

Package ‘scds’

December 11, 2024

Type Package

Title In-Silico Annotation of Doublets for Single Cell RNA Sequencing Data

Version 1.23.0

Description In single cell RNA sequencing (scRNA-seq) data combinations of cells are sometimes considered a single cell (doublets). The scds package provides methods to annotate doublets in scRNA-seq data computationally.

License MIT + file LICENSE

Encoding UTF-8

biocViews SingleCell, RNASeq, QualityControl, Preprocessing, Transcriptomics, GeneExpression, Sequencing, Software, Classification

RoxygenNote 6.1.1

Depends R (>= 3.6.0)

Imports Matrix, S4Vectors, SingleCellExperiment, SummarizedExperiment, xgboost, methods, stats, dplyr, pROC

Suggests BiocStyle, knitr, rsvd, Rtsne, scater, cowplot, rmarkdown

VignetteBuilder knitr

git_url <https://git.bioconductor.org/packages/scds>

git_branch devel

git_last_commit f0cf1fa

git_last_commit_date 2024-10-29

Repository Bioconductor 3.21

Date/Publication 2024-12-10

Author Dennis Kostka [aut, cre],
Bais Abha [aut]

Maintainer Dennis Kostka <kostka@pitt.edu>

Contents

bcds	2
cxds	3
cxds_bcds_hybrid	4
cxds_getTopPairs	4
get_dblCalls_ALL	5
get_dblCalls_dist	6
get_dblCalls_ROC	6
sce_chcl	7

Index	8
--------------	----------

bcds	<i>Find doublets/multiplets in UMI scRNA-seq data;</i>
------	--

Description

Annotates doublets/multiplets using a binary classification approach to discriminate artificial doublets from original data.

Usage

```
bcds(sce, ntop = 500, srat = 1, verb = FALSE, retRes = FALSE,
     nmax = "tune", varImp = FALSE, estNdbl = FALSE)
```

Arguments

sce	single cell experiment (SingleCellExperiment) object to analyze; needs counts in assays slot.
ntop	integer, indicating number of top variance genes to consider. Default: 500
srat	numeric, indicating ratio between original number of "cells" and simulated doublets; Default: 1
verb	progress messages. Default: FALSE
retRes	logical, should the trained classifier be returned? Default: FALSE
nmax	maximum number of training rounds; integer or "tune". Default: "tune"
varImp	logical, should variable (i.e., gene) importance be returned? Default: FALSE
estNdbl	logical, should the number of doublets be estimated from the data. Enables doublet calls. Default:FALSE. Use with caution.

Value

sce input sce object SingleCellExperiment with doublet scores added to colData as "bcds_score" column, and possibly more (details)

Examples

```
data("sce_chcl")
## create small data set using only 100 cells
sce_chcl_small = sce_chcl[, 1:100]
sce_chcl_small = bcdds(sce_chcl_small)
```

cxds

*Find doublets/multiplets in UMI scRNA-seq data;***Description**

Annotates doublets/multiplets using co-expression based approach

Usage

```
cxds(sce, ntop = 500, binThresh = 0, verb = FALSE, retRes = FALSE,
     estNdbl = FALSE)
```

Arguments

sce	single cell experiment (SingleCellExperiment) object to analyze; needs counts in assays slot.
ntop	integer, indimessageing number of top variance genes to consider. Default: 500
binThresh	integer, minimum counts to consider a gene "present" in a cell. Default: 0
verb	progress messages. Default: FALSE
retRes	logical, whether to return gene pair scores & top-scoring gene pairs? Default: FALSE.
estNdbl	logical, should the numer of doublets be estimated from the data. Enables doublet calls. Default:FALSE. Use with caution.

Value

sce input sce object SingleCellExperiment with doublet scores added to colData as "cxds_score" column.

Examples

```
data("sce_chcl")
## create small data set using only 100 cells
sce_chcl_small = sce_chcl[, 1:100]
sce_chcl_small = cxds(sce_chcl_small)
```

cxds_bcds_hybrid *Find doublets/multiples in UMI scRNA-seq data;*

Description

Annotates doublets/multiplets using the hybrid approach

Usage

```
cxds_bcds_hybrid(sce, cxdsArgs = NULL, bcdsArgs = NULL, verb = FALSE,
  estNdbl = FALSE, force = FALSE)
```

Arguments

sce	single cell experiment (SingleCellExperiment) object to analyze; needs counts in assays slot.
cxdsArgs	list, arguments for cxds function in list form. Default: NULL
bcdsArgs	list, arguments for bcds function in list form. Default: NULL
verb	logical, switch on/off progress messages
estNdbl	logical, should the number of doublets be estimated from the data. Enables doublet calls. Default:FALSE. Use with caution.
force	logical, force a (re)run of cxds and bcds. Default: FALSE

Value

sce input sce object SingleCellExperiment with doublet scores added to colData as "hybrid_score" column.

