kolda - Bader notations cite{Kolda08}

maps onto a matrix element (i_n, j) , where

$$j=1+\sum_{p\neq n}(i_p-1)J_p,\quad \text{with}\quad J_p=\begin{cases} 1, & \text{if}\ \ p=1\ \ \text{or if}\ \ p=2\ \ \text{and}\ \ n=1,\\ \prod_{m\neq n}^{p-1}I_m, & \text{otherwise}. \end{cases}$$

Python function:

```
matricization (rdims=None, cdims=None, tsize=None) mode-n unfolding of a tensor reimplementation of the tenmat class
```

Parameters K: Tensor

rdims : int
cdims : list
tsize : int

Returns M: Matrix

Implementation:

```
def matricization (self, rdims = None, cdims = None, tsize = None):
           import numpy as np
2
           if tsize is None: tsize = self.shape
           nn = np.mgrid[1:self.ndims()+1]
           if bool(rdims) ^ bool(cdims):
                   if rdims is None: rdims = np.setdiff1d(nn, np.array(cdims))
                   if cdims is None: cdims = np.setdiff1d(nn, np.array(rdims))
10
           else:
11
                   raise ValueError("You have to specify either rdims or cdims")
12
           rdims = np.array(rdims, ndmin = 1)
13
           cdims = np.array(cdims, ndmin = 1)
           rcdims = np.hstack((rdims, cdims))
16
           if np.setdiff1d(rcdims, nn) or np.setdiff1d(nn, rcdims):
17
                   raise ValueError("Incorrect specification of dimensions." +
18
                                                      "\n RDIMS = %s\n CDIMS = %s" % (re
19
20
           T = self.permute(rcdims-1);
21
22
           row = reduce(np.multiply, [tsize[i-1] for i in rdims])
```

```
col = reduce(np.multiply, [tsize[i-1] for i in cdims])
return T.data.reshape([row, col])
```

1.2.9 N-vect

Python function:

```
nvecs (n, r, flipsign=True)
```

Compute the leading mode-n vectors for a tensor

computes the r leading eigenvalues of Xn*Xn' (where Xn is the mode-n matricization of X), which provides information about the mode-n fibers. In two-dimensions, the r leading mode-1 vectors are the same as the r left singular vectors and the r leading mode-2 vectors are the same as the r right singular vectors.

Parameters X: Tensor

n: int, mode-n matricization of X

r: int, nnumber of leading eigenvalues to return

flipsign: bool, make each column's largest element positive / Make the largest magnitude element be positive

Returns M: Matrix

Implementation:

```
from numpy import dot
   from scipy.sparse.linalg.eigen.arpack import eigen_symmetric
  Xn = self.matricization(n)
   Y = dot(Xn, Xn.T)
  v = eigen_symmetric(Y, r, which = 'LM')
  if flipsign:
           """ not implemented """
10
           pass
11
  return v[1]
           scipy.sparse.linalg.eigen.arpack.eigEindskyeigenvalues and eigenvectors of
                                                      the real symmetric
   seealso:
           scipy.sparse.linalg.eigen.arpack
                                                      Eigenvalue solver using iterative
                                                      methods.
```

Functions summary

tensor.khatrirao	Khatri-Rao product of a and b
tensor.mttkrp	Matricized tensor times Khatri-Rao product for tensor
tensor.tensor.nvecs	Compute the leading mode-n vectors for a tensor
tensor.tensor.matricization	mode-n unfolding of a tensor
tensor.tensor.ttm	mode-n tensor-matrix product
tensor.tensor.ttv	mode-n tensor-vector product
tensor.tensor.norm	Frobenius norm of a Tensor
tensor.tensor.ndims	The Tensor's number of dimensions
tensor.tensor.permute	returns a tensor permuted by the order specified.
ktensor.ktensor.norm	Frobenius norm for a K-Tensor
ktensor.ktensor.innerprod	Inner product of a tensor and a K-tensor

Functions from Python Libraries

numpy.inner	Inner product of two arrays.
numpy.outer	Compute the outer product of two vectors.
numpy.tensordot	Compute tensor dot product along specified
	axes for arrays \geq 1-D.
numpy.ndarray.flatten	Return a copy of the array collapsed into one
	dimension.
numpy.kron	Kronecker product of two arrays.
scipy.linalg.kron	Kronecker product of a and b.
scipy.linalg.norm	Matrix or vector norm.
scipy.sparse.linalg.eigen.arpack.	Find k eigenvalues and eigenvectors of the
	real symmetric
scipy.sparse.linalg.eigen.arpack	Eigenvalue solver using iterative methods.

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TWO

NONNEGATIVE MATRIX FACTORISATION

Warning: Documentation Under Construction

- 2.1 Hierachical Alternating Least Squares
- 2.1.1 Fast HALS
- 2.1.2 Fast beta HALS



TENSOR DECOMPOSITION WITH PARAFAC MODEL

Warning: Documentation Under Construction

A key feature of the analysis of three-way arrays by Candecomp/Parafac is the essential uniqueness of the trilinear decomposition. Kruskal has previously shown that the three component matrices involved are essentially unique when the sum of their k-ranks is at least twice the rank of the decomposition plus 2. It was proved that Kruskal's sufficient condition is also necessary when the rank of the decomposition is 2 or 3. If the rank is 4 or higher, the condition is not necessary for uniqueness. However, when the k-ranks of the component matrices equal their ranks, necessity of Kruskal's condition still holds in the rank-4 case. Ten Berge and Sidiropoulos conjectured that Kruskal's condition is necessary for all cases of rank 4 and higher where ranks and k-ranks coincide. In the present paper we show that this conjecture is false. http://portal.acm.org/citation.cfm?id=1647955.1648010

3.1 Cadecomp-PARAFAC model

Python function:

Compute a CP decomposition of any type of tensor.

