Package 'RcppPlanc'

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```
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Title Parallel Low-Rank Approximation with Nonnegativity Constraints
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Description 'Rcpp' bindings for 'PLANC', a highly parallel
      and extensible NMF/NTF (Non-negative Matrix/Tensor Factorization) library.
      Wraps algorithms described in
      Kannan et. al (2018) <doi:10.1109/TKDE.2017.2767592> and
      Eswar et. al (2021) <doi:10.1145/3432185>.
      Implements algorithms described in
      Welch et al. (2019) <doi:10.1016/j.cell.2019.05.006>,
      Gao et al. (2021) <doi:10.1038/s41587-021-00867-x>, and
      Kriebel & Welch (2022) <doi:10.1038/s41467-022-28431-4>.
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Author Andrew Robbins [aut, cre] (<a href="https://orcid.org/0009-0001-7961-7489">https://orcid.org/0009-0001-7961-7489</a>),
      Yichen Wang [aut],
      Joshua Welch [cph] (<a href="https://orcid.org/0000-0002-5869-2391">https://orcid.org/0000-0002-5869-2391</a>),
      Ramakrishnan Kannan [cph] (<a href="https://orcid.org/0000-0002-5852-4806">https://orcid.org/0000-0002-5852-4806</a>),
      UT-Batelle [cph] (The original PLANC code)
```

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Maintainer Andrew Robbins < robbiand@umich.edu>

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bppnnls

Block Principal Pivoted Non-Negative Least Squares

Description

Use the BPP algorithm to get the nonnegative least squares solution. Regular NNLS problem is described as optimizing $\min_{x\geq 0}||CX-B||_F^2$ where C and B are given and X is to be solved. bppnnls takes C and B as input. bppnnls_prod takes $C^\mathsf{T}C$ and $C^\mathsf{T}B$ as input to directly go for the intermediate step of BPP algorithm. This can be useful when the dimensionality of C and B is large while pre-calculating $C^\mathsf{T}C$ and $C^\mathsf{T}B$ is cheap.

Usage

```
bppnnls(C, B, nCores = 2L)
bppnnls_prod(CtC, CtB, nCores = 2L)
```

Arguments

C	Input dense C matrix
В	Input B matrix of either dense or sparse form
nCores	The number of parallel tasks that will be spawned. Default 2
CtC	The $C^{T}C$ matrix, see description.
CtB	The $C^{T}B$ matrix, see description.

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Value

The calculated solution matrix in dense form.

Examples

```
set.seed(1)
C <- matrix(rnorm(250), nrow = 25)
B <- matrix(rnorm(375), nrow = 25)
res1 <- bppnnls(C, B)
dim(res1)
res2 <- bppnnls_prod(t(C) %*% C, t(C) %*% B)
all.equal(res1, res2)</pre>
```

ctrl.sparse

Example single-cell transcriptomic data in sparse form

Description

The two datasets, namingly ctrl.sparse and stim.sparse, are single-cell transcriptomic data preprocessed and subsampled from the study of Hyun Min Kang and et al., Nat Biotech., 2018. The raw datasets were two sparse matrices of integer values indicating the counts of genes (rows) per cell (columns). We normalized each column of both matrices by its library size (sum), and selected common variable genes across the datasets. Finally, we scaled the genes without centering them, in order to keep the non-negativity. The processed datasets were then randomly subsampled for a minimal example.

Usage

```
ctrl.sparse
```

Format

An object of class dgCMatrix with 173 rows and 300 columns.

An object of class dgCMatrix with 173 rows and 300 columns.

Source

https://www.nature.com/articles/nbt.4042

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dim.H5SpMat

Retrieve the dimension of H5SpMat argument list

Description

Retrieve the dimension of H5SpMat argument list

Usage

```
## S3 method for class 'H5SpMat'
dim(x)
## S3 replacement method for class 'H5SpMat'
dim(x) <- value</pre>
```

Arguments

x H5SpMat argument list object

value Numeric vector of two, for number of rows and number of columns.

Value

Retriever returns a vector of two (nrow and ncol), setter sets the value of that in the argument list.

Examples

format.H5Mat

Prepare character information of a H5Mat object

Description

Prepare character information of a H5Mat object

Usage

