

# Package ‘scds’

November 4, 2024

**Type** Package

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

**Version** 1.22.0

**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

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

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### 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)
```

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

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**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.

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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)

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get_dblCalls_ROC	<i>Derive doublet calls from classification probabilities</i>
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### 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)

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sce_chcl	<i>Example single cell experiment (SingleCellExperiment) object</i>
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### 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](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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