Package ‘CyTOFpower’

Type Package
Title Power analysis for CyTOF experiments
Version 1.8.0
Description This package is a tool to predict the power of CyTOF experiments in the context of differential state analyses. The package provides a shiny app with two options to predict the power of an experiment: i. generation of in-silico CyTOF data, using users input ii. browsing in a grid of parameters for which the power was already precomputed.

biocViews FlowCytometry, SingleCell, CellBiology, StatisticalMethod, Software
License LGPL-3
Encoding UTF-8
Depends R (>= 4.1)
Imports CytoGLMM, diffcyt, DT, dplyr, ggplot2, magrittr, methods, rlang, stats, shiny, shinyFeedback, shinyjs, shinyMatrix, SummarizedExperiment, tibble, tidyr

RoxygenNote 7.1.2
VignetteBuilder knitr
Suggests testthat (>= 3.0.0), BiocStyle, knitr
Config/testthat/edition 3
git_url https://git.bioconductor.org/packages/CyTOFpower
git_branch RELEASE_3_18
git_last_commit d62a254
git_last_commit_date 2023-10-24
Repository Bioconductor 3.18
Date/Publication 2024-01-12

Author Anne-Maud Ferreira [cre, aut] (<https://orcid.org/0000-0002-4749-746X>), Catherine Blish [aut], Susan Holmes [aut]
Maintainer Anne-Maud Ferreira <anne-maud.ferreira@stanford.edu>
R topics documented:

compute_effectsize ......................................................... 2
compute_pwr ................................................................. 3
compute_variance ............................................................ 3
CyTOFpower ................................................................. 4
function_apply_modelcomputations_modelchoice ...................... 4
function_apply_one_simulation_withmarkerinfo ...................... 5
function_check_nbDEmarkers ............................................ 6
function_check_nbmarkers ................................................ 6
function_compute_diffcyt_features ..................................... 7
function_create_mock_dataset_withmarkerinfo ....................... 7
function_DEmarkers_sup_nbmarkers .................................... 8
function_desigmat_contrast_diffcytDSLIMMA_fixedeffect .......... 9
function_desigmat_contrast_diffcytDSLIMMA_randomeffect ........ 9
function_extract_marker_names ........................................ 10
function_formula_contrast_diffcytDSLIMMA_randomeffect ........ 10
function_is_data_paired .................................................. 11
function_names_DE_markers .............................................. 12
function_run_bootstrapcytoGLMM ...................................... 12
function_run_cytoGLMM .................................................. 13
function_run_diffcytDSLIMMA ......................................... 13
function_run_diffcytDSLIMM ............................................ 14
function_run_diffcyt_full_pipeline .................................. 15
function_summary_results_models ..................................... 15
function_to_compute_model_computation_one_simulation_modelchoice ......................................................... 16
function_to_transform_data .............................................. 17
function_value_onemarker ............................................... 17

Index 19

compute_effectsize  Compute effect size

Description

Compute effect size

Usage

compute_effectsize(raw_data_lg)

Arguments

raw_data_lg  data.frame, cells values in long format.

Details

Compute observed Cohen’s effect size and observed fold change.
compute_pwr

Value
data.frame, Cohen’s effect size and fold change that were observed in the data for each marker.

---

compute_pwr  Compute power

Description
Compute power

Usage
compute_pwr(model_values, alpha = 0.05)

Arguments
- model_values: data.frame, output of run_models().
- alpha: numeric, significance level.

Details
Compute the power based on the model values.

Value
numeric, power.

---

compute_variance  Compute variance

Description
Compute variance

Usage
compute_variance(raw_data_lg)

Arguments
- raw_data_lg: data.frame, cells values in long format.

Details
Compute the observed variance in the data.

Value
numeric, observed variance mean.
CyTOFpower

CyTOFpower: R-package to predict the power of a CyTOF experiment

Description
This package provides functions and a shiny app to predict the power of a CyTOF experiment. Interactive shiny app to predict the power of a CyTOF experiment.

Usage
CyTOFpower()

Value
Interactive shiny app.

Examples
# Launch the shiny app
if (interactive()) {
  CyTOFpower()
}

function_apply_modelcomputations_modelchoice

Run DS tests for one simulation.

Description
Run DS tests for one simulation.

Usage
function_apply_modelcomputations_modelchoice(
  list_combined_output,
  model = c("cytoglmm", "cytoglm", "testDS_limma_random", "testDS_limma_fixed", "testDS_lmm")
)

Arguments
  list_combined_output
    list, of simulated data (output of the function_apply_onesimulation_withmarkerinfo function).
  model
    vector, name(s) of models to test.
Details

Wrapper to run the models through the different simulations.

Value

data.frame of results for each simulation.