```
## S3 method for class 'H5Mat' format(x, ...)
```

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Arguments

x H5Mat argument list object

... Not used.

Value

A character scalar of the displayed message

Examples

format.H5SpMat

prepare character information of a H5SpMat object

Description

prepare character information of a H5SpMat object

Usage

```
## S3 method for class 'H5SpMat' format(x, \ldots)
```

Arguments

x H5SpMat argument list object

... Not used.

Value

A character scalar of the displayed message

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H5Mat

Argument list object for using a dense matrix stored in HDF5 file

Description

For running inmf, onlineINMF or uinmf with dense matrix stored in HDF5 file, users will need to construct an argument list for the filename of the HDF5 file as well as the path in the file storing the matrix. H5Mat is provided as an instructed constructor. Meanwhile, since the INMF functions require that all datasets should be of the same type, as . H5Mat is provided for writing in-memory data into a new HDF5 file on disk and returning the constructed argument list.

Usage

```
H5Mat(filename, dataPath)
as.H5Mat(x, filename, dataPath = "data", overwrite = FALSE, ...)
## S3 method for class 'matrix'
as.H5Mat(x, filename, dataPath = "data", overwrite, ...)
## S3 method for class 'dgCMatrix'
as.H5Mat(x, filename, dataPath = "data", overwrite = FALSE, ...)
## Default S3 method:
as.H5Mat(x, filename, dataPath = "data", ...)
```

Arguments

filename	Filename of the HDF5 file
dataPath	Path in the HDF5 file that points to a 2D dense matrix. Default "data" when using as. H5Mat.
X	For as . H5Mat, matrix of either dense or sparse type to be written; for print, a H5Mat argument list object
overwrite	Logical, whether to overwrite the file if already exists at the given path. Default FALSE.
	Passed down to hdf5r.Extra::h5Write

Value

H5Mat object, indeed a list object.

```
if (require("withr")) {
H5MatEx <- function(){
withr::local_dir(withr::local_tempdir())</pre>
```

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H5SpMat

Argument list object for using a sparse matrix stored in HDF5 file

Description

For running inmf, onlineINMF or uinmf with sparse matrix stored in HDF5 file, users will need to construct an argument list for the filename of the HDF5 file as well as the paths in the file storing the arrays that construct the CSC (compressed sparse column) matrix. H5SpMat is provided as an instructed constructor. Meanwhile, since the INMF functions require that all datasets should be of the same type, as . H5SpMat is provided for writing in-memory data into a new HDF5 file on disk and returning the constructed argument list.

Usage

```
H5SpMat(filename, valuePath, rowindPath, colptrPath, nrow, ncol)
as.H5SpMat(x, filename, dataPath, overwrite = FALSE)
## S3 method for class 'matrix'
as.H5SpMat(x, filename, dataPath = "", overwrite = FALSE)
## S3 method for class 'dgCMatrix'
as.H5SpMat(x, filename, dataPath = "", overwrite = FALSE)
## Default S3 method:
as.H5SpMat(x, filename, dataPath = "", overwrite = FALSE, ...)
```

Arguments

filename Filename of the HDF5 file

valuePath Path in the HDF5 file that points to a 1D array storing the non-zero values of the

sparse matrix. Default "data" when using as . H5SpMat.

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rowindPath	Path in the HDF5 file that points to a 1D integer array storing the row indices of non-zero values in each column of the sparse matrix. Default "indices" when using as. H5SpMat.
colptrPath	Path in the HDF5 file that points to a 1D integer array storing the number of non-zero values in each column of the sparse matrix. Default "indptr" when using as.H5SpMat.
nrow, ncol	Integer, the true dimensionality of the sparse matrix.
X	For as . H5SpMat, matrix of either dense or sparse type to be written; for print, a H5SpMat argument list object.
dataPath	For as . H5SpMat methods, the H5Group name for the sparse matrix. Default "".
overwrite	Logical, whether to overwrite the file if already exists at the given path. Default FALSE.
	not used

Value

H5SpMat object, indeed a list object.

Examples

inmf

Perform Integrative Non-negative Matrix Factorization

Description

Performs integrative non-negative matrix factorization (iNMF) (J.D. Welch, 2019) to return factorized H, W, and V matrices. The objective function is stated as

$$\arg\min_{H\geq 0, W\geq 0, V\geq 0} \sum_{i}^{d} ||E_{i} - (W+V_{i})Hi||_{F}^{2} + \lambda \sum_{i}^{d} ||V_{i}H_{i}||_{F}^{2}$$

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where E_i is the input non-negative matrix of the i'th dataset, d is the total number of datasets. E_i is of size $m \times n_i$ for m features and n_i sample points, H_i is of size $k \times n_i$, V_i is of size $m \times k$, and W is of size $m \times k$.

inmf optimizes the objective with ANLS strategy, while online INMF optimizes the same objective with an online learning strategy.

Usage

