Package ‘DR.SC’

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Type Package

Title Joint Dimension Reduction and Spatial Clustering

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Description Joint dimension reduction and spatial clustering is conducted for
Single-cell RNA sequencing and spatial transcriptomics data, and more details can be referred to
Wei Liu, Xu Liao, Yi Yang, Huazhen Lin, Joe Yeong, Xi-
ang Zhou, Xingjie Shi and Jin Liu. (2022) <doi:10.1093/nar/gkac219>. It is not only computa-
tionally efficient and scalable to the sample size increment, but also is capable of choos-
ing the smoothness parameter and the number of clusters as well.

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Depends parallel, spatstat.geom, R (>= 4.0.0)

Imports CompQuadForm, cowplot, ggplot2, GiRaF, MASS, Matrix, mclust,
methods, purrr, S4Vectors, RColorBrewer, Rcpp (>= 1.0.5),
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dlpfc151510

A human dorsolateral prefrontal cortex data

Description
A human dorsolateral prefrontal cortex dataset measured on the Visium platform, which includes 4634 spots and 500 genes, a subset of raw dataset at https://github.com/LieberInstitute/spatialLIBD.

Note
nothing

Author(s)
Wei Liu

References
None

Examples
data("dlpfc151510")

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Description

Joint dimension reduction and spatial clustering for scRNA-seq and spatial transcriptomics data

Usage

```r
# S3 method for class 'Seurat'
DR.SC(seu, K, q=15, platform= "Visium", ...)
```

Arguments

- `seu`: an object of class "Seurat". The details of this object are given under 'Details'.
- `q`: a positive integer, specify the number of latent features to be extracted, default as 15.
- `K`: a positive integer or integer vector, specify the number of clusters. When \( K \) is a vector, it is automatically selected by MBIC criteria. Users can also use BIC and AIC to select \( K \) or refine model with MBIC by argument `pen.const` in the function `selectModel`.
- `platform`: a string, specify the platform of the provided data, default as "Visium". There are more platforms to be chosen, including ("Visium", "ST", "seqfish", 'merfish', 'slide-seqv2') and "scRNAseq", where the first group means there are spatial coordinates information in the metadata of `seu`, named "row" and "col" and a Hidden Markov random field is used to model the spatial coordinates, and the last one "scRNAseq" means there is no spatial information in object `seu` and a multinomial model is used to model the unobserved class labels. The platform helps to calculate the adjacency matrix.
- `...`: Other arguments to pass into `DR.SC_fit` function.

Details

`seu` is an object named `Seurat`, which can easily created by R package `Seurat`. If the data is collected by the spatial transcriptomics technologies such as 10X Visium, ST, seqFISH, MERFISH and Slide-seq, then there are spatial coordinates information in the metadata of `seu`, named "row" and "col". DR-SC model uses a Hidden Markov random field to model the spatial coordinates. If the data is collected by the single cell RNA sequencing technologies which means there is no spatial information in object `seu` then a multinomial model is used to model the unobserved class labels.
DR.SC returns a revised Seurat object. There are two revisions in the seu. 1. the metadata is added a new column named `spatial.drsc.cluster` that represents the clustering results from DR-SC model, and the `Idents(seu)` is assigned with `spatial.drsc.cluster`. 2. a DimReduc object named `dr-sc` is added in the slot `reductions`, which represents the features extracted by DR-SC model.

Note
nothing

Author(s)
Wei Liu

References

See Also
None

Examples
```r
## we generate the spatial transcriptomics data with lattice neighborhood, i.e. ST platform.
seu <- gendata_RNAExp(height=10, width=10,p=50, K=4,platform="ST")
library(Seurat)
seu <- NormalizeData(seu, verbose=FALSE)
# choose 100 highly variable features
# seu <- FindVariableFeatures(seu, nfeatures = 100)
# maxIter = 2 is only used for illustration, and user can use default.
# seu1 <- DR.SC(seu, K=4, platform = 'ST', maxIter=2,verbose=FALSE)
# choose spatially variable features (SVGs)
seu <- FindSVGs(seu, nfeatures = 40, verbose=FALSE)
# use SVGs to fit DR.SC model
# maxIter = 2 is only used for illustration, and user can use default.
seu1 <- DR.SC(seu, K=4,platform = 'ST', maxIter=2, verbose=TRUE)
```
**DR.SC_fit**

