

Package ‘spillR’

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Type Package

Title Spillover Compensation in Mass Cytometry Data

Version 1.1.0

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

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LazyData false

Config/testthat/edition 3

RoxygenNote 7.2.3

Imports dplyr, tibble, tidyselect, stats, ggplot2, tidyr, spatstat.geom, 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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compCytof	<i>Compute spillover probability and correct for spillover</i>
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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::compCytotf(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

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

Value

A list of class `spillr` containing

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

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

<code>tb_real</code>	Data frame or tibble with proteins counts of real experiment
<code>tb_bead</code>	Data frame or tibble with proteins counts of bead experiment
<code>target_marker</code>	Marker name in real experiment
<code>spillover_markers</code>	Marker names in bead experiment
<code>impute_value</code>	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 coverage 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>
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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>
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Description

Compute spillover probability and correct for spillover

Usage

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

Arguments

sce	A <code>SingleCellExperiment</code> 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::compCytOf(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

Value

A transformed count

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