```
inmf(
  objectList,
  k = 20,
  lambda = 5,
  niter = 30,
  nCores = 2,
  Hinit = NULL,
  Vinit = NULL,
  winit = NULL,
  verbose = FALSE
)
```

Arguments

objectList	list of input datasets. List elements should all be of the same class. Viable classes include: matrix, dgCMatrix, H5Mat, H5SpMat.
k	Integer. Inner dimensionality to factorize the datasets into. Default 20.
lambda	Regularization parameter. Larger values penalize dataset-specific effects more strongly (i.e. alignment should increase as lambda increases). Default 5.
niter	Integer. Total number of block coordinate descent iterations to perform. Default 30.
nCores	The number of parallel tasks that will be spawned. Default 2
Hinit	Initial values to use for H matrices. A list object where each element is the initial H matrix of each dataset. Each should be dense matrix of size $n_i \times k$. Default NULL.
Vinit	Similar to Hinit, but each should be of size $m \times k$.
Winit	Initial values to use for W matrix. A matrix object of size $m \times k$. Default NULL.
verbose	Logical scalar. Whether to show information and progress. Default FALSE.

Value

A list of the following elements:

- H a list of result H_i matrices of size $n_i \times k$
- V a list of result V_i matrices
- ullet W the result W matrix
- objErr the final objective error value.

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Author(s)

Yichen Wang

References

Joshua D. Welch and et al., Single-Cell Multi-omic Integration Compares and Contrasts Features of Brain Cell Identity, Cell, 2019

Examples

```
library(Matrix)
set.seed(1)
result <- inmf(list(ctrl.sparse, stim.sparse), k = 10, niter = 10, verbose = FALSE)</pre>
```

nmf

Perform Non-negative Matrix Factorization

Description

Regularly, Non-negative Matrix Factorization (NMF) is factorizes input matrix X into low rank matrices W and H, so that $X \approx WH$. The objective function can be stated as $\arg\min_{W \geq 0, H \geq 0} ||X - WH||_F^2$. In practice, X is usually regarded as a matrix of m features by n sample points. And the result matrix W should have the dimensionality of $m \times k$ and H with $n \times k$ (transposed). This function wraps the algorithms implemented in PLANC library to solve NMF problems. Algorithms includes Alternating Non-negative Least Squares with Block Principal Pivoting (ANLS-BPP), Alternating Direction Method of Multipliers (ADMM), Hierarchical Alternating Least Squares (HALS), and Multiplicative Update (MU).

Usage

