Package ‘spillR’

May 30, 2024

Type Package
Title Spillover Compensation in Mass Cytometry Data
Version 1.0.0
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
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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

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**compCytof**

*Compute spillover probability and correct for spillover*

**Description**

Compute spillover probability and correct for spillover

**Usage**

```r
compCytof(
  sce, 
  sce_bead, 
  marker_to_barc, 
  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_barc**: 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

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

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

Value

A `SingleCellExperiment` object

Examples

```r
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_barc <- 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_barc, impute_value = NA)
```

compensate  
`Compute spillover probability and correct for spillover`

Description

Compute spillover probability and correct for spillover

Usage

```r
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
compensate_naive

Value

A list of class spillr containing

- `tb_compensate` corrected real cells
- `tb_spill_prob` probability curve
- `convergence` convergence 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

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compensate_naive  Compute spillover probability and correct for spillover from beads only

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Description

Compute spillover probability and correct for spillover from beads only

Usage

```r
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
**generate_bead**

Value

A list of class **spillr** containing

- `tb_compensate` corrected real cells
- `tb_spill_prob` probability curve
- `convergence` convergence 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

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**generate_bead**

*Generate dataset for vignettes and simulation studies*

**Description**

Generate dataset for vignettes and simulation studies

**Usage**

```r
generate_bead()
```

**Value**

**tibble** data frame

**Examples**

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

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**generate_real**

*Generate dataset for vignettes and simulation studies*

**Description**

Generate dataset for vignettes and simulation studies

**Usage**

```r
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_barc <- 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_barc, impute_value = NA)
plotDiagnostics(sce, "Yb173Di")
tfm

Description
Variance stabilizing transform of counts

Usage
tfm(x)

Arguments
x Raw count

Value
A transformed count
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