Usage

function_apply_onesimulation_withmarkerinfo(variation)

Arguments

variation list, list of list containing the different input parameter variations @describeIn function_create_mock_dataset_withmarkerinfo.

Details

Apply one simulation for a given parameter combination number times (iterations), when we have prior information about the markers distribution parameters (mean and dispersion of the negative binomial).

Value

list of simulated data. Each list member contains 5 slots: - variation: the variation of input parameters which has been used in input; - df_info: experimental information (donor IDs, group IDs, samples IDs); - DE_markers_names: name of the differentially expressed markers; - ls_mock_data: list of data.frames, each data.frame being one simulation of the cell values using the input parameters provided (list is length nb_sim).
function_check_nbDEmarkers

Number of DE markers greater than 1.

Description
Number of DE markers greater than 1.

Usage
function_check_nbDEmarkers(nb_DEmarker)

Arguments
nb_DEmarker numeric, number of differentially expressed markers.

Details
Function to check that the number of DE markers is greater than 1.

Value
error message

function_check_nbmarkers

Number of markers greater than 2.

Description
Number of markers greater than 2.

Usage
function_check_nbmarkers(nb_marker)

Arguments
nb_marker numeric, total number of markers.

Details
Function to check that the number of markers is greater than 2.

Value
error message if the total number of markers is lower than 3.
**function_compute_diffcyt_features**

*Compute cells counts and medians.*

**Description**

Compute cells counts and medians.

**Usage**

```r
function_compute_diffcyt_features(mock_flowset)
```

**Arguments**

- `mock_flowset`: data.frame, cell values for each marker.

**Details**

Function to calculate features for diffcyt package models.

**Value**

list with cell counts and medians for each markers.

---

**function_create_mock_dataset_withmarkerinfo**

*Compute simulated cell values for one simulation with markers NB information.*

**Description**

Compute simulated cell values for one simulation with markers NB information.

**Usage**

```r
function_create_mock_dataset_withmarkerinfo(variation)
```

**Arguments**

- `variation`: list, list of data.frames containing the different variable input parameters to generate the data: - `marker_name`: name of the marker (character); - `nb_donor`: number of donors; - `rho`: fold change; - `subject_effect`: standard deviation for the normal distribution from which the donor’s means will be drawn; - `mu0`: mean of the negative binomial for the gamma distribution from which the means of the different donor will be drawn; - `dispersion`: dispersion of the negative binomial from which the DE marker’s cell values will be drawn; - `nb_cell_per_sample`: number of cells per sample.
Details

Function to compute the simulated cell values using a combination of variable parameters, when we have prior information about the markers distribution parameters (mean and dispersion of the negative binomial).

Value

list with 4 slots: - df_info: data.frame of experimental information; - DEmarkers_names: vector of DE marker names; - raw_data: data.frame of raw cell values; - data: data.frame of transformed cell values.

function_DEmarkers_sup_nbmarkers

Check on the number of DE markers.

Description

Check on the number of DE markers.

Usage

function_DEmarkers_sup_nbmarkers(nb_markers, nb_DEmarker)

Arguments

- nb_markers numeric, total number of markers.
- nb_DEmarker numeric, number of differentially expressed markers.

Details

Function to check that number of DE markers greater than number of markers.

Value

error message if the number of DE markers is greater than the total number of markers.
function_desigmat_contrast_diffcytDSlimma_fixedeffect

Design and contrast matrices for diffcyt-DS-limma with fixed effect.

Description

Design and contrast matrices for diffcyt-DS-limma with fixed effect.

Usage

function_desigmat_contrast_diffcytDSlimma_fixedeffect(df_experiment_info)

Arguments

df_experiment_info
data.frame, information about the experiment (donor IDs, group IDs and sample IDs).

Details

Function to create the design matrix and contrast for the diffcyt-DS-limma model with fixed effect.

Value

list with 3 slots: - design_matrix: the design matrix; - contrast: the contrast matrix; - effect: the specification of the "fixed" effect.

function_desigmat_contrast_diffcytDSlimma_randomeffect

Design and contrast matrices for diffcyt-DS-limma with random effect.

Description

Design and contrast matrices for diffcyt-DS-limma with random effect.

Usage

function_desigmat_contrast_diffcytDSlimma_randomeffect(df_experiment_info)

Arguments

df_experiment_info
data.frame, information about the experiment (donor IDs, group IDs and sample IDs).
**Details**

Function to create the design matrix and contrast for the diffcyt-DS-limma model with random effect from the diffcyt package.

**Value**

list with 3 slots: - design_matrix: the design matrix; - contrast: the contrast matrix; - effect: the specification of the "random" effect.

---

**function_extract_marker_names**

*Extract marker names.*

---

**Description**

Extract marker names.

