Package 'scds'

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Type Package

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

Version 2.0.0

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.

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Encoding UTF-8

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

RoxygenNote 7.3.3

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

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Contents

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

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 orginal 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 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 "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 = bcds(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 numer 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 colulmns, 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, respecitvely.

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 basedon 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.

Format

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

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