Package ‘wpm’

Type Package

Title Well Plate Maker

Version 1.14.0

Description The Well-Plate Maker (WPM) is a shiny application deployed as an R package. Functions for a command-line/script use are also available. The WPM allows users to generate well plate maps to carry out their experiments while improving the handling of batch effects. In particular, it helps controlling the "plate effect" thanks to its ability to randomize samples over multiple well plates. The algorithm for placing the samples is inspired by the backtracking algorithm: the samples are placed at random while respecting specific spatial constraints.

License Artistic-2.0

biocViews GUI, Proteomics, MassSpectrometry, BatchEffect, ExperimentalDesign

Depends R (>= 4.1.0)

Imports utils, methods, cli, Biobase, SummarizedExperiment, config, golem, shiny, DT, ggplot2, dplyr, rlang, stringr, shinydashboard, shinyWidgets, shinycustomloader, RColorBrewer, logging

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NeedsCompilation no

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backtracking Backtracking Function

Description

Function used to launch the backtracking algorithm on a dataframe with the corresponding plate parameters, number of iterations and special wells
Usage

backtracking(
  max_iter = 20,
  user_data,
  wells,
  rows,
  columns,
  nb_plates,
  constraint,
  prog = NULL
)

Arguments

max_iter         numeric, the maximal number of iterations to do, default value is 20
user_data       dataframe, user samples to place randomly on the plate
wells            dataframe, special wells not to be placed randomly on the plate
rows             numeric, number of lines on the plate(s)
columns         numeric, number of columns on the plate(s)
nb_plates      numeric, number of plates
constraint   character, spatial mode
prog            progress bar used for shiny app only

Value

da dataframe containing user samples and special wells with their coordinates for the corresponding plates.

balancedGrpDistrib(d, nb_p, df_max_size)

Description

This function makes it possible to distribute the samples equitably on several plates, taking into account the numbers in the groups (if there are any). This means that, for example, if 2 plates are to be filled, then 50 generally, all the plates are assigned the same number of elements. When the numbers do not allow it (in particular when the total number of elements to be allocated is not a multiple of the number of plates), there will be a slight difference in the number of samples on the plates.

Usage

balancedGrpDistrib(d, nb_p, df_max_size)
Arguments

d the user dataframe
nb_p the number of plates to fill
df_max_size the maximum number of samples that can be placed on the current plate

Value

a list of dataframes each corresponding to a plate to fill.

checkConstraints  Check for spatial constraints

Description

Finds the neighbors of the current element (row, col) in the matrix m, depending on the chosen constraint pattern. Currently, there are only 3 valid patterns (NS, WE and NEWS)

Usage

checkConstraints(m, row, col, mode)

Arguments

m matrix
row current selected row in the matrix m
col current selected column in the matrix m
mode spatial constraint

Value

A vector containing the neighbors of element (row,col) of the matrix m.
**checkWpmInputs**  \(\text{Check the inputs for the wrapper function}\)

**Description**

Checks if all the inputs given to the function WrapperWPM are correct and intercompatible.

**Usage**

```r
checkWpmInputs(
  user_df,
  plate_dims,
  nb_plates,
  spatial_constraint,
  max_iteration
)
```

**Arguments**

- `user_df`: expected dataframe, returns adapted message error
- `plate_dims`: expected list of plate dimensions (rows and columns)
- `nb_plates`: expected number of plates
- `spatial_constraint`: expected character for spatial constraint
- `max_iteration`: expected number of iterations

**Value**

returns an error message if a problem is found with some parameter.

---

**convertCSV**  \(\text{Convert a CSV File into a valid dataframe for WPM}\)

**Description**

This function converts a CSV into a dataframe to make it usable by the shiny application of wpm as well as by the wrapper function (version of wpm in command line). Be sure that the first column of the CSV file corresponds to samples names.

**Usage**

```r
convertCSV(dt_path, row_names = FALSE, gp_field = NULL, ...)
```
**Arguments**

- `dt_path`: file path.
- `row_names`: logical value, indicates if the file has rownames or not.
- `gp_field`: the column name indicating the grouping factor for the samples in the csv. If there is no grouping factor, then `gp_field` must be set to NULL or "none".
- ... parameters to give to read.csv2 function

**Value**

a list containing a dataframe containing the data of the imported CSV and a dataframe containing 3 fields (Sample, Group and ID) which will be used by WPM. Or NULL if there is an error when giving wrong parameters.