**Usage**

```r
function_extract_marker_names(mock_dataset)
```

**Arguments**

- `mock_dataset` data.frame, containing the cell values for each marker.

**Details**

Function to extract the marker names.

**Value**

vector of marker names.

---

**function_formula_contrast_diffcytDSLMM_randomeffect**

*Formula and contrast matrix for diffcyt-DS-LMM with random effect.*

---

**Description**

Formula and contrast matrix for diffcyt-DS-LMM with random effect.

**Usage**

```r
function_formula_contrast_diffcytDSLMM_randomeffect(df_experiment_info)
```
function_is_data_paired

**Arguments**

- **df_experiment_info**
  - data.frame, information about the experiment (donor IDs, group IDs and sample IDs).

**Details**

Function to create formula and contrast for diffcyt-DS-LMM with random effect.

**Value**

- list with 3 slots: - formula: the formula for the model; - contrast: the contrast matrix.

---

function_is_data_paired

Data paired.

---

**Description**

Data paired.

**Usage**

function_is_data_paired(data)

**Arguments**

- **data**
  - data.frame, experimental information containing (sample IDs, donor IDs).

**Details**

Function to check if the data is paired.

**Value**

- logical, TRUE is the data are paired - FALSE if the data are not paired
function_names_DE_markers

Generate name of the DE markers.

Description
Generate name of the DE markers.

Usage
function_names_DE_markers(total_nb_marker, nb_DE_marker)

Arguments
- total_nb_marker: numeric, total number of markers.
- nb_DE_marker: numeric, number of DE markers.

Details
Function to generate the name of the DE markers.

Value
vector of marker names.

function_run_bootstrapcytoGLMM

Run cytoglm.

Description
Run cytoglm.

Usage
function_run_bootstrapcytoGLMM(mock_dataset, nb_bootstrap = 500)

Arguments
- mock_dataset: data.frame, cell values for each marker.
- nb_bootstrap: numeric, number of bootstrap (by defaults nb_bootstrap = 1000).

Details
Function to run the Generalized Linear Model with Bootstrap, from the CytoGLMM package.
**function_run_cytoGLMM**

**Value**

- model_fit: fit of the model;
- plot: plot of the effects;
- results_summary: data.frame containing the results of the models for each marker.

**Description**

Run cytoGLMM

**Usage**

function_run_cytoGLMM(mock_dataset)

**Arguments**

- mock_dataset: data.frame, cell values for each marker.

**Details**

Function to run GLMM model from CytoGLMM package.

**Value**

- model_fit: fit of the model;
- plot: plot of the effects;
- results_summary: data.frame containing the results of the models for each marker.

**function_run_diffcytDSlimma**

Run diffcyt-DS-limma model.

**Description**

Run diffcyt-DS-limma model.

**Usage**

function_run_diffcytDSlimma(
    ls_desigmat_contrast,
    df_experiment_info,
    ls_features
)
function_run_diffcytDSLMM

**Arguments**

- `ls_desigmat_contrast`  
  list, with design and contrast matrices.

- `df_experiment_info`  
  data.frame, information about the experiment (donor IDs, group IDs and sample IDs).

- `ls_features`  
  list, with cell counts and medians for each markers.

**Details**

Function to run diffcyt-DS-limma model from the diffcyt package.

**Value**

list with 2 slots: - `model_fit`: the model fit; - `result_summary`: results of the model for each marker.

---

**Description**

Run diffcyt-DS-LMM model.

**Usage**

`function_run_diffcytDSLMM(ls_form_contrast, df_experiment_info, ls_features)`

**Arguments**

- `ls_form_contrast`  
  list, with formula and constraint matrix.

- `df_experiment_info`  
  data.frame, information about the experiment (donor IDs, group IDs and sample IDs).

- `ls_features`  
  list, with cell counts and medians for each markers.

**Details**

Function to run diffcyt-DS-LMM model from the diffcyt package.

**Value**

list with 2 slots: - `model_fit`: the model fit; - `result_summary`: results of the model for each marker.
function_run_diffcyt_full_pipeline

Run diffcyt pipeline

Description
Run diffcyt pipeline

Usage
function_run_diffcyt_full_pipeline(
  onevariation,
  model = c("limma", "LMM"),
  effect = c("random", "fixed")
)

Arguments
- onevariation: list, of simulated data (output of the function_wrapper_apply_simulation_nbtimes function).
- model: character, model to run: "limma" or "LMM".
- effect: character, effect: "random" or "fixed".

Details
Function to run diffcyt pipeline. We do not used the diffcyt function directly because of the limma model run differently with the effects.

Value
list with 2 slots: - model_fit: the model fit; - result_summary: results of the model for each marker.

function_summary_results_models

Summarize data and results.