Joint dimension reduction and spatial clustering for scRNA-seq and spatial transcriptomics data

**Usage**

```r
DR.SC_fit(X, K, Adj_sp=NULL, q=15,
error.heter= TRUE, beta_grid=seq(0.5, 5, by=0.5),
maxIter=25, epsLogLik=1e-5, verbose=FALSE, maxIter_ICM=6,
wpca.int=FALSE, coreNum = 5)
```

**Arguments**

- **X**
  a sparse matrix with class dgCMatrix or matrix, specify the log-normalization gene expression matrix used for DR-SC model.

- **K**
  a positive integer allowing scalar or vector, specify the number of clusters in model fitting.

- **Adj_sp**
  an optional sparse matrix with class dgCMatrix, specify the adjoint matrix used for DR-SC model. We provide this interface for those users who would like to define the adjoint matrix by their own.

- **q**
  a positive integer, specify the number of latent features to be extracted, default as 15.

- **error.heter**
  an optional logical value, whether use the heterogenous error for DR-SC model, default as TRUE. If error.heter=FALSE, then the homogenous error is used for probabilistic PCA model in DR-SC.

- **beta_grid**
  an optional vector of positive value, the candidate set of the smoothing parameter to be searched by the grid-search optimization approach.

- **maxIter**
  an optional positive value, represents the maximum iterations of EM.

- **epsLogLik**
  an optional positive value, tolerance value of relative variation rate of the observed pseudo log-loglikelihood value, default as ’1e-5’.

- **verbose**
  an optional logical value, whether output the information of the ICM-EM algorithm.

- **maxIter_ICM**
  an optional positive value, represents the maximum iterations of ICM.

- **wpca.int**
  an optional logical value, means whether use the weighted PCA to obtain the initial values of loadings and other parameters, default as FALSE which means the ordinary PCA is used.

- **coreNum**
  an optional positive integer, means the number of thread used in parallel computing, default as 5. If the length of K is one, then coreNum will be set as 1 automatically.
Details

Nothing

Value

DR.SC_fit returns a list with class "drscObject" with the following three components:

- **Objdrsc**: a list including the model fitting results, in which the number of elements is same as the length of K.
- **out_param**: a numeric matrix used for model selection in MBIC.
- **K_set**: a scalar or vector equal to input argument K.

In addition, each element of "Objdrsc" is a list with the following components:

- **cluster**: inferred class labels
- **hZ**: extracted latent features.
- **beta**: estimated smoothing parameter
- **Mu**: mean vectors of mixtures components.
- **Sigma**: covariance matrix of mixtures components.
- **W**: estimated loading matrix
- **Lam_vec**: estimated variance of errors in probabilistic PCA model
- **loglik**: pseudo observed log-likelihood.

Note

nothing

Author(s)

Wei Liu

References


See Also

None
Examples

```r
## we generate the spatial transcriptomics data with lattice neighborhood, i.e. ST platform.
seu <- gendata_RNAExp(height=10, width=10, p=50, K=4)
library(Seurat)
seu <- NormalizeData(seu, verbose=FALSE)
# choose 40 highly variable features using FindVariableFeatures in Seurat
# seu <- FindVariableFeatures(seu, nfeatures = 40)
# or choose 40 spatially variable features using FindSVGs in DR.SC
seu <- FindSVGs(seu, nfeatures = 40, verbose=FALSE)
# users define the adjacency matrix
Adj_sp <- getAdj(seu, platform = 'ST')
var.features <- seu@assays$RNA@var.features
X <- Matrix::t(seu[["RNA"]][data[var.features,]])
# maxIter = 2 is only used for illustration, and user can use default.
drscList <- DR.SC_fit(X, Adj_sp=Adj_sp, K=4, maxIter=2, verbose=TRUE)
```

---

**drscPlot**

* tNSE or UMAP plot visualization

### Description

Intuitive way of visualizing how cell types changes across the spatial locations.