**Examples**

```r
test <- data.frame("Sample" = c("s1","s2","s3","s4"),
                       "Group" = c("A","A","B", "C"))
tf <- tempfile()
write.csv2(test, tf, row.names = FALSE)
convertCSV(tf, gp_field = "Group", header = TRUE, sep = ";")

# if there are row names in the CSV file
write.csv2(test, tf)
convertCSV(tf, row_names = TRUE, gp_field="Group", header = TRUE, sep = ";")

# if there is no grouping factor in the CSV file
convertCSV(tf, row_names = TRUE, gp_field ="none", header = TRUE, sep = ";")
# gives the same output as the previous example
convertCSV(tf, row_names = TRUE, header = TRUE, sep = ";")
```

---

**convertESet**

*Convert the phenotype data of an ExpressionSet or MsnSet into a dataframe for WPM*

**Description**

This function converts an ExpressionSet/MsnSet object into a dataframe to make it usable by the shiny application of wpm as well as by the wrapper function (version of wpm in command line).

**Usage**

`convertESet(eSet_obj, gp_field = NULL)`

**Arguments**

- `eSet_obj`: an ExpressionSet/MsnSet object containing the phenotype data
- `gp_field`: character, corresponding to the phenotype data used to categorize samples into distinct groups if any
convertSE

Convert the phenotype data of a SummarizedExperiment into a dataframe for WPM

Description
Convert the phenotype data of a SummarizedExperiment into a dataframe for WPM

Usage
convertSE(se_object, gp_field = NULL)

Arguments
se_object
a SummarizedExperiment object containing the phenotype data

gp_field
character, corresponding to the phenotype data used to categorize samples into distinct groups if any

Value
a dataframe containing 3 fields: Sample, Group and ID.

Examples
nrows <- 200
cols <- 6
counts <- matrix(runif(nrows * cols, 1, 1e4), nrows)
colData <- data.frame(Treatment=rep(c("ChIP", "Input"), 3), row.names=LETTERS[1:6])
se <- SummarizedExperiment::SummarizedExperiment(assays=list(counts=counts), colData=colData)
convertSE(se, "Treatment")
convertVector2Df  

Convert a vector of plate coordinates into a dataframe

Description

Function converting the format of "Letter-Digit" coordinates into a dataframe containing these coordinates in Row, Column.

Usage

convertVector2Df(chr_wells, max_Row, max_Col, status = NA)

Arguments

- chr_wells: character string containing the wells
- max_Row: integer, maximal number of lines in the plate
- max_Col: integer, maximal number of columns in the plate
- status: character, the status of the wells

Value

result, dataframe containing wells coordinates

Examples

# convert the vector of well coordinates into a dataframe
convertVector2Df("A1,C2,A3,B12,C42",3,42,"specify_status")

# supports uppercase / lowercase letters
convertVector2Df("a1,C2,A3,b12,C42",3,42,"specify_status")

data_test  

Fictitious clinical data for demonstration.

Description

A demo dataset containing the age and other attributes of 193 fictitious patients. It aims to help the user to test the shiny application of the wpm package.

Usage

data(data_test)
**defineBufferCoords**

**Format**

A data frame with 193 rows and 7 variables

- **samples**  the samples to be analyzed representing fictitious patients.
- **age**  age of the patients under 5 age groups, in years (20-30;30-40;40-50;50-60;60-70)
- **gender**  gender of the patients, F (for Female) and M (for Male)
- **treatment**  the treatment each patient received, Ctrl (Control), treatment A, treatment B and treatment C
- **diabetes**  presence of diabetes, 0 (no) and 1 (yes)
- **gender-treatment**  A combination between the gender and treatment fields
- **age-diabetes**  A combination between the age and the diabetes fields

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**defineBufferCoords**  Determines buffer wells coordinates on a plate

**Description**

function to place the buffer solutions on the plate according to the selected mode: it generates a dataframe containing the row and column coordinates for each buffer solution.