Examples

```
data("sce_chcl")
## create small data set using only 100 cells
sce_chcl_small = sce_chcl[, 1:100]
sce_chcl_small = cxds_bcds_hybrid(sce_chcl_small)
```

cxds_getTopPairs *Extract top-scoring gene pairs from an SingleCellExperiment where cxds has been run*

Description

Extract top-scoring gene pairs from an SingleCellExperiment where cxds has been run

Usage

```
cxds_getTopPairs(sce, n = 100)
```

Arguments

sce single cell experiment to analyze; needs "counts" in assays slot.
n integer. The number of gene pairs to extract. Default: 100

Value

matrix Matrix with two columns, each containing gene indexes for gene pairs (rows).

get_dblCalls_ALL *Wrapper for getting doublet calls*

Description

Wrapper for getting doublet calls

Usage

```
get_dblCalls_ALL(scrs_real, scrs_sim, rel_loss = 1)
```

Arguments

scrs_real numeric vector, the scores for the real/original data
scrs_sim numeric vector, the scores for the artificial doublets
rel_loss numeric scalar, relative weight of a false positive classification compared with a false negative. Default:1 (same loss for fp and fn).

Value

numeric, matrix containing the (estimated) number of doublets, the score threshold and the fraction of artificial doublets missed (false negative rate, of sorts) as columns and four types of estimating: "youden", "balanced" and a false negative rate of artificial doublets of 0.1 and 0.01, respectively.

get_dblCalls_dist *Derive doublet calls from doublset scores*

Description

Given score vectors for real data and artificial doubles, derive doublet calls based on determining doublet score cutoffs.

Usage

```
get_dblCalls_dist(scrs_real, scrs_sim, type = "balanced")
```

Arguments

scrs_real	numeric vector, the scores for the real/original data
scrs_sim	numeric vector, the scores for the artificial doublets
type	character or numeric, describes how the score threshold for calling doublets is determined. Either "balanced" or a number between zero and one that indicates the fraction of artificial doublets missed when making calls. Default: "balanced".

Value

numeric, vector containing the (estimated) number of doublets, the score threshold and the fraction of artificial doublets missed (false negative rate, of sorts)

get_dblCalls_ROC *Derive doublet calls from classification probabilities*

Description

Given class probabilities (or scores) discriminating real data from artificial doublets, derive doublet calls. Based on selecting a ROC cutoff, see *The Inconsistency of "Optimal" Cutpoints Obtained using Two Criteria based on the Receiver Operating Characteristic Curve*, (doi).

Usage

```
get_dblCalls_ROC(scrs_real, scrs_sim, rel_loss = 1)
```

Arguments

scrs_real	numeric vector, the scores for the real/original data
scrs_sim	numeric vector, the scores for the artificial doublets
rel_loss	numeric scalar, relative weight of a false positive classification compared with a false negative. Default:1 (same loss for fp and fn).

Value

numeric, vector containing the (estimated) number of doublets, the score threshold and the fraction of artificial doublets missed (false negative rate, of sorts)

`sce_chcl`*Example single cell experiment (SingleCellExperiment) object*

Description

Example data set, created by randomly sampling genes and cells from a real data set (`ch_cl`, i.e., the cell lines data from https://satijalab.org/seurat/hashing_vignette.html). Contains raw counts in the `counts` assay slot.

Usage

```
sce_chcl
```

Format

a single cell experiment object (`SingleCellExperiment`) with raw counts in the `counts` in assays, and `colData` with experimental annotations.

Index

[bcds](#), [2](#)

[cxds](#), [3](#)

[cxds_bcds_hybrid](#), [4](#)

[cxds_getTopPairs](#), [4](#)

[get_dblCalls_ALL](#), [5](#)

[get_dblCalls_dist](#), [6](#)

[get_dblCalls_ROC](#), [6](#)

[sce_chcl](#), [7](#)