Package 'RCSL'

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Type Package

Title Rank Constrained Similarity Learning for single cell RNA sequencing data

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Description A novel clustering algorithm and toolkit RCSL (Rank Constrained Similarity Learning) to accurately identify various cell types using scRNA-seq data from a complex tissue. RCSL considers both lo-cal similarity and global similarity among the cells to discern the subtle differences among cells of the same type as well as larger differences among cells of different types. RCSL uses Spearman's rank correlations of a cell's expression vector with those of other cells to measure its global similar-ity, and adaptively learns neighbour representation of a cell as its local similarity. The overall similarity of a cell to other cells is a linear combination of its global similarity and local similarity.

URL https://github.com/QinglinMei/RCSL

Depends R (>= 4.1)

License Artistic-2.0

VignetteBuilder knitr

biocViews SingleCell, Software, Clustering, DimensionReduction, RNASeq, Visualization, Sequencing

Suggests testthat, knitr, BiocStyle, rmarkdown, mclust, tidyverse, tinytex

Imports RcppAnnoy, igraph, NbClust, Rtsne, ggplot2(>= 3.4.0), methods, pracma, umap, grDevices, graphics, stats, Rcpp (>= 0.11.0), MatrixGenerics, SingleCellExperiment

LazyData TRUE

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RoxygenNote 7.3.1

NeedsCompilation no

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Contents

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ann *Cell type annotations of 'yan' datasets by Yan et al.*

Description

Cell type annotations of 'yan' datasets by Yan et al.

Usage

```
ann
```

Format

An object of class `data.frame` with 90 rows and 1 columns.

Source

http://dx.doi.org/10.1038/nsmb.2660

Each row corresponds to one cell of 'yan' dataset

BDSM *Calculate the bolock-diagnal matrix B min_B>=0, B*1=1, F'*F=I ||B - A||_1 + r*||B||^2 + 2*lambda*trace(F'*L*F)*

Description

Calculate the bolock-diagnal matrix B min_B>=0, B*1=1, F'*F=I ||B - A||_1 + r*||B||^2 + 2*lambda*trace(F'*L*F)

Usage

```
BDSM(S, C)
```

Arguments

S	the calculated initial similarity matrix S
C	the estimated number of clusters C

Value

B block-diagonal matrix

y clustering results

Examples

```
gfData <- GenesFilter(yan)
res_SimS <- SimS(gfData)
C <- EstClusters(res_SimS$drData,res_SimS$S)
BDSM(res_SimS$S,C)
```

EProjSimplexdiag *Solve the problem: min 1/2*x'*L*x-x'*d s.t. x>=0, 1'x=1*

Description

Solve the problem: min 1/2*x'*L*x-x'*d s.t. x>=0, 1'x=1

Usage

```
EProjSimplexdiag(d, l)
```

Arguments

d	matrix or vector
l	matrix or vector

Value

x

EstClusters *Estimate the optimal number of clusters C for clustering*

Description

Estimate the optimal number of clusters C for clustering

Usage

```
EstClusters(drData, S)
```

Arguments

drData	gene expression matrix after PCA processing
S	the calculated similarity matrix S from "SimS"

Value

C the estimated number of clusters

Examples

```
gfData <- GenesFilter(yan)
res_SimS <- SimS(gfData)
EstClusters(res_SimS$drData,res_SimS$S)
```

EucDist *Solve the problem: ||A-B||^2 = ||A||^2 + ||B||^2 - 2*A'*B*

Description

Solve the problem: ||A-B||^2 = ||A||^2 + ||B||^2 - 2*A'*B

Usage

```
EucDist(A, B)
```

Arguments

A	matrix or vector
B	matrix or vector

Value

d matrix or vector

GenesFilter — *Perform the step of gene filtering to normalizaed gene expression data*

Description

Perform the step of gene filtering to normalizaed gene expression data

Usage

```
GenesFilter(data, gfRatio = 0.025)
```

Arguments

data	the normalized gene expression matrix
gfRatio	the ratio of genes filtering

Value

the gene expression matrix after genes filtering gfData

Examples

```
data(yan)
GenesFilter(yan)
```

getLineage — *Infer the development lineage based on the clustering results from RCSL and the pseudotime*

Description

Infer the development lineage based on the clustering results from RCSL and the pseudotime