```
nmf(
    x,
    k,
    niter = 30L,
    algo = "anlsbpp",
    nCores = 2L,
    Winit = NULL,
    Hinit = NULL
)
```

Arguments

x Input matrix for factorization. Can be either dense or sparse.
k Integer. Factor matrix rank.
niter Integer. Maximum number of NMF interations.
algo Algorithm to perform the factorization, choose from "anlsbpp", "admm", "hals" or "mu". See detailed sections.

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nCores	The number of parallel tasks that will be spawned. Only applies to anlsbpp. Default 2
Winit	Initial left-hand factor matrix, must be of size m x k.
Hinit	Initial right-hand factor matrix, must be of size n x k.

Value

A list with the following elements:

- W the result left-hand factor matrix
- H the result right hand matrix.
- objErr the objective error of the factorization.

References

Ramakrishnan Kannan and et al., A High-Performance Parallel Algorithm for Nonnegative Matrix Factorization, PPoPP '16, 2016, 10.1145/2851141.2851152

onlineINMF	Perform Integrative Non-negative Matrix Factorization Using Online Learning	

Description

Performs integrative non-negative matrix factorization (iNMF) (J.D. Welch, 2019, C. Gao, 2021) using online learning approach to return factorized $H,\,W,\,$ and V matrices. The objective function is stated as

$$\arg \min_{H \geq 0, W \geq 0, V \geq 0} \sum_{i}^{d} ||E_i - (W + V_i)Hi||_F^2 + \lambda \sum_{i}^{d} ||V_iH_i||_F^2$$

where E_i is the input non-negative matrix of the *i*'th dataset, *d* is the total number of datasets. E_i is of size $m \times n_i$ for m features and n_i sample points, H_i is of size $k \times n_i$, V_i is of size $m \times k$, and W is of size $m \times k$.

Different from inmf which optimizes the objective with ANLS approach, onlineINMF optimizes the same objective with online learning strategy, where it updates mini-batches of H_i solving the NNLS problem, and updates V_i and W with HALS multiplicative method.

This function allows online learning in 3 scenarios:

- 1. Fully observed datasets;
- 2. Iterative refinement using continually arriving datasets;
- 3. Projection of new datasets without updating the existing factorization

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Usage

```
onlineINMF(
  objectList,
  newDatasets = NULL,
  project = FALSE,
  k = 20,
  lambda = 5,
 maxEpoch = 5,
 minibatchSize = 5000,
 maxHALSIter = 1,
  permuteChunkSize = 1000,
  nCores = 2,
 Hinit = NULL,
  Vinit = NULL,
 Winit = NULL,
 Ainit = NULL,
 Binit = NULL,
  verbose = FALSE
)
```

Arguments

objectList list of input datasets. List elements should all be of the same class. Viable

classes include: matrix, dgCMatrix, H5Mat, H5SpMat.

newDatasets Same requirements as for new arriving datasets. Default NULL for scenario 1,

specify for scenario 2 or 3.

project Logical scalar, whether to run scenario 3. See description. Default FALSE.

k Integer. Inner dimensionality to factorize the datasets into. Default 20.

lambda Regularization parameter. Larger values penalize dataset-specific effects more

strongly (i.e. alignment should increase as lambda increases). Default 5.

maxEpoch The number of epochs to iterate through. Default 5.

minibatchSize Total number of cells in each mini-batch. Default 5000.

maxHALSIter Maximum number of block coordinate descent (HALS algorithm) iterations to

perform for each update of W and V. Default 1. Changing this parameter is not

recommended.

permuteChunkSize

Number of cells in a chunk being shuffled before subsetting to minibatches. Only appliable to in-memory data and for Scenario 1 and 2. Default 1000.

nCores The number of parallel tasks that will be spawned. Default 2

Hinit, Vinit, Winit, Ainit, Binit

Pass the previous factorization result for datasets existing in objectList, in order to run scenario 2 or 3. All should have length(objectList) matrices inside. See description for dimensionality of H_i , V_i and W_i . A_i should be of

size $k \times k$ and B_i should be of size $m \times k$

verbose Logical scalar. Whether to show information and progress. Default FALSE.

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Value

A list of the following elements:

- H a list of result H_i matrices of size $n_i \times k$
- V a list of result V_i matrices
- ullet W the result W matrix
- A a list of result A_i matrices, $k \times k$
- B a list of result B_i matrices, $m \times k$
- objErr the final objective error value.

Author(s)

Yichen Wang

References

Joshua D. Welch and et al., Single-Cell Multi-omic Integration Compares and Contrasts Features of Brain Cell Identity, Cell, 2019

Chao Gao and et al., Iterative single-cell multi-omic integration using online learning, Nat Biotechnol., 2021

