

Package ‘spillR’

December 11, 2024

Type Package

Title Spillover Compensation in Mass Cytometry Data

Version 1.3.0

Description Channel interference in mass cytometry can cause spillover and may result in miscounting of protein markers. We develop a nonparametric finite mixture model and use the mixture components to estimate the probability of spillover. We implement our method using expectation-maximization to fit the mixture model.

biocViews FlowCytometry, ImmunoOncology, MassSpectrometry, Preprocessing, SingleCell, Software, StatisticalMethod, Visualization, Regression

License LGPL-3

Encoding UTF-8

LazyData false

Config/testthat/edition 3

RoxygenNote 7.3.1

Imports dplyr, tibble, tidyselect, stats, ggplot2, tidyr, spatstat.univar, S4Vectors, parallel

Depends R (>= 4.3.0), SummarizedExperiment, CATALYST

Suggests knitr, rmarkdown, cowplot, testthat (>= 3.0.0), BiocStyle, hexbin

VignetteBuilder knitr

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

git_branch devel

git_last_commit 7a34e97

git_last_commit_date 2024-10-29

Repository Bioconductor 3.21

Date/Publication 2024-12-10

Author Marco Guazzini [aut, cre] (ORCID: <https://orcid.org/0009-0007-8111-5772>),
 Alexander G. Reisach [aut] (ORCID: <https://orcid.org/0009-0003-5057-6278>),
 Sebastian Weichwald [aut] (ORCID: <https://orcid.org/0000-0003-0169-7244>),
 Christof Seiler [aut] (ORCID: <https://orcid.org/0000-0001-8802-3642>)

Maintainer Marco Guazzini <m.guazzini@student.maastrichtuniversity.nl>

Contents

compCytof	2
compensate	3
compensate_naive	4
generate_bead	5
generate_real	6
plotDiagnostics	6
tfm	7

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

compCytof	<i>Compute spillover probability and correct for spillover</i>
-----------	--

Description

Compute spillover probability and correct for spillover

Usage

```
compCytof(
  sce,
  sce_bead,
  marker_to_barcode,
  impute_value,
  overwrite = FALSE,
  n_cores = 1,
  naive = FALSE
)
```

Arguments

sce	SingleCellExperiment for the real cells
sce_bead	SingleCellExperiment for the bead experiment
marker_to_barcode	Table that maps the marker to the barcode in the beads experiment
impute_value	Imputed value for counts that are declared as spillover

overwrite	logical; if TRUE data are overwritten if FALSE data are saved in new columns
n_cores	Number of computing cores
naive	logical; if TRUE use the naive version

Value

A `SingleCellExperiment` object

Examples

```
library(CATALYST)
library(dplyr)
bc_key <- c(139, 141:156, 158:176)
sce_bead <- prepData(ss_exp)
sce_bead <- assignPrelim(sce_bead, bc_key, verbose = FALSE)
sce_bead <- applyCutoffs(estCutoffs(sce_bead))
sce_bead <- computeSpillmat(sce_bead)
data(mp_cells, package = "CATALYST")
sce <- prepData(mp_cells)
marker_to_barcode <- rowData(sce_bead)[, c("channel_name", "is_bc")] |>
  as_tibble() |>
  filter(is_bc == TRUE) |>
  mutate(barcode = bc_key) |>
  select(marker = channel_name, barcode)
spillR::compCytobf(sce, sce_bead, marker_to_barcode, impute_value = NA)
```

 compensate

Compute spillover probability and correct for spillover

Description

Compute spillover probability and correct for spillover

Usage

```
compensate(
  tb_real,
  tb_bead,
  target_marker,
  spillover_markers,
  impute_value = NA,
  n_iter = 1000
)
```

Arguments

tb_real	Data frame or tibble with proteins counts of real experiment
tb_bead	Data frame or tibble with proteins counts of bead experiment
target_marker	Marker name in real experiment
spillover_markers	Marker names in bead experiment
impute_value	Value for counts that are declared as spillover
n_iter	Maximum number of EM steps

Value

A list of class `spillr` containing

tb_compensate	corrected real cells
tb_spill_prob	probability curve
convergence	covergence table of EM algorithm
tb_real	input real cells
tb_bead	input bead cells
target_marker	input marker in real experiment
spillover_markers	input markers in bead experiment

compensate_naive	<i>Compute spillover probability and correct for spillover from beads only</i>
------------------	--

Description

Compute spillover probability and correct for spillover from beads only

Usage

```
compensate_naive(
  tb_real,
  tb_bead,
  target_marker,
  spillover_markers,
  impute_value = NA
)
```

Arguments

tb_real	Data frame or tibble with proteins counts of real experiment
tb_bead	Data frame or tibble with proteins counts of bead experiment
target_marker	Marker name in real experiment
spillover_markers	Marker names in bead experiment
impute_value	Value for counts that are declared as spillover

Value

A list of class `spillr` containing

tb_compensate	corrected real cells
tb_spill_prob	probability curve
convergence	covergence table of EM algorithm
tb_real	input real cells
tb_bead	input bead cells
target_marker	input marker in real experiment
spillover_markers	input markers in bead experiment

generate_bead	<i>Generate dataset for vignettes and simulation studies</i>
---------------	--

Description

Generate dataset for vignettes and simulation studies

Usage

```
generate_bead()
```

Value

`tibble` data frame

Examples

```
set.seed(23)
generate_bead()
```

generate_real *Generate dataset for vignettes and simulation studies*

Description

Generate dataset for vignettes and simulation studies

Usage

```
generate_real()
```

Value

[tibble](#) data frame

Examples

```
set.seed(23)
generate_real()
```

plotDiagnostics *Compute spillover probability and correct for spillover*

Description

Compute spillover probability and correct for spillover

Usage

```
plotDiagnostics(sce, ch)
```

Arguments

sce A [SingleCellExperiment](#) object
ch Character string specifying the channel to plot

Value

A list of [ggplot2](#) plots

Examples

```
library(CATALYST)
library(dplyr)
bc_key <- c(139, 141:156, 158:176)
sce_bead <- prepData(ss_exp)
sce_bead <- assignPrelim(sce_bead, bc_key, verbose = FALSE)
sce_bead <- applyCutoffs(estCutoffs(sce_bead))
sce_bead <- computeSpillmat(sce_bead)
data(mp_cells, package = "CATALYST")
sce <- prepData(mp_cells)
marker_to_barcode <- rowData(sce_bead)[, c("channel_name", "is_bc")] |>
  as_tibble() |>
  filter(is_bc == TRUE) |>
  mutate(barcode = bc_key) |>
  select(marker = channel_name, barcode)
sce <- spillR::compCytotof(sce, sce_bead, marker_to_barcode, impute_value = NA)
plotDiagnostics(sce, "Yb173Di")
```

tfm

Variance stabilizing transform of counts

Description

Variance stabilizing transform of counts

Usage

```
tfm(x)
```

Arguments

x Raw count

Value

A transformed count

Index

compCytof, [2](#)
compensate, [3](#)
compensate_naive, [4](#)

generate_bead, [5](#)
generate_real, [6](#)
ggplot2, [6](#)

plotDiagnostics, [6](#)

SingleCellExperiment, [2](#), [3](#), [6](#)

tfm, [7](#)
tibble, [5](#), [6](#)