**Usage**

```
defineBufferCoords(p_lines, p_cols, mod = "none", start_buffer)
```

**Arguments**

- **p_lines**  number of rows on the plate
- **p_cols**  number of columns on the plate
- **mod**  character, can be "none", "by_column", "by_row" or "checkerboard"
- **start_buffer**  character, "even" means that the buffers will be positioned on the even rows of the plate. Otherwise, they will be positioned on the odd rows.

**Value**

a dataframe containing the buffer wells with their coordinates.
drawMap

Generate a ggplot object of a plate plan

drawMap(function to plot the input dataframe containing the Sample names, the Row, Column coordinates, the group and the status)

drawMap(df, sample_gps, gp_levels, plate_lines, plate_cols, project_title)

Arguments

df: dataframe containing user data and special wells if any.
sample_gps: number of distinct groups in the file before adding the special wells to df
gp_levels: is Group column levels before adding the special wells to df
plate_lines: integer, number of plate’s lines
plate_cols: integer, number of plate’s columns
project_title: character, the user’s project title

Value

g, a ggplot object corresponding to the generated plate map.

Examples

# example of data containing 5 biological samples, 2 forbidden wells,
# 2 buffers and 3 not random wells
user_data <- data.frame("Sample" = c(as.character(seq_len(5)), rep_len(NA, 7)),
  "Group" = c(c("A","B","C","A","B"),
  rep_len("forbidden", 2),
  rep_len("buffer", 2),
  rep_len("fixed", 3)),
  "ID" = c(seq_len(5),rep_len(NA,7)),
  "Well" = c("A1","B2","C3","B4","A3","A1","A4","B2","C2","B1","C1","C4"),
  "Status" = c(rep_len("toRandom", 5),
  rep_len("forbidden", 2),
  rep_len("buffer", 2),
  rep_len("fixed", 3)),
  "Row" = c(1,2,3,2,1,1,2,3,2,3,3,4),
  "Column" = c(2,3,3,4,3,1,4,2,2,1,1,4))

p <- "My Project"
gp_lvl <- levels(as.factor(c("A","B","C")))
drawMap(df = user_data, sample_gps = 3, gp_levels = gp_lvl, plate_lines = 3,
plate_cols = 4, project_title = p)
# also works when giving a plate with more wells than the number of samples to place.
drawMap(df = user_data, sample_gps = 3, gp_levels = gp_lvl, plate_lines = 8,
plate_cols = 12, project_title = p)

findNEWsneighbors  

Find the 4 cardinal neighbors of an element of a matrix

**Description**

Function for spatial constraints: the North, East, West and South neighbors of the current element (i,j) of the matrix m.

**Usage**

findNEWsneighbors(m, i, j)

**Arguments**

- m: matrix
- i: integer, line index in the matrix
- j: integer, column index in the matrix

**Value**

A vector containing the North, East, West and South neighbors of the element (i,j) of the matrix being processed.

findNSneighbors  

Find the top and bottom neighbors of an element of a matrix

**Description**

Function for spatial constraint that only looks for North (top) and South (bottom) neighbors of the current element (i,j) of the matrix m.

**Usage**

findNSneighbors(m, i, j)

**Arguments**

- m: matrix
- i: integer, line index in the matrix
- j: integer, column index in the matrix
**Value**

A vector containing the North and South neighbors of the element $(i,j)$ of the matrix being processed.

---

**findWEneighbors**  
*Find the left and right neighbors of an element of a matrix*

**Description**

Function for spatial constraint that only looks for West (left) and East (right) neighbors of the current element $(i,j)$ of the matrix $m$.

**Usage**

```r
findWEneighbors(m, i, j)
```

**Arguments**

- `m`: matrix
- `i`: integer, line index in the matrix
- `j`: integer, column index in the matrix

**Value**

A vector containing the West and East neighbors of the element $(i,j)$ of the matrix being processed.

---

**generateMap**  
*Generate a plate map according to the input parameters*

**Description**

This function generates a plate map using a backtracking algorithm and returns a dataframe if success. If it fails to find a solution, returns NULL. If there are not enough wells to place all the samples, returns 0.

