

Package ‘SCORPION’

October 12, 2022

Type Package

Title Single Cell Oriented Reconstruction of PANDA Individual
Optimized Networks

Version 1.0.1

Description Constructs gene regulatory networks from single-cell gene expression data using the PANDA (Passing Attributes between Networks for Data Assimilation) algorithm.

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Encoding UTF-8

LazyData true

Imports cli, methods, irlba, igraph, RANN, Matrix, pbapply,
RhpcBLASctl

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NeedsCompilation no

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scorpion	<i>Constructs PANDA gene regulatory networks from single-cell gene expression data</i>
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Description

Constructs gene regulatory networks from single-cell gene expression data using the PANDA (Passing Attributes between Networks for Data Assimilation) algorithm.

Usage

```
scorpion(
  tfMotifs = NULL,
  gexMatrix,
  ppiNet = NULL,
  nCores = 1,
  gammaValue = 10,
  nPC = 25,
  assocMethod = "pearson",
  alphaValue = 0.1,
  hammingValue = 0.001,
  nIter = Inf,
  outNet = c("regulatory", "coregulatory", "cooperative"),
  zScaling = TRUE,
  showProgress = TRUE,
  randomizationMethod = "None",
  scaleByPresent = FALSE
)
```

Arguments

tfMotifs	A motif dataset, a data.frame or a matrix containing 3 columns. Each row describes an motif associated with a transcription factor (column 1) a gene (column 2) and a score (column 3) for the motif.
gexMatrix	An expression dataset, with genes in the rows and barcodes (cells) in the columns.
ppiNet	A Protein-Protein-Interaction dataset, a data.frame or matrix containing 3 columns. Each row describes a protein-protein interaction between transcription factor 1(column 1), transcription factor 2 (column 2) and a score (column 3) for the interaction.
nCores	Number of processors to be used if BLAS or MPI is active.
gammaValue	Graining level of data (proportion of number of single cells in the initial dataset to the number of super-cells in the final dataset)
nPC	Number of principal components to use for construction of single-cell kNN network.
assocMethod	Association method. Must be one of 'pearson', 'spearman' or 'pcNet'.

alphaValue	Value to be used for update variable.
hammingValue	Value at which to terminate the process based on Hamming distance.
nIter	Sets the maximum number of iterations PANDA can run before exiting.
outNet	A vector containing which networks to return. Options include "regulatory", "coregulatory", "cooperative".
zScaling	Boolean to indicate use of Z-Scores in output. False will use [0,1] scale.
showProgress	Boolean to indicate printing of output for algorithm progress.
randomizationMethod	Method by which to randomize gene expression matrix. Default "None". Must be one of "None", "within.gene", "by.genes". "within.gene" randomization scrambles each row of the gene expression matrix, "by.gene" scrambles gene labels.
scaleByPresent	Boolean to indicate scaling of correlations by percentage of positive samples

Value

A list of matrices describing networks achieved by convergence with PANDA algorithm.

Author(s)

