Package ‘scds’

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Type Package

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

Version 1.18.0

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

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Description
Annotates doublets/multiplets using a binary classification approach to discriminate artificial doubles 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 doubles; 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

```r
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

Find doublets/multiplets in UMI scRNA-seq data;

#### Description

Annotates doublets/multiplets using co-expression based approach

#### Usage

```r
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, indi messaging 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 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 "cxds_score" column.

#### Examples

```r
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**

```r
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**

```r
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 doublet 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)

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**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.
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