

Package ‘corral’

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Title Correspondence Analysis for Single Cell Data

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Description Correspondence analysis (CA) is a matrix factorization method, and is similar to principal components analysis (PCA). Whereas PCA is designed for application to continuous, approximately normally distributed data, CA is appropriate for non-negative, count-based data that are in the same additive scale. The corral package implements CA for dimensionality reduction of a single matrix of single-cell data, as well as a multi-table adaptation of CA that leverages data-optimized scaling to align data generated from different sequencing platforms by projecting into a shared latent space. corral utilizes sparse matrices and a fast implementation of SVD, and can be called directly on Bioconductor objects (e.g., SingleCellExperiment) for easy pipeline integration. The package also includes the option to apply CA-style processing to continuous data (e.g., proteomic TOF intensities) with the Hellinger distance adaptation of CA.

Imports ggplot2, ggthemes, grDevices, gridExtra, irlba, Matrix, methods, MultiAssayExperiment, pals, SingleCellExperiment, SummarizedExperiment, transport

Suggests ade4, BiocStyle, CellBench, DuoClustering2018, knitr, testthat

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add_embeddings2sclist

Add embeddings to list of SCEs

Description

Add embeddings to list of SCEs

Usage

```
add_embeddings2sclist(sclist, embeddings, slotname = "corralm")
```

Arguments

sclist	list of SingleCellExperiments; to which the corresponding embeddings should be added
embeddings	matrix; the embeddings outputted from a dimension reduction, e.g. <code>corralm</code> . Rows in this table correspond to columns in the SCEs in <code>sclist</code> (if all the SCEs were column-bound), and row indices should correspond to cells.
slotname	character; name of the slot for the reduced dim embedding; defaults to <code>corral</code>

Value

list of SingleCellExperiments with respective embeddings stored in them

Examples

```
library(DuoClustering2018)
sce <- sce_full_Zhengmix4eq()
sclist <- list(sce,sce)
embeddings <- matrix(sample(seq(0,20,1),dim(sce)[2]*6,replace = TRUE),nrow = dim(sce)[2]*2)
sclist <- add_embeddings2sclist(sclist, embeddings)
```

all_are	<i>all_are</i>
---------	----------------

Description

Checks if all elements of a list or List are of a (single) particular type typechar

Usage

```
all_are(inplist, typechar)
```

Arguments

inplist	list or List to be checked
typechar	char of the type to check for

Value

boolean, for whether the elements of inplist are all typechar

Examples

```
x <- list(1,2)
all_are(x, 'numeric')
all_are(x, 'char')

y <- list(1,2, 'c')
all_are(y, 'numeric')
all_are(y, 'char')
```

compsvd	<i>compsvd: Compute Singular Value Decomposition (SVD)</i>
---------	--

Description

Computes SVD.

Usage

```
compsvd(mat, method = c("irl", "svd"), ncomp = 30, ...)
```

Arguments

mat	matrix, pre-processed input; can be sparse or full (pre-processing can be performed using corral_preproc from this package)
method	character, the algorithm to be used for svd. Default is irl. Currently supports 'irl' for irlba::irlba or 'svd' for stats::svd
ncomp	numeric, number of components; Default is 30
...	(additional arguments for methods)

Value

SVD result - a list with the following elements:

`d` a vector of the diagonal singular values of the input `mat`. Note that using `svd` will result in the full set of singular values, while `irlba` will only compute the first `ncomp` singular values.

`u` a matrix of with the left singular vectors of `mat` in the columns

`v` a matrix of with the right singular vectors of `mat` in the columns

`eigsum` sum of the eigenvalues, for calculating percent variance explained

Examples

```
mat <- matrix(sample(0:10, 2500, replace=TRUE), ncol=50)
compsvd(mat)
compsvd(mat, method = 'svd')
compsvd(mat, method = 'irl', ncomp = 5)
```

corralm_matlist	<i>Multi-table correspondence analysis (list of matrices)</i>
-----------------	---

Description

This multi-table adaptation of correspondence analysis applies the same scaling technique and enables data alignment by finding a set of embeddings for each dataset within shared latent space.