The PARAFAC can be formulated as follows (see Figures 1.26 and 1.27 for graphical representations). Given a data tensor YeRIxTxQ and the positive index J, find three-component matrices, also called loading matrices or factors, $A = [a1, a2, \ldots, aJ]$ RIJ, $B = [b1, b2, \ldots, bJ]$ RTJ and $C = [c1, c2, \ldots, cJ]$ RQJ which perform the following approximate factorization:

Y = J = 1 aj ? bj ? cj + E = A, B, C + E, (1.123)

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or equivalently in the element-wise form (see Table 1.2 for various representations of PARAFAC)

yitq =J j=1 aijbtjcqj + eitq. (1.124)

FOUR

TENSOR FACTORISATION WITH TUCKER MODEL

Warning: Documentation Under Construction

Two of the most commonly used decompositions are the Tucker decomposition and PARAFAC (also known as CANDECOMP or simply CP) which are often considered (thought of) as higher-order generalizations of the matrix singular value decomposition (SVD) or principal component analysis (PCA).

- Cadecomp-PARAFAC model
- Tucker model
- nmf ntd ntf

```
1 >>> for i in range(10):
2 ... print i
Y = AX + E = ABT + E
```

4.1 Tucker model

Python function:

tucker_als (*X*, *R*, fitchangetol=1.000000000000001e-05, maxiters=200, verbose=1, init='eigs')

The original Tucker model makes the assumption of orthogonality of the factor matrices (in analogy to SVD), [17,79,83,84,107,117]. We will, however, ignore these constraints. By imposing nonnegativity constraints the problem of estimating the component matrices and a core tensor is converted into a generalized NMF problem called the Nonnegative Tucker Decomposition (NTD) (see Chapter 7 for details). The first implementations of Tucker decomposition with nonnegativity constraints together with a number of other constraints were

given by Kiers, Smilde and Bro in [17,79]. The NTD imposes nonnegativity constraints for all component matrices and a core tensor, while a semi-NTD (in analogy to semi-NMF) imposes nonnegativity constraints to only some components matrices and/or some elements of the core tensor.

```
class ttensor (core, uIn)

copy()
size()

totensor()
    returns a tensor object that is represented by the tucker tensor

tucker_als(X, R, fitchangetol=1.000000000000001e-05, maxiters=200, verbose=1, init='eigs')
```

FIVE

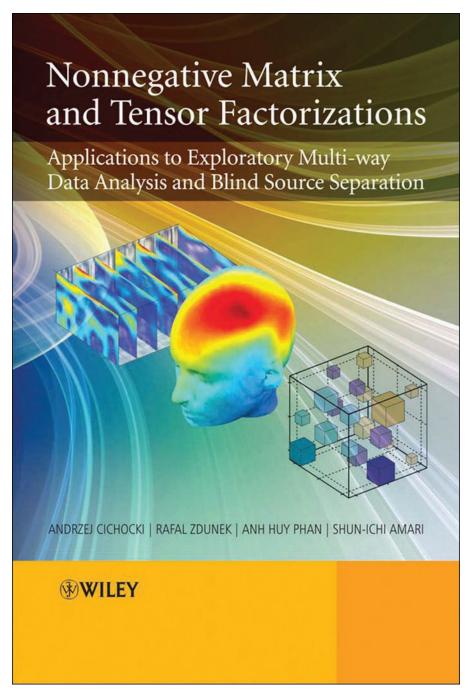
ABOUT — DRAFT & TESTS

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Many modern applications generate large amounts of data with multiple aspects and high dimensionality for which tensors (i.e., multi-way arrays) provide a natural representation.



- 1. This project is developed in the Laboratory for Advanced Brain Signal Processing, RIKEN Brain Science Institute
- 2. Large parts of this documentation originate from Andrzej CICHOCKI's book Nonnegative Matrix and Tensor factorization.

5.1 Testings

Operation	Result	Notes
x or y	if x is <i>environment</i> , then y, else x	(1)
x and y	if x is false, then x , else y	(2)
not x	if x is false, then True, else False	(3)

$$y = ax^2 + bx + c (5.1)$$

$$f(x) = x^2 + 2xy + y^2 (5.2)$$

Imports:

.. literalinclude:: ../../src/tensor.py

:pyobject: khatrirao
:language: python

:linenos:

:start-after: #!End

5.2 Todo list

Documentation

- **Solve the conflict between** *begin{gather} begin{split} and begin{eqnarray}* on the :math: extention http://sphinx.pocoo.org/latest/ext/math.html : nowarp:?
- Completion of the Index
- Completion of the Module page
- Feed the glossary
- Write functions parameters definition
- NMF documentation
- NTF documentation
- NTD documentation
- MTTKRP documentation
- Nvec documentation
- Setup the doctest extention http://docs.python.org/library/doctest.htm

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Programmation

- Proper testing sets
 - Check Mathematic properties
 - Check consistency with extisting matlab code
- Visualisation for Benchmarks

+++

5.3 Glossary

Numpy http://www.numpy.org

Scipy Python's Open Source Library of Scientific Tools. www.scipy.org

environment A structure where information about all documents under the root is saved, and used for cross-referencing. The environment is pickled after the parsing stage, so that successive runs only need to read and parse new and changed documents.

source directory The directory which, including its subdirectories, contains all source files for one Sphinx project.

5.4 Acknowledgements

- Many of those algorithms were borrowed or inspired from the work of KOLDA et. al. ...
- This project meant to implement algorithms of the *Nonnegative Matrix and Tensor Factor-izations* book by...

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