

# Package ‘scds’

October 16, 2025

**Type** Package

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

**Version** 1.24.0

**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** RELEASE\_3\_21

**git\_last\_commit** 41355d9

**git\_last\_commit\_date** 2025-04-15

**Repository** Bioconductor 3.21

**Date/Publication** 2025-10-15

**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 |

|              |          |
|--------------|----------|
| <b>Index</b> | <b>8</b> |
|--------------|----------|

---

|      |                                                        |
|------|--------------------------------------------------------|
| 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 | <i>Find doublets/multiples in UMI scRNA-seq data;</i> |
|------------------|-------------------------------------------------------|

---

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

---

### 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 | <i>Wrapper for getting doublet calls</i> |
|------------------|------------------------------------------|

---

**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 | <i>Derive doublet calls from doublset scores</i> |
|-------------------|--------------------------------------------------|

---

### 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 | <i>Derive doublet calls from classification probabilities</i> |
|------------------|---------------------------------------------------------------|

---

### 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](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](#)