Usage

```
corralm_matlist(
  matlist,
  method = c("irl", "svd"),
  ncomp = 30,
  rtype = "indexed",
  rw_contrib = NULL,
  ...
)

corralm_sce(
  sce,
  splitby,
  method = c("irl", "svd"),
  ncomp = 30,
  whichmat = "counts",
  fullout = FALSE,
  rw_contrib = NULL,
  ...
)

corralm(inp, whichmat = "counts", fullout = FALSE, ...)

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

Arguments

matlist	(for corralm_matlist) list of input matrices; input matrices should be counts (raw or log). Matrices should be aligned row-wise by common features (either by sample or by gene)
method	character, the algorithm to be used for svd. Default is irl. Currently supports 'irl' for irlba::irlba or 'svd' for stats::svd
ncomp	numeric, number of components; Default is 30
rtype	character indicating what type of residual should be computed. For corralm, defaults to indexed. Options are "indexed", "standardized", and "hellinger." indexed and standardized compute the respective chi-squared residuals and are appropriate for count data. The hellinger option is appropriate for continuous data.
rw_contrib	numeric vector, same length as the matlist. Indicates the weight that each dataset should contribute to the row weights. When set to NULL the row weights are <i>not</i> combined and each matrix is scaled independently (i.e., using their observed row weights, respectively). When set to a vector of all the same values, this is equivalent to taking the mean. Another option is to the number of observations per matrix to create a weighted mean. Regardless of input scale, row weights for each table must sum to 1 and thus are scaled.
...	(additional arguments for methods)
sce	(for corralm_sce) SingleCellExperiment; containing the data to be integrated. Default is to use the counts, and to include all of the data in the integration. These can be changed by passing additional arguments. See sce2matlist function documentation for list of available parameters.
splitby	character; name of the attribute from colData that should be used to separate the SCE.
whichmat	char, when using SingleCellExperiment or other SummarizedExperiment, can be specified. default is 'counts'.
fullout	boolean; whether the function will return the full corralm output as a list, or a SingleCellExperiment; defaults to SingleCellExperiment (FALSE). To get back the corralm_matlist -style output, set this to TRUE.
inp	list of matrices (any type), a SingleCellExperiment, list of SingleCellExperiments, list of SummarizedExperiments, or MultiAssayExperiment. If using SingleCellExperiment or SummarizedExperiment, then include the whichmat argument to specify which slot to use (defaults to counts). Additionally, if it is one SingleCellExperiment, then it is also necessary to include the splitby argument to specify the batches. For a MultiAssayExperiment, it will take the intersect of the features across all the assays, and use those to match the matrices; to use a different subset, select desired subsets then call corral
x	(print method) corralm object; the list output from corralm_matlist

Details

corralm is a wrapper for [corralm_matlist](#) and [corralm_sce](#), and can be called on any of the acceptable input types (see inp below).

Value

When run on a list of matrices, a list with the correspondence analysis matrix decomposition result, with indices corresponding to the concatenated matrices (in order of the list):

d a vector of the diagonal singular values of the input mat (from SVD output)
 u a matrix of with the left singular vectors of mat in the columns (from SVD output)
 v a matrix of with the right singular vectors of mat in the columns. When cells are in the columns, these are the cell embeddings. (from SVD output)
 eigsum sum of the eigenvalues for calculating percent variance explained

For SingleCellExperiment input, returns the SCE with embeddings in the reducedDim slot 'corralm'

For a list of [SingleCellExperiments](#), returns a list of the SCEs with the embeddings in the respective reducedDim slot 'corralm'

Examples

```
listofmats <- list(matrix(sample(seq(0,20,1),1000,replace = TRUE),nrow = 25),
                  matrix(sample(seq(0,20,1),1000,replace = TRUE),nrow = 25))
result <- corralm_matlist(listofmats)
library(DuoClustering2018)
library(SingleCellExperiment)
sce <- sce_full_Zhengmix4eq()[1:100,sample(1:3500,100,replace = FALSE)]
colData(sce)$Method <- matrix(sample(c('Method1','Method2'),100,replace = TRUE))
result <- corralm_sce(sce, splitby = 'Method')
```

```
listofmats <- list(matrix(sample(seq(0,20,1),1000,replace = TRUE),nrow = 20),
                  matrix(sample(seq(0,20,1),1000,replace = TRUE),nrow = 20))
corralm(listofmats)
```