### Usage

```r
drscPlot(seu, dims=1:5, visu.method='tSNE',...)
```

### Arguments

- `seu` an object of class "Seurat" obtained by DR.SC.
- `dims` a positive integer to specify the number of latent features for visualiztion.
- `visu.method` a string including 'tSNE' or 'UMAP'.
- `...` Other arguments passing to DimPlot function.

### Details

Nothing

### Value

return a ggplot2 object.

### Note

nothing
FindSVGs

Find spatially variable genes

Description

Identifies features that have spatially variation along spots.

Usage

FindSVGs(seu, nfeatures=2000, covariates=NULL, num_core=1, verbose=TRUE)

Arguments

- **seu**: an object of class "Seurat".
- **nfeatures**: a positive integer, means how many spatially variable genes to be chosen. If there are less than 2000 features in seu, then all features are identified.
- **covariates**: a covariate matrix named control variable matrix whose number of rows is equal to the number of columns of seu.
- **num_core**: an optional positive integer, specify the cores used for identifying the SVGs in parallel.
- **verbose**: an optional logical value, whether output the related information.

Examples

```r
# we generate the spatial transcriptomics data with lattice neighborhood, i.e. ST platform.
seu <- gendata_RNAExp(height=10, width=10, p=50, K=4)
library(Seurat)
seu <- NormalizeData(seu)
# choose spatially variable features
seu <- FindSVGs(seu)

# use SVGs to fit DR.SC model
# maxIter = 2 is only used for illustration, and user can use default.
seu1 <- DR.SC(seu, K=4, platform = "ST", maxIter = 2, verbose=FALSE)
drscPlot(seu1)
```
**gendata_RNAExp**

**Details**

Nothing

**Value**

return a revised Seurat object by adding three columns named "is.SVGs", "order.SVGs" and "adjusted.pval.SVGs" in the meta.features of default Assay.

**Note**

nothing

**References**


**See Also**

topSVGs

**Examples**

```r
seu <- gendata_RNAExp(height=20, width=20, p=200, K=4)
seu <- FindSVGs(seu, nfeatures=100)
topSVGs(seu)
```

---

**Description**

Generate simulated spatial transcriptomics data or scRNAseq data.

**Usage**

gendata_RNAExp(height=30, width=30, platform="ST", p =100, q=10, K=7, G=4, sigma2=1, tau=8, seed=1, view=FALSE)
Arguments

- **height, width**: Height and width of lattice grids for generating spatial coordinates. \( n = \text{height} \times \text{width} \) cells for scRNAseq data.
- **platform**: Set the platform for the simulated data, only support 'ST' and 'scRNAseq'.
- **p**: Number of genes to generate.
- **q**: Number of true latent features to generate gene expression.
- **K**: Number of clusters (cell types).
- **seed**: Random seed for generating data.
- **G**: The number of neighbors. The latter must be one of \( G = 4 \) or \( G = 8 \), which respectively correspond to a first order and a second order dependency structure. By default, \( G = 4 \).
- **sigma2**: Variance of error term in probabilistic PCA model.
- **tau**: A positive factor of mixture mean values.
- **view**: Logical value indicating whether the draw should be printed. Do not display the optional borders.

Details

Nothing

Value

Return a "Seurat" object. If `platform="ST"`, then the metadata of this Seurat object will include two columns with names "row" and "col" which are the spatial coordinates; If `platform="scRNAseq"`, then the metadata of this Seurat object will not have them.

Note

Nothing

Author(s)

Wei Liu

References

None

See Also

None
### Examples

```r
## we generate the spatial transcriptomics data with lattice neighborhood, i.e. ST platform.
seu <- gendata_RNAExp(height=20, width=20, p=200, K=4)
seu

## generate scRNAseq data
seu <- gendata_RNAExp(height=20, width=20, platform="scRNAseq", p=100, K=4)
seu
```

### getAdj

**Calculate the adjacency matrix given the spatial coordinates**

#### Description

Calculate the adjacency matrix for the spatial transcriptomics data measured on 10X Visium or other platforms as a Seurat object.

