

Package ‘spillR’

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Type Package

Title Spillover Compensation in Mass Cytometry Data

Version 1.4.0

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

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compCytot	<i>Compute spillover probability and correct for spillover</i>
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Description

Compute spillover probability and correct for spillover

Usage

```
compCytot(  
  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::compCytof(sce, sce_bead, marker_to_barcode, impute_value = NA)
```

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

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 <code>spillr</code> 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>
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Description

Generate dataset for vignettes and simulation studies

Usage

```
generate_bead()
```

Value

tibble data frame

Examples

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

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

Description

Generate dataset for vignettes and simulation studies

Usage

```
generate_real()
```

Value

[tibble](#) data frame

Examples

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

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

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::compCytob(sce, sce_bead, marker_to_barcode, impute_value = NA)
plotDiagnostics(sce, "Yb173Di")
```

tfm	<i>Variance stabilizing transform of counts</i>
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Description

Variance stabilizing transform of counts

Usage

```
tfm(x)
```

Arguments

x	Raw count
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Value

A transformed count

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