```
library(DuoClustering2018)
library(SingleCellExperiment)
sce <- sce_full_Zhengmix4eq()[seq(1,100,1),sample(seq(1,3500,1),100,replace = FALSE)]
colData(sce)$Method <- matrix(sample(c('Method1','Method2'),100,replace = TRUE))
result <- corralm(sce, splitby = 'Method')
```

```
# default print method for corralm objects
```

corral_mat

corral: Correspondence analysis on a single matrix

Description

corral can be used for dimensionality reduction to find a set of low-dimensional embeddings for a count matrix.

corral is a wrapper for [corral_mat](#) and [corral_sce](#), and can be called on any of the acceptable input types.

Usage

```
corral_mat(
  inp,
  method = c("irl", "svd"),
  ncomp = 30,
```

```

    row.w = NULL,
    col.w = NULL,
    ...
)

corral_sce(
  inp,
  method = c("irl", "svd"),
  ncomp = 30,
  whichmat = "counts",
  fullout = FALSE,
  subset_row = NULL,
  ...
)

corral(inp, ...)

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

```

Arguments

inp	matrix (any type), SingleCellExperiment, or SummarizedExperiment. If using SingleCellExperiment or SummarizedExperiment, then include the whichmat argument to specify which slot to use (defaults to counts).
method	character, the algorithm to be used for svd. Default is irl. Currently supports 'irl' for irlba::irlba or 'svd' for stats::svd
ncomp	numeric, number of components; Default is 30
row.w	numeric vector; the row weights to use in chi-squared scaling. Defaults to 'NULL', in which case row weights are computed from the input matrix.
col.w	numeric vector; the column weights to use in chi-squared scaling. For instance, size factors could be given here. Defaults to 'NULL', in which case column weights are computed from the input matrix.
...	(additional arguments for methods)
whichmat	character; defaults to counts, can also use logcounts or normcounts if stored in the sce object
fullout	boolean; whether the function will return the full corral output as a list, or a SingleCellExperiment; defaults to SingleCellExperiment (FALSE). To get back the corral_mat -style output, set this to TRUE.
subset_row	numeric, character, or boolean vector; the rows to include in corral, as indices (numeric), rownames (character), or with booleans (same length as the number of rows in the matrix). If this parameter is NULL, then all rows will be used.
x	(print method) corral object; the list output from corral_mat

Value

When run on a matrix, a list with the correspondence analysis matrix decomposition result:

d a vector of the diagonal singular values of the input mat (from SVD output)

u a matrix of with the left singular vectors of mat in the columns (from SVD output)

v a matrix of with the right singular vectors of mat in the columns. When cells are in the columns, these are the cell embeddings. (from SVD output)

eigsum sum of the eigenvalues for calculating percent variance explained

SCu and SCv standard coordinates, left and right, respectively

PCu and PCv principal coordinates, left and right, respectively

When run on a [SingleCellExperiment](#), returns a SCE with the embeddings (PCv from the full corral output) in the reducedDim slot corral (default). Also can return the same output as `corral_mat` when `fullout` is set to TRUE.

For matrix and SummarizedExperiment input, returns list with the correspondence analysis matrix decomposition result (u,v,d are the raw svd output; SCu and SCv are the standard coordinates; PCu and PCv are the principal coordinates)

For SummarizedExperiment input, returns the same as for a matrix.

.

Examples

```
mat <- matrix(sample(0:10, 5000, replace=TRUE), ncol=50)
result <- corral_mat(mat)
result <- corral_mat(mat, method = 'svd')
result <- corral_mat(mat, method = 'irl', ncomp = 5)

library(DuoClustering2018)
sce <- sce_full_Zhengmix4eq()[1:100,1:100]
result_1 <- corral_sce(sce)
result_2 <- corral_sce(sce, method = 'svd')
result_3 <- corral_sce(sce, method = 'irl', ncomp = 30, whichmat = 'logcounts')

library(DuoClustering2018)
sce <- sce_full_Zhengmix4eq()[1:100,1:100]
corral_sce <- corral(sce, whichmat = 'counts')

mat <- matrix(sample(0:10, 500, replace=TRUE), ncol=25)
corral_mat <- corral(mat, ncomp=5)

mat <- matrix(sample(1:100, 10000, replace = TRUE), ncol = 100)
corral(mat)
```

Description

This function performs the row and column scaling pre-processing operations, prior to SVD, for the corral methods. See `corral` for single matrix correspondence analysis and `corralm` for multi-matrix correspondence analysis.

Usage