Description
Summarize data and results.

Usage
function_summary_results_models(summary_from_model, package)
function_to_compute_model_computation_onesimulation_modelchoice

Arguments

  summary_from_model  list, output from the functions running the models.
  package            character, package used to run the test: "CytoGLMM" or "diffcyt".

Details

  Function to do a summary of the tested data and model's results for the CytoGLMM and diffcyt packages.

Value

  data.frame of results for each simulation.

function_to_compute_model_computation_onesimulation_modelchoice

Run DS tests for one simulation.

Description

  Run DS tests for one simulation.

Usage

  function_to_compute_model_computation_onesimulation_modelchoice(
    onevariation,
    model
  )

Arguments

  onevariation  list, of simulated data (output of the function_wrapper_apply_simulation_nbtimes function).
  model         vector, name(s) of models to test.

Details

  Function to run the DS tests through the different models.

Value

  data.frame of results for each simulation all models combined.
**function_to_transform_data**

arcsinh transformation.

**Description**

arcsinh transformation.

**Usage**

function_to_transform_data(data, cofactor = 5)

**Arguments**

data    data.frame, cell values to transform.
cofactor numeric, co-factor used in the arcsinh (by default cofactor = 5).

**Details**

Function to transform the data with the recommended transformation for cyTOF data: arcsinh with cofactor equals to 5.

**Value**

data.frame of transformed data.

**function_value_onemarker**

Compute simulated cell values for one marker with markers NB informations

**Description**

Compute simulated cell values for one marker with markers NB informations

**Usage**

function_value_onemarker(
    marker_name,
    mu0,
    dispersion,
    subject_effect,
    nb_donor,
    nb_cell_per_sample,
    rho = 1
)
Arguments

- `marker_name` character, name of the marker.
- `mu0` numeric, general donor mean from which the individual mu0i will be drawn.
- `dispersion` numeric, dispersion of the markers.
- `subject_effect` numeric, standard deviation for the normal distribution from which the donor’s means will be drawn (by default `subject_effect = 0.01`).
- `nb_donor` numeric, number of donors.
- `nb_cell_per_sample` numeric, number of cells per sample (by default `nb_cell_per_sample = 500`).
- `rho` numeric, fold change.

Details

Function to generate value for one marker with a mean and dispersion specified for the negative binomial.

Value

data.frame of cell values.
Index

* internal
  compute_effectsize, 2
  compute_pwr, 3
  compute_variance, 3
  function_apply_modelcomputations_modelchoice, 4
  function_apply_onesimulation_withmarkerinfo, 5
  function_check_nbDEmarkers, 6
  function_check_nbmarkers, 6
  function_compute_diffcyt_features, 7
  function_create_mock_dataset_withmarkerinfo, 7
  function_DEmarkers_sup_nbmarkers, 8
  function_desigmat_contrast_diffcytDSlimma_fixedeffect, 9
  function_desigmat_contrast_diffcytDSlimma_randomeffect, 9
  function_extract_marker_names, 10
  function_formula_contrast_diffcytDSLMM_randomeffect, 10
  function_is_data_paired, 11
  function_names_DE_markers, 12
  function_run_bootstrapcytoGLMM, 12
  function_run_cytoGLMM, 13
  function_run_diffcyt_full_pipeline, 15
  function_run_diffcytDSlimma, 13
  function_run_diffcytDSLMM, 14
  function_summary_results_models, 15
  function_to_compute_model_computation_onesimulation_modelchoice, 16
  function_to_transform_data, 17
  function_value_onemarker, 17

compute_effectsize, 2
compute_pwr, 3
CyTOFpower, 4
function_apply_modelcomputations_modelchoice, 4
function_apply_onesimulation_withmarkerinfo, 5
function_check_nbDEmarkers, 6
function_check_nbmarkers, 6
function_compute_diffcyt_features, 7
function_create_mock_dataset_withmarkerinfo, 7
function_DEmarkers_sup_nbmarkers, 8
function_desigmat_contrast_diffcytDSlimma_fixedeffect, 9
function_desigmat_contrast_diffcytDSlimma_randomeffect, 9
function_extract_marker_names, 10
function_formula_contrast_diffcytDSLMM_randomeffect, 10
function_is_data_paired, 11
function_names_DE_markers, 12
function_run_bootstrapcytoGLMM, 12
function_run_cytoGLMM, 13
function_run_diffcyt_full_pipeline, 15
function_run_diffcytDSlimma, 13
function_run_diffcytDSLMM, 14
function_summary_results_models, 15
function_to_compute_model_computation_onesimulation_modelchoice, 16
function_to_transform_data, 17
function_value_onemarker, 17