#### Usage

```r
getAdj(obj, platform = c("Visium", "ST", "SeqFISH", "merfish", "slide-seqv2", "seqscope"))
```

#### Arguments

- **obj**: an object with class "Seurat", there are spatial coordinates information in the metadata of obj, named "row" and "col", where first column is x-axis coordinate, the second column is y-axis coordinate. `getAdj_manual` and `getAdj_auto` supports multi-dimensional spatial coordinates with a matrix as input.
- **platform**: a string, specify the platform of the provided data, default as "Visium". There are many platforms to be supported, including ("Visium", "ST", "SeqFISH", "merFISH", "slide-seqv2", "seqscope", "HDST"), which means there are spatial coordinates information in the metadata of seu, named "row" and "col". The platform helps to calculate the adjacency matrix by defining the neighborhoods.

#### Details

For lattice grids, i.e., two-dimensional coordinates, the interior spot has four neighbors (left, right, up and down), the boundary spot has three neighbors, and the spot in the corner has two neighbors. For hexagon grids, such as spatial coordinate in 10X Visium platform, the interior spot has six neighbors. More flexible definition can be used if there are some additional information. And then use `getAdj_manual` function to evaluate the adjacency matrix as a input for `DR.SC_fit` to run DR-SC model.
Value

Return a `dgCMatrix` object recording the information of neighborhoods about each spot.

Note

nothing

Author(s)

Wei Liu

References

None

See Also

ggetAdj_auto, getAdj_manual.

Examples

```r
## S3 method for class "Seurat"
seu <- gendata_RNAExp(height=20, width=20, p=200, K=4)
Adj_sp <- getAdj(seu, platform = 'ST')
```
getAdj_manual

See Also

getAdj, getAdj_manual.

---

getAdj_manual

*Calculate adjacency matrix by user-specified radius*

**Description**

An efficient function to find the neighborhood based on the matrix of position and a pre-defined radius.

**Usage**

getAdj_manual(pos, radius)

**Arguments**

- **pos**: is a n-by-d matrix of position, where n is the number of spots, and d is the dimension of coordinates.
- **radius**: is a threshold of Euclidean distance to decide whether a spot is a neighborhood of another spot. For example, if the Euclidean distance between spot A and B is less than radius, then A is taken as the neighborhood of B.

**Value**

A sparse matrix containing the neighborhood

See Also

getAdj_auto, getAdj.

---

getneighborhood_fast

**Description**

An efficient function to find the neighborhood based on the matrix of position and a pre-defined cutoff

**Usage**

getneighborhood_fast(x, radius)
**mbicPlot**

**Arguments**

- **x** is a n-by-2 matrix of position.
- **radius** is a threshold of Euclidean distance to decide whether a spot is a neighborhood of another spot. For example, if the Euclidean distance between spot A and B is less than cutoff, then A is taken as the neighborhood of B.

**Value**

A sparse matrix containing the neighborhood

---

**mbicPlot**

*MBIC plot visualization*

**Description**

Intuitive way of visualizing how modified BIC values changes across different number of clusters

**Usage**

`mbicPlot(seu, criteria="MBIC")`

**Arguments**

- **seu** an object of class `Seurat` revised by `DR.SC` with argument `K=NULL`.
- **criteria** a string specifying the information criteria such as AIC, BIC and MBIC to be plotted, default as MBIC.

**Details**

Nothing

**Value**

return a `ggplot2` object.

**Note**

nothing

**Author(s)**

Wei Liu

**References**

None
**read10XVisium**

**Description**

Read the spatial transcriptomics data measured on 10X Visium platform as a Seurat object, where the spatial coordinates are saved in the metadata, named "row" and "col".