```
corral_preproc(
  inp,
  rtype = c("standardized", "indexed", "hellinger"),
  row.w = NULL,
  col.w = NULL
)
```

Arguments

inp	matrix, numeric, counts or logcounts; can be sparse Matrix or matrix
rtype	character indicating what type of residual should be computed; options are "indexed", "standardized", and "hellinger"; defaults to "standardized." indexed and standardized compute the respective chi-squared residuals and are appropriate for count data. The hellinger option is appropriate for continuous data.
row.w	numeric vector; Default is NULL, to compute row.w based on inp. Use this parameter to replace computed row weights with custom row weights
col.w	numeric vector; Default is NULL, to compute col.w based on inp. Use this parameter to replace computed column weights with custom column weights

Value

sparse matrix, processed for input to compsvd to finish CA routine

Examples

```
mat <- matrix(sample(0:10, 500, replace=TRUE), ncol=25)
mat_corral <- corral_preproc(mat)
corral_output <- compsvd(mat_corral, ncomp = 5)
```

earthmover_dist	<i>Earthmover distance (and general Wasserstein distance)</i>
-----------------	---

Description

i.e., wasserstein distance with L1 ($p_param = 1$); can also use other penalties > 1 (Not technically earthmover distance if using other p_param values)

Usage

```
earthmover_dist(batch1, batch2, whichdim = 1, numbins = 100, p_param = 1)
```

Arguments

batch1	matrix; subset of observations from an embedding corresponding to some attribute (e.g., batch or phenotype)
batch2	matrix; subset of observations from an embedding corresponding to some attribute (e.g., batch or phenotype)
whichdim	int; which dimension (i.e., column) from the embeddings is used. defaults on first

numbins int; number of bins for the probability discretization (defaults to 100)

p_param int; penalty parameter for general Wasserstein distance. Defaults to 1, which corresponds to earthmover.

Value

num; the distance

Examples

```
# To compare distributions of reduced dimension values to assess similarity,
# e.g. as a metric for batch integration
embedding <- matrix(sample(x = seq(0,10,.1),1000, replace = TRUE),ncol = 5)
batch <- matrix(sample(c(1,2),200, replace = TRUE))
earthmover_dist(embedding[which(batch == 1),],embedding[which(batch == 2),])
```

get_pct_var_exp_svd *Compute percent of variance explained*

Description

Compute percent of variance explained

Usage

```
get_pct_var_exp_svd(thissvd, preproc_mat = thissvd$d)
```

Arguments

thissvd list outputted from an svd function (svd, irlba; can also take output from [corral_mat](#) and [corralm_matlist](#))

preproc_mat matrix of pre-processed values (optional) - important to include if the svd is only partial as this is used to compute the sum of eigenvalues

Value

vector of percent variance explained values, indexed by PC

Examples

```
mat <- matrix(sample(seq(0,20,1),100,replace = TRUE),nrow = 10)
my_svd <- svd(mat)
get_pct_var_exp_svd(my_svd) # this works if my_svd is a full svd
my_irl <- irlba::irlba(mat,nv = 2)
get_pct_var_exp_svd(my_irl, preproc_mat = mat) # ... otherwise use this
```

get_weights	<i>Get weights</i>
-------------	--------------------

Description

Computes row weights and column weights

Usage

```
get_weights(inp_mat)
```

Arguments

inp_mat matrix for which weights should be calculated (sparse or full)

Value

list of 2 elements: 'row.w' and 'col.w' contain the row and column weights respectively

Examples

```
mat <- matrix(sample(seq(0,20,1),100,replace = TRUE),nrow = 10)
ws <- get_weights(mat)
```

list2mat	<i>List to Matrix</i>
----------	-----------------------

Description

List to Matrix

Usage

```
list2mat(matlist, direction = c("c", "r")[1])
```

Arguments

matlist list of matrices to concatenate
direction character, r or c, to indicate whether should be row-wise (i.e., rbind to match on columns) or column-wise (i.e., cbind to match on rows). Defaults to columnwise (matching on rows) to match convention of SingleCellExperiments

Value

matrix

Examples