```
library(Matrix)
# Scenario 1 with sparse matrices
set.seed(1)
res1 <- onlineINMF(list(ctrl.sparse, stim.sparse),</pre>
                   minibatchSize = 50, k = 10, verbose = FALSE)
# Scenario 2 with H5 dense matrices
h5dense1 <- H5Mat(filename = system.file("extdata", "ctrl_dense.h5",
                             package = "RcppPlanc", mustWork = TRUE),
                                          dataPath = "scaleData")
h5dense2 <- H5Mat(filename = system.file("extdata", "stim_dense.h5",
                             package = "RcppPlanc", mustWork = TRUE),
                                          dataPath = "scaleData")
res2 <- onlineINMF(list(ctrl = h5dense1), minibatchSize = 50, k = 10, verbose = FALSE)
res3 <- onlineINMF(list(ctrl = h5dense1),
                   newDatasets = list(stim = h5dense2),
                   Hinit = res2$H, Vinit = res2$V, Winit = res2$W,
                   Ainit = res2$A, Binit = res2$B,
                   minibatchSize = 50, k = 10, verbose = FALSE)
# Scenario 3 with H5 sparse matrices
h5sparse1 <- H5SpMat(filename = system.file("extdata", "ctrl_sparse.h5",
                                package = "RcppPlanc", mustWork = TRUE),
                                valuePath = "scaleDataSparse/data",
                                rowindPath = "scaleDataSparse/indices",
```

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```
colptrPath = "scaleDataSparse/indptr",
                                nrow = nrow(ctrl.sparse),
                                ncol = ncol(ctrl.sparse))
h5sparse2 <- H5SpMat(filename = system.file("extdata", "stim_sparse.h5",
                                package = "RcppPlanc", mustWork = TRUE),
                                valuePath = "scaleDataSparse/data",
                                rowindPath = "scaleDataSparse/indices",
                                colptrPath = "scaleDataSparse/indptr",
                                nrow = nrow(stim.sparse),
                                ncol = nrow(stim.sparse))
res4 <- onlineINMF(list(ctrl = h5sparse1), minibatchSize = 50, k = 10, verbose = FALSE)
res5 <- onlineINMF(list(ctrl = h5sparse1),</pre>
                   newDatasets = list(stim = h5sparse2), project = TRUE,
                   Hinit = res4$H, Vinit = res4$V, Winit = res4$W,
                   Ainit = res4$A, Binit = res4$B,
                   minibatchSize = 50, k = 10, verbose = FALSE)
```

print.H5Mat

Show information of a H5Mat object

Description

Show information of a H5Mat object

Usage

```
## S3 method for class 'H5Mat'
print(x, ...)
```

Arguments

x H5Mat argument list object

... Not used.

Value

NULL. Information displayed.

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print.H5SpMat

Show information of a H5SpMat object

Description

Show information of a H5SpMat object

Usage

```
## S3 method for class 'H5SpMat'
print(x, ...)
```

Arguments

x H5SpMat argument list object

... Not used.

Value

NULL. Information displayed.

Examples

symNMF

Perform Symmetric Non-negative Matrix Factorization

Description

Symmetric input matrix X of size $n \times n$ is required. Two approaches are provided. Alternating Non-negative Least Squares Block Principal Pivoting algorithm (ANLSBPP) with symmetric regularization, where the objective function is set to be $\arg\min_{H\geq 0,W\geq 0}||X-WH||_F^2+\lambda||W-H||_F^2$, can be run with algo = "anlsbpp". Gaussian-Newton algorithm, where the objective function is set to be $\arg\min_{H\geq 0}||X-H^\mathsf{T}H||_F^2$, can be run with algo = "gnsym". In the objectives, W is of size $n\times k$ and H is of size $k\times n$. The returned results will all be $n\times k$.