Usage

```
getLineage(drData, clustRes, pseudoTime, simMeasure = "kendall")
```

Arguments

drData	preprocessed gene expression data (each column represent a cell)
clustRes	the clustering results identified by RCSL
pseudoTime	inferred by PlotPseudoTime() using the similarity matrix S and starting cell
simMeasure	the calculation method of measuring the cluster centers' similarity

Value

lineage the cell lineages connected all the cluster centers based on the clustering results from RCSL

Examples

```
gfData <- GenesFilter(yan)
TrueLabel <- ann$cell_type1
res_SimS <- SimS(gfData)
C <- EstClusters(res_SimS$drData,res_SimS$S)
res_BDSM <- BDSM(res_SimS$S,C)
Pseudo <- PlotPseudoTime(res_SimS$S,TrueLabel,startPoint=1)
getLineage(res_SimS$drData,res_BDSM$y,Pseudo$pseudoTime)
```

`NeigRepresent` *Calculate the neighbor representation of cells to the low-dimensional gene expression matrix*

Description

Calculate the neighbor representation of cells to the low-dimensional gene expression matrix

Usage

```
NeigRepresent(
  drData,
  NN.method = "KNN",
  Dis.method = "Euclidean",
  LSH.TreeNum = 30,
  LSH.Dim = 500,
  LSH.Dis = "angular",
  neiRatio = 0.65
)
```

Arguments

`drData`	gene expression matrix after dimensionality reduced by PCA
`NN.method`	the method of finding neighbors
`Dis.method`	the distance metric in finding neighbors
`LSH.TreeNum`	the tree number of LSH
`LSH.Dim`	the dimension in LSH
`LSH.Dis`	the distance metric in LSH
`neiRatio`	ratio of the number of selected

Value

the similarity matrix measured by neighbor representation NR

Examples

```
gfData <- GenesFilter(yan)
res_SimS <- SimS(gfData)
NeigRepresent(res_SimS$drData)
```

PlotMST *Plot the visualization of constructed Minimum Spanning Tree based on the clustering results of RCSL*

Description

Plot the visualization of constructed Minimum Spanning Tree based on the clustering results of RCSL

Usage

```
PlotMST(
  drData,
  clustRes,
  TrueLabel,
  dataName = "",
  fontSize = 12,
  VisualMethod = "umap"
)
```

Arguments

drData	preprocessed gene expression data
clustRes	the clustering results identified by RCSL
TrueLabel	the real cell types to color the dots in plot
dataName	the name of the data that will be showed in the plot
fontSize	the font size of the plot
VisualMethod	the method for 2D visualization including UMAP,t-SNE and PCA

Value

MSTPlot ggplot object of the visualization of constructed MST

Examples

```
gfData <- GenesFilter(yan)
TrueLabel <- ann$cell_type1
res_SimS <- SimS(gfData)
C <- EstClusters(res_SimS$drData,res_SimS$S)
res_BDSM <- BDSM(res_SimS$S,C)
PlotMST(res_SimS$drData,res_BDSM$y,TrueLabel)
```

PlotPseudoTime *Infer the pseudo-temporal ordering between the cell types using the distance from a cell type to the predefined starting cell type.*

Description

Infer the pseudo-temporal ordering between the cell types using the distance from a cell type to the predefined starting cell type.

Usage

```
PlotPseudoTime(
  S,
  TrueLabel,
  startPoint,
  fontSize = 12,
  dataName = "",
  sim = TRUE
)
```

Arguments

S	the similarity matrix calculated by SimS() function
TrueLabel	the real cell types used to indicate the vertical axis
startPoint	the posiition of the starting cell in the matrix
fontSize	the font size of the plot
dataName	the name of the data that will be showed in the plot
sim	indicate the input data is simialrity matrix or not

Value

PstudoTime

PseudoTimePlot ggplot object of the pseudo-temporal ordering of cells

Examples

```
gfData <- GenesFilter(yan)
TrueLabel <- ann$cell_type1
res_SimS <- SimS(gfData)
PlotPseudoTime(res_SimS$S,TrueLabel,startPoint=1)
```

PlotTrajectory *Infer the developmental trajectories based on the clustering results from RCSL*

Description

Infer the developmental trajectories based on the clustering results from RCSL

Usage

```
PlotTrajectory(
  gfData,
  clustRes,
  TrueLabel,
  lineage,
  fontSize = 12,
  dataName = "",
  VisualMethod = "umap"
)
```

Arguments

gfData	preprocessed gene expression data (each column represent a cell)
clustRes	the clustering results identified by RCSL
TrueLabel	the real cell types
lineage	the lineage obtained by getLineage()
fontSize	the size of font in the plot
dataName	the name of the data that will be showed in the plot
VisualMethod	the display method of 2-D visualization