```
listofmats <- list(matrix(sample(seq(0,20,1),100,replace = TRUE),nrow = 10),
                  matrix(sample(seq(0,20,1),1000,replace = TRUE),nrow = 10))
newmat <- list2mat(listofmats) # to "cbind" them
listofmats_t <- lapply(listofmats,t)
newmat_t <- list2mat(listofmats_t, 'r') # to "rbind" them
```

na2zero	<i>Set na to 0</i>
---------	--------------------

Description

Set na to 0

Usage

```
na2zero(x)
```

Arguments

x matrix of values for which na values should be changed to 0

Value

matrix, where na values are set to 0

Examples

```
x <- matrix(sample(0:10, 5000, replace = TRUE), ncol = 25)
x[sample(1:5000, 10)] <- NA

na2zero(x)
```

pairwise_rv	<i>Pairwise rv coefficient</i>
-------------	--------------------------------

Description

Pairwise rv coefficient

Usage

```
pairwise_rv(matlist)
```

Arguments

matlist list of matrices (or matrix-like; see rv function) for which to compute pairwise RV coefficients

Value

matrix of the pairwise coefficients

Examples

```

a <- matrix(sample(1:10,100,TRUE), nrow = 10)
b <- matrix(sample(1:10,50,TRUE), nrow = 5)
c <- matrix(sample(1:10,20,TRUE), nrow = 2)

matlist <- list(a,b,c)
pairwise_rv(matlist)
pairwise_rv(lapply(matlist, t))

```

plot_embedding

Plot selected PCs from an embedding

Description

Plot selected PCs from an embedding

Usage

```

plot_embedding(
  embedding,
  xpc = 1,
  ypc = xpc + 1,
  plot_title = paste0("Dim", xpc, " by Dim", ypc),
  color_vec = NULL,
  color_title = NULL,
  ellipse_vec = NULL,
  facet_vec = NULL,
  psize = 0.8,
  saveplot = FALSE,
  plotfn = paste(plot_title, xpc, sep = "_"),
  showplot = TRUE,
  returngg = FALSE,
  color_pal_vec = NULL,
  dimname = "Dim"
)

```

Arguments

embedding	matrix or other tabular format where columns correspond to PCs and rows correspond to cells (entries). corral and corralm objects are also accepted.
xpc	int; which PC to put on the x-axis (defaults to 1)
ypc	int; which PC to put on the y-axis (defaults to the one after xpc)
plot_title	char; title of plot (defaults to titling based on xpc and ypc)
color_vec	vector; length should correspond to the number of rows in embedding, and each element of the vector classifies that cell (entry) in the embedding to that particular class, which will be colored the same. (e.g., this could be indicating which batch each cell is from)
color_title	char; what attribute the colors represent

ellipse_vec	vector; length should correspond to the number of rows in embedding, and each element of the vector classifies that cell (entry) in the embedding to that particular class, and elements of the same class will be circled in an ellipse. (e.g., this could be indicating the cell type or cell line; works best for attributes intended to be compact)
facet_vec	vector; length should correspond to the number of rows in embedding, and each element of the vector classifies that cell (entry) in the embedding to that particular class. Plot will be faceted by this attribute.
ptsize	numeric; the size of the points as passed to <code>geom_point()</code> . Defaults to 0.8.
saveplot	boolean; whether or not to save the plot, defaults FALSE
plotfn	char; what the filename is to be called. (defaults to making a name based on <code>plot_title</code> and <code>xpc</code>)
showplot	boolean; whether or not to show the plot, defaults TRUE
returngg	boolean; whether or not to return a <code>ggplot2</code> object, defaults FALSE
color_pal_vec	char; hex codes for the color palette to be used. Default is to use the <code>ggthemes</code> <code>few</code> for plots with less than 9 colors, and to use <code>"stretch"</code> pals polychrome if more colors are needed.
dimname	char; the name of the dimensions. defaults to "Dim"

Value

default none; options to display plot (`showplot`), save plot (`saveplot`), and/or return `ggplot2` object (`returngg`)

Examples