Daniel Osorio <daniecos@uio.no>

Examples

```
# Loading example data
data(scorpionTest)

# The structure of the data
str(scorpionTest)

# List of 3
# $ gex:Formal class 'dgCMatrix' [package "Matrix"] with 6 slots
# .. ..@ i      : int [1:4456] 1 5 8 11 22 30 33 34 36 38 ...
# .. ..@ p      : int [1:81] 0 47 99 149 205 258 306 342 387 423 ...
# .. ..@ Dim     : int [1:2] 230 80
# .. ..@ Dimnames:List of 2
# .. .. ..$ : chr [1:230] "MS4A1" "CD79B" "CD79A" "HLA-DRA" ...
# .. .. ..$ : chr [1:80] "ATGCCAGAACGACT" "CATGGCCTGTGCAT" "GAACCTGATGAACC" "TGACTGGATTCTCA" ...
# .. ..@ x      : num [1:4456] 1 1 3 1 1 4 1 5 1 1 ...
# .. ..@ factors : list()
# $ tf :'data.frame': 4485 obs. of 3 variables:
# ..$ tf      : chr [1:4485] "ADNP" "ADNP" "ADNP" "AEBP2" ...
# ..$ target: chr [1:4485] "PRF1" "TMEM40" "TNFRSF1B" "CFP" ...
# ..$ mor     : num [1:4485] 1 1 1 1 1 1 1 1 1 1 ...
# $ ppi:'data.frame': 12754 obs. of 3 variables:
# ..$ X.node1  : chr [1:12754] "ADNP" "ADNP" "ADNP" "AEBP2" ...
# ..$ node2    : chr [1:12754] "ZBTB14" "NFIA" "CDC5L" "YY1" ...
# ..$ combined_score: num [1:12754] 0.769 0.64 0.581 0.597 0.54 0.753 0.659 0.548 0.59 0.654 ...

# Running SCORPION with large alphaValue for testing purposes.
```

```

scorpionOutput <- scorpion(tfMotifs = scorpionTest$tf,
                          gexMatrix = scorpionTest$gex,
                          ppiNet = scorpionTest$ppi,
                          alphaValue = 0.8)

# -- SCORPION -----
# + Initializing and validating
# + Verified sufficient samples
# i Normalizing networks
# i Learning Network
# i Using tanimoto similarity
# + Successfully ran SCORPION on 214 Genes and 783 TFs

# Structure of the output.
str(scorpionOutput)

# List of 6
# $ regNet :Formal class 'dgeMatrix' [package "Matrix"] with 4 slots
# .. ..@ x      : num [1:167562] -0.413 1.517 -1.311 0.364 -1.041 ...
# .. ..@ Dim    : int [1:2] 783 214
# .. ..@ Dimnames:List of 2
# .. .. ..$ : chr [1:783] "ADNP" "AEBP2" "AIRE" "ALX1" ...
# .. .. ..$ : chr [1:214] "ACAP1" "ACRBP" "ACSM3" "ADAR" ...
# .. ..@ factors : list()
# $ coregNet:Formal class 'dgeMatrix' [package "Matrix"] with 4 slots
# .. ..@ x      : num [1:45796] 7.07e+06 -4.06 1.76e+01 -1.16e+01 -1.62e+01 ...
# .. ..@ Dim    : int [1:2] 214 214
# .. ..@ Dimnames:List of 2
# .. .. ..$ : chr [1:214] "ACAP1" "ACRBP" "ACSM3" "ADAR" ...
# .. .. ..$ : chr [1:214] "ACAP1" "ACRBP" "ACSM3" "ADAR" ...
# .. ..@ factors : list()
# $ coopNet :Formal class 'dgeMatrix' [package "Matrix"] with 4 slots
# .. ..@ x      : num [1:613089] 5.65e+06 -5.16 -3.79 -3.63 2.94 ...
# .. ..@ Dim    : int [1:2] 783 783
# .. ..@ Dimnames:List of 2
# .. .. ..$ : chr [1:783] "ADNP" "AEBP2" "AIRE" "ALX1" ...
# .. .. ..$ : chr [1:783] "ADNP" "AEBP2" "AIRE" "ALX1" ...
# .. ..@ factors : list()
# $ numGenes: int 214
# $ numTFs  : int 783
# $ numEdges: int 167562

```

scorpionTest

Example single-cell gene expression, motif, and ppi data

Description

This data is a list containing three objects. The motif data.frame describes a set of pairwise connections where a specific known sequence motif of a transcription factor was found upstream of the corresponding gene. The expression dgCMatrix is a set of 230 gene expression levels measured

across 80 cells. Finally, the `ppi` `data.frame` describes a set of known pairwise protein-protein interactions.

Usage

```
data(scorpionTest)
```

Format

A list containing three datasets.

`gex` A subsetted version of 10X Genomics' 3k PBMC dataset provided by the Seurat package.

`tf` Subset of the transcription-factor and target gene list provided by the dorothea package for Homo sapiens.

`ppi` The known protein-protein interactions and the combined score downloaded from the STRING database

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# .. ..@ p      : int [1:81] 0 47 99 149 205 258 306 342 387 423 ...
# .. ..@ Dim    : int [1:2] 230 80
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# .. .. ..$ : chr [1:80] "ATGCCAGAACGACT" "CATGGCCTGTGCAT" "GAACCTGATGAACC" "TGACTGGATTCTCA" ...
# .. ..@ x      : num [1:4456] 1 1 3 1 1 4 1 5 1 1 ...
# .. ..@ factors : list()
# $ tf :'data.frame': 4485 obs. of 3 variables:
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# ..$ combined_score: num [1:12754] 0.769 0.64 0.581 0.597 0.54 0.753 0.659 0.548 0.59 0.654 ...
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