**Usage**

```r
read10XVisium(dirname)
```

**Arguments**

- `dirname` A string, the directory of Visium datasets

**Details**

Nothing

**Value**

return a Seurat object.

**Note**

nothing

**Author(s)**

Wei Liu

---

### Examples

```r
## we generate the spatial transcriptomics data with lattice neighborhood, i.e. ST platform.
seu <- gendata_RNAExp(height=20, width=20,p=100, K=4)
library(Seurat)
seu <- NormalizeData(seu)
# choose spatially variable features
seu <- FindSVGs(seu)
## Just for illustrating the usage of mbicPlot
seu["RNA"]@misc["Var"] <- data.frame(K=2:5, MBIC=c(105, 101, 99, 108))
mbicPlot(seu)
```
readscRNAseq

Description

Read the single cell RNA sequencing data measured on scRNA sequencing platform as a Seurat object.

Usage

readscRNAseq(mtx, cells, features, ...)

Arguments

- **mtx**: a string, ane or remote URL of the mtx file
- **cells**: a string, Name or remote URL of the cells/barcodes file
- **features**: a string, Name or remote URL of the features/genes file
- **...**: the arguments passing to ReadMtx

Details

Nothing

Value

return a Seurat object including expression matrix.

Note

nothing
RunWPCA

Author(s)
Wei Liu

References
None

See Also
None

Examples

## Not run:
### set the file directory, then read it.
seu <- readscRNAseq(mtx="GSM3755564_16_Liver_Treg_matrix.mtx.gz",
features='GSM3755564_16_Liver_Treg_genes.tsv.gz',
cells='GSM3755564_16_Liver_Treg_barcode.tsv.gz')

seu

## End(Not run)

---

RunWPCA Run Weighted Principal Component Analysis

Description
Run a weighted PCA dimensionality reduction

Usage

RunWPCA(object, q=15)
### S3 method for class "Seurat"
## RunWPCA(object, q=15)

### S3 method for class "matrix"
## RunWPCA(object, q=15)

### S3 method for class "dgCMatrix"
## RunWPCA(object, q=15)

Arguments

- **object**: an object named "Seurat", "matrix" or "dgCMatrix". The object of class "Seurat" must include slot "scale.data".
- **q**: an optional positive integer, specify the number of features to be extracted.
Details

Nothing

Value

For Seurat object, return a Seurat object. For object "matrix" and "dgCMatrix", return a object "matrix" with rownames same as the colnames of \( X \), and colnames "WPCA1" to "WPCAq".

Note

nothing

Author(s)

Wei Liu

References


See Also

None

Examples

```r
## Not run:
library(Seurat)
seu <- gendata_RNAExp(height=20, width=20, p=100, K=4)
## log-normalization
seu <- NormalizeData(seu)
##
## Run WPCA
seu <- RunWPCA(seu)
## Run tSNE based on wpca
seu <- RunTSNE(seu, reduction='wpca')
seu
## Find SVGs
seu <- FindSVGs(seu, nfeatures=80)
(genes <- topSVGs(seu, ntop=10))
Idents(seu) <- factor(paste0("cluster", seu$true_clusters), levels=paste0("cluster",1:4))
RidgePlot(seu, features = genes[1:2], ncol = 2)
FeaturePlot(seu, features = genes[1:2], reduction = 'tsne', ncol=2)

## End(Not run)
```
selectModel

Select the number of clusters

Description
Select the number of clusters by specified criteria.

Usage

```r
selectModel(obj, criteria = 'MBIC', pen.const=1)  
## S3 method for class 'drscObject'
selectModel(obj, criteria = 'MBIC', pen.const=1)  
## S3 method for class 'Seurat'
selectModel(obj, criteria = 'MBIC', pen.const=1)
```

Arguments

- **S**
  an object with class Seurat by DR.SC or class drscObject by DR.SC_fit.

- **criteria**
  a string, specify the criteria used for selecting the number of clusters, supporting "MBIC", "BIC" and "AIC".

- **pen.const**
  an optional positive value, the adjusted constant used in the MBIC criteria. It usually takes value between 0.1 to 1.