**Usage**

```r
generateMap(
  user_df, nb_rows, nb_cols, df_forbidden, mod, max_it, updateProgress = NULL
)
```
joinDataframes

Arguments

- **user_df**: dataframe containing 9 features: Sample, ID, Group, Sample.name, Well, Status, Row, Column, Plate. See details.
- **nb_rows**: numeric, number of lines on the plate
- **nb_cols**: numeric, number of columns on the plate
- **df_forbidden**: dataframe with the same structure than user_df, but for the forbidden, buffer solutions and Not randomized wells.
- **mod**: character, neighborhood spatial constraint
- **max_it**: numeric, maximum number of attempts to generate a plate plan before returning a failure.
- **updateProgress**: shiny object, reports progress to the user.

Details

The dataframe is generated using dedicated functions of the wpm package: 'convertCSV()', 'convertESet()' or 'convertSE()'. But the user can also generate it by hand.

A number of attempts is allowed. Consequently, if the maximal number if attempts is reached and no solution was found with the backtracking (i.e., the randomWalk does not return a dataframe), this function prints a warning message and returns NULL. If a solution is found, then it returns the dataframe.

Value

Returns a dataframe containing all the data of the plate map(s)

joinDataframes  Binds multiple dataframes together

Description

Function that merges dataframes that contain wells of different types. To do this, it verifies that all the conditions provided are compatible with each other in order to be able to launch WPM on this data.

Usage

```r
joinDataframes(
  forbidden_w = NULL,
  buffer_w = NULL,
  fixed_w = NULL,
  nb_samples,
  totalNbWells,
  nb_p
)
```
Arguments

- forbidden_w: dataframe, the forbidden wells
- buffer_w: dataframe, the buffer wells
- fixed_w: dataframe, the quality control wells
- nb_samples: numeric, the number of samples to place using the backtracking algorithm.
- totalNbWells: numeric, the total number of wells that can be filled.
- nb_p: numeric, number of plates to fill

Value

a dataframe containing all the special wells

randomWalk

Random walk of the matrix to fill

Description

Returns the user dataframe updated after choosing randomly a well on the plate (matrix) and randomly choosing a sample ID that satisfies all the constraints.

Usage

randomWalk(m, toVisit, d, constraint)

Arguments

- m: is a matrix corresponding to the plate to be filled.
- toVisit: contains the wells in form "A1", and contains only the wells authorized to be filled in
- d: is the dataframe containing the data supplied by the user.
- constraint: character string corresponding to the spatial constraint selected by the user

Value

a dataframe corresponding to the user-supplied data. This dataframe is an updated version, where the columns ‘Row’ and ‘Column’ are filled with the coordinates of the chosen well. If no solution is found for the current selected well, then this function returns 1.
resample

Randomly take a number of elements in a vector

Description
This function allows to pick up the last element in a vector when the parameter size is equal to 1. Passes parameters to `sample.int` like size.

Usage
resample(x, ...)

Arguments
- x is a vector
- ... parameters given to the function sample.int

Value
a vector of length equal to size parameter.

solveCell
Affects a sample to the chosen cell in the plate

Description
This function chooses a sample randomly from among those who respect the neighborhood constraints and who have not yet been assigned to a well.

Usage
solveCell(m, d, i, j, already_drawn, constraint)

Arguments
- m Matrix representing the plate plan.
- d Dataframe containing the samples to place.
- i Line index of the chosen well.
- j Column index of the chosen well.
- already_drawn Vector of samples already affected to wells.
- constraint Character. Corresponds to the neighborhood constraint mode.

Value
If there is no possibility to find a valid sample, the function returns an error value (1). If a sample is chosen, then this function returns two objects: *m* The matrix updated with the new added sample. *already_drawn* The vector of already placed samples updated.
**wpm**

*Run the Shiny Application of Well Plate Maker*

**Description**

Run the Shiny Application of Well Plate Maker

**Usage**

```r
wpm(...)```

**Arguments**

... A series of options to be used inside the app.

**Value**

a shiny application object with golem options

**Examples**

```r
if(interactive()) {wpm()}
```

---

**wrapperWPM**

*Generate plate plans in a single step*

**Description**

Wrapper function that generates plate plans like the wpm shiny application. This feature allows the user to use the wpm package from the command line rather than going through a web application.

**Usage**

```r
wrapperWPM(
  user_df,
  plate_dims,
  nb_plates,
  forbidden_wells = NULL,
  buffer_wells = NULL,
  