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Usage

```
symNMF(
    x,
    k,
    niter = 30L,
    lambda = 0,
    algo = "gnsym",
    nCores = 2L,
    Hinit = NULL
)
```

Arguments

х	Input matrix for factorization. Must be symmetric. Can be either dense or sparse.
k	Integer. Factor matrix rank.
niter	Integer. Maximum number of symNMF interations. Default 30
lambda	Symmetric regularization parameter. Must be non-negative. Default 0.0 uses the square of the maximum value in x.
algo	Algorithm to perform the factorization, choose from "gnsym" or "anlsbpp". Default "gnsym" $$
nCores	The number of parallel tasks that will be spawned. Only applies to anlsbpp. Default 2
Hinit	Initial right-hand factor matrix, must be of size n x k. Default NULL.

Value

A list with the following elements:

- W the result left-hand factor matrix, non-empty when using "anlsbpp"
- H the result right hand matrix.
- objErr the objective error of the factorization.

References

Srinivas Eswar and et al., Distributed-Memory Parallel Symmetric Nonnegative Matrix Factorization, SC '20, 2020, 10.5555/3433701.3433799

uinmf 17

uinmf	Perform Mosaic Integrative Non-negative Matrix Factorization with
	Unshared Features

Description

Performs mosaic integrative non-negative matrix factorization (UINMF) (A.R. Kriebel, 2022) to return factorized H, W, V and U matrices. The objective function is stated as

$$\arg\min_{H\geq 0, W\geq 0, V\geq 0, U\geq 0} \sum_{i}^{d} || \begin{bmatrix} E_i \\ P_i \end{bmatrix} - (\begin{bmatrix} W \\ 0 \end{bmatrix} + \begin{bmatrix} V_i \\ U_i \end{bmatrix}) Hi||_F^2 + \lambda_i \sum_{i}^{d} || \begin{bmatrix} V_i \\ U_i \end{bmatrix} H_i||_F^2$$

where E_i is the input non-negative matrix of the i'th dataset, P_i is the input non-negative matrix for the unshared features, d is the total number of datasets. E_i is of size $m \times n_i$ for m shared features and n_i sample points, P_i is of size $u_i \times n_i$ for u_i unshared features, H_i is of size $k \times n_i$, V_i is of size $m \times k$, W is of size $m \times k$ and W_i is of size $w \times k$.

Similar to inmf, uinmf also optimizes the objective with ANLS algorithm.

Usage

```
uinmf(
  objectList,
  unsharedList,
  k = 20,
  lambda = 5,
  niter = 30,
  nCores = 2,
  verbose = FALSE
)
```

Arguments

objectList	list of input datasets. List elements should all be of the same class. Viable classes include: matrix, dgCMatrix, H5Mat, H5SpMat.
unsharedList	$List \ of \ input \ unshared \ feature \ matrices, \ with \ the \ same \ requirement \ as \ object List.$
k	Integer. Inner dimensionality to factorize the datasets into. Default 20.
lambda	Regularization parameter. Use one number for all datasets or a vector to specify for each dataset. Larger values penalize dataset-specific effects more strongly (i.e. alignment should increase as lambda increases). Default 5.
niter	Integer. Total number of block coordinate descent iterations to perform. Default 30.
nCores	The number of parallel tasks that will be spawned. Default 2.
verbose	Logical scalar. Whether to show information and progress. Default FALSE.

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Value

A list of the following elements:

- H a list of result H_i matrices of size $n_i \times k$
- V a list of result V_i matrices
- ullet W the result W matrix
- U a list of result A_i matrices
- objErr the final objective error value.

Author(s)

Yichen Wang

References

April R. Kriebel and Joshua D. Welch, UINMF performs mosaic integration of single-cell multiomic datasets using nonnegative matrix factorization, Nat. Comm., 2022

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