Value

TrajectoryPlot ggplot object of the inferred developmental trajectories

Examples

```
gfData <- GenesFilter(yan)
TrueLabel <- ann$cell_type1
res_SimS <- SimS(gfData)
C <- EstClusters(res_SimS$drData,res_SimS$S)
res_BDSM <- BDSM(res_SimS$S,C)
Pseudo <- PlotPseudoTime(res_SimS$S,TrueLabel,startPoint=1)
Linea <- getLineage(res_SimS$drData,res_BDSM$y,Pseudo$pseudoTime)
PlotTrajectory(gfData,res_BDSM$y,TrueLabel,lineage=Linea)
```

RCSL *Perform the RCSL program*

Description

Perform the RCSL program

Usage

```
RCSL(
  data,
  GF = TRUE,
  gfRatio = 0.025,
  pcRatio = 0.95,
  NN.method = "KNN",
  Dis.method = "Euclidean",
  neiRatio = 0.65
)
```

Arguments

data	normalizaed gene expression matrix(each column represents a cell)
GF	should I need the gene filter step?
gfRatio	the ratio of the gene filter
pcRatio	the ratio between the variance of the
NN.method	the method of finding neighbors
Dis.method	the distance metric in finding neighbors
neiRatio	ratio of the number of selected

Value

gfData gene expression matrix after genes filtering

B block-diagonal matrix

C estimated number of clusters

y clustering results

Examples

```
data(yan)
data <- log2(yan+1)
RCSL(yan[,1:20])
```

SimS *Calculate the initial similarity matrix*

Description

Calculate the initial similarity matrix

Usage

```
SimS(
  data,
  pcRatio = 0.95,
  gamma = 0.8,
  NN.method = "KNN",
  Dis.method = "Euclidean",
  LSH.TreeNum = 30,
  LSH.Dim = 1000,
  LSH.Dis = "angular",
  neiRatio = 0.65
)
```

Arguments

data	gene expression matrix after genes filtering
pcRatio	the ratio between the variance of the
gamma	the ratio of the global simialrity
NN.method	the method of finding neighbors
Dis.method	the distance metric in finding neighbors
LSH.TreeNum	the tree number of LSH
LSH.Dim	the dimension in LSH
LSH.Dis	the distance metric in LSH
neiRatio	ratio of the number of selected

Value

initial similarity matrix S

gene expression matrix after PCA processing drData

Examples

```
gfData <- GenesFilter(yan)
SimS(gfData)
```

`TrajectoryAnalysis` *Trajectory analysis*

Description

Trajectory analysis

Usage

```
TrajectoryAnalysis(
  gfData,
  drData,
  S,
  clustRes,
  fontSize = 12,
  TrueLabel,
  startPoint,
  dataName = "",
  sim = TRUE,
  simMeasure = "kendall",
  VisualMethod = "umap"
)
```

Arguments

`gfData`	preprocessed gene expression data (each column represent a cell)
`drData`	preprocessed gene expression data (each column represent a cell)
`S`	the similarity matrix calculated by SimS() function
`clustRes`	the clustering results identified by RCSL
`fontSize`	the size of font in the plot
`TrueLabel`	the real cell types used to indicate the vertical axis
`startPoint`	the posiition of the starting cell in the matrix
`dataName`	the name of the data that will be showed in the plot
`sim`	indicate the input data is simialrity matrix or not
`simMeasure`	the calculation method of measuring the cluster centers' similarity
`VisualMethod`	the display method of 2-D visualization

Value

PseudoTimePlot, MSTPlot, TrajectoryPlot

Examples

```
gfData <- GenesFilter(yan)
TrueLabel <- ann$cell_type1
res_SimS <- SimS(gfData)
C <- EstClusters(res_SimS$drData,res_SimS$S)
res_BDSM <- BDSM(res_SimS$S,C)
TrajectoryAnalysis(gfData,res_SimS$drData,res_SimS$S,res_BDSM$y,
                   TrueLabel=TrueLabel,startPoint=1)
```

yan *A public scRNA-seq dataset by Yan et al.*

Description

A public scRNA-seq dataset by Yan et al.

Usage

```
yan
```

Format

An object of class `data.frame` with 20214 rows and 90 columns.

Source

http://dx.doi.org/10.1038/nsmb.2660

Columns represent cells, rows represent genes expression values.

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