```
listofmats <- list(matrix(sample(seq(0,20,1),1000,replace = TRUE),nrow = 20),
                  matrix(sample(seq(0,20,1),1000,replace = TRUE),nrow = 20))
corralm_obj <- corralm(listofmats, ncomp = 5)
embed_mat <- corralm_obj$v
cell_type_vec <- sample(c('type1', 'type2', 'type3'),100,replace = TRUE)
plot_embedding(embedding = embed_mat,
              xpc = 1,
              plot_title = 'corralm plot',
              color_vec = cell_type_vec,
              color_title = 'cell type',
              saveplot = FALSE)

# or, call directly on the corralm object
plot_embedding(corralm_obj)
```

plot_embedding_sce	<i>Plot selected PCs from an embedding saved in a SingleCellExperiment object</i>
--------------------	---

Description

Plot selected PCs from an embedding saved in a SingleCellExperiment object

Usage

```
plot_embedding_sce(
  sce,
  which_embedding,
  color_attr = NULL,
  color_title = color_attr,
  ellipse_attr = NULL,
  facet_attr = NULL,
  ...
)
```

Arguments

sce	SingleCellExperiment object; contains the embedding within the reducedDim slot
which_embedding	character; for the embedding to plot
color_attr	character; name of the attribute within colData to use for assigning colors (in lieu of color_vec in the plot_embedding function)
color_title	character; title to use for colors legend, defaults to the same as color_attr
ellipse_attr	character; name of the attribute within colData to use for drawing ellipse(s) (in lieu of ellipse_vec in the plot_embedding function)
facet_attr	character; name of the attribute within colData to use for faceting (in lieu of facet_vec in the plot_embedding function)
...	additional optional arguments - see plot_embedding function for details on other potential arguments: xpc, ypc, plot_title, color_title (if title is different from color_attr), ptsize, saveplot, plotfn, showplot, returngg, color_pal_vec, dimname

Value

default none; options to display plot (showplot), save plot (saveplot), and/or return [ggplot2](#) object (returngg)

Examples

```
library(DuoClustering2018)
library(SingleCellExperiment)
sce <- sce_full_Zhengmix4eq()[1:100,sample(1:3500,100,replace = FALSE)]
colData(sce)$Method <- matrix(sample(c('Method1','Method2'),100,replace = TRUE))
sce <- corralm(sce, splitby = 'Method')

# to plot and show only
plot_embedding_sce(sce = sce,
  which_embedding = 'corralm',
  xpc = 1,
  plot_title = 'corralm: PC1 by PC2',
  color_attr = "Method",
  ellipse_attr = 'phenoid',
  saveplot = FALSE)

# to return ggplot2 object and display, but not save
```

```
corralm_ggplot <- plot_embedding_sce(sce = sce,
  which_embedding = 'corralm',
  xpc = 1,
  plot_title = 'corralm: PC1 by PC2',
  color_attr = 'Method',
  ellipse_attr = 'phenoid',
  returngg = TRUE,
  saveplot = FALSE)
```

rv *rv coefficient*

Description

rv coefficient

Usage

```
rv(mat1, mat2)
```

Arguments

mat1	matrix (or matrix-like, e.g., df); either columns or rows should be matched with mat2
mat2	matrix (or matrix-like, e.g., df); either columns or rows should be matched with mat1

Value

numeric; RV coefficient between the matched matrices

Examples

```
a <- matrix(sample(1:10,100, TRUE), nrow = 10)
b <- matrix(sample(1:10,50, TRUE), nrow = 5)

rv(a, b) # matched by columns
rv(t(a), t(b)) # matched by rows
```

sce2matlist	<i>SingleCellExperiment to list of matrices</i>
-------------	---

Description

SingleCellExperiment to list of matrices

Usage

```
sce2matlist(sce, splitby, to_include = NULL, whichmat = "counts")
```

Arguments

sce	SingleCellExperiment that is to be separated into list of count matrices
splitby	character; name of the attribute from colData that should be used to separate the SCE
to_include	(optional) character vector; determines which values from the "splitby" column will be included in the outputted matlist. NULL is the default, and will result in selecting all elements
whichmat	character; defaults to counts, can also use logcounts or normcounts if stored in the sce object

Value

list of matrices

Examples

```
library(DuoClustering2018)
sce <- sce_full_Zhengmix4eq()
matlist <- sce2matlist(sce = sce, splitby = 'phenoid', whichmat = 'logcounts')
```

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