Value

For S3 method of Seurat, it return a revised "Seurat" object with updated Idents(seu), spatial.drsc.cluster in the metadata and DimReduc object named dr-sc in the slot reductions. For S3 method of drscObject, it returns a list with the following components:

- **bestK**
  the selected number of clusters.

- **cluster**
  inferred class labels

- **hZ**
  extracted latent features.

- **icMat**
  a numeric matrix including the criteria value for each number of clusters K.

Note

nothing

Author(s)

Wei Liu
References
None

See Also
DR.SC, DR.SC_fit.

Examples
```r
seu <- gendata_RNAExp(height=10, width=10, p=50, K=4)
library(Seurat)
seu <- NormalizeData(seu, verbose=FALSE)
# or choose 40 spatially variable features using FindSVGs in DR.SC
seu <- FindSVGs(seu, nfeatures = 40, verbose=FALSE)
# users define the adjacency matrix
Adj_sp <- getAdj(seu, platform = 'ST')
var.features <- seu@assays$RNA@var.features
X <- Matrix::t(seu@"RNA"@data[var.features,])
# maxIter = 2 is only used for illustration, and user can use default.
drscList <- DR.SC_fit(X, Adj_sp=Adj_sp , K=4, maxIter=2, verbose=TRUE)
drsc1 <- selectModel(drscList)
str(drsc1)
```

---

**spatialPlotClusters**

Spatial coordinates plot visualization

**Description**
Intuitive way of visualizing how cell types changes across the spatial locations.

**Usage**
```r
spatialPlotClusters(seu)
```

**Arguments**

- `seu` an object of class "Seurat" obtained by **DR.SC**.

**Details**
Nothing

**Value**
return a ggplot2 object.

**Note**
nothing
sp_means_Rcpp

Author(s)

Wei Liu

References

None

See Also

None

Examples

```r
## we generate the spatial transcriptomics data with lattice neighborhood, i.e. ST platform.
seu <- gendata_RNAExp(height=10, width=10,p=50, K=4)
library(Seurat)
seu <- NormalizeData(seu)
# choose spatially variable features using Seurat
seu <- FindSVGs(seu)
# use SVGs to fit DR.SC model
# maxIter = 2 is only used for illustration, and user can use default.
seu1 <- DR.SC(seu, K=4,platform = 'ST', maxIter=2,verbose=FALSE)
spatialPlotClusters(seu1)
```

---

**sp_means_Rcpp**  
*Calculate column-wise or row-wise mean*

**Description**

Calculate column-wise or row-wise mean

**Usage**

```r
sp_means_Rcpp(sp_data, rowMeans = FALSE)
```

**Arguments**

- `sp_data`  
  A sparse matrix
- `rowMeans`  
  A boolean value, whether to calculate row-wise mean

**Value**

A n x 1 or p x 1 matrix
sp_sums_Rcpp  
*Calculate column-wise or row-wise sum*

**Description**
Calculate column-wise or row-wise sum

**Usage**
```r
sp_sums_Rcpp(sp_data, rowSums = FALSE)
```

**Arguments**
- `sp_data`: A sparse matrix
- `rowSums`: A boolean value, whether to calculate row-wise sum

**Value**
A n x 1 or p x 1 matrix

---

topSVGs  
*Return the top n SVGs*

**Description**
Return top n spatially variable genes given a Seurat object performed by `FindSVGs`.

**Usage**
```r
topSVGs(seu, ntop=5)
```

**Arguments**
- `seu`: an object of class "Seurat".
- `ntop`: an optional positive integer, means how many spatially variable genes to access.

**Details**
Nothing

**Value**
return a character vector including the names of SVGs.
topSVGs

**Note**
nothing

**Author(s)**
Wei Liu

**References**
None

**See Also**
topSVGs

**Examples**
```r
seu <- gendata_RNAExp(height=20, width=20, p=200, K=4)
seu <- FindSVGs(seu, nfeatures=100, verbose=FALSE)
(genes <- topSVGs(seu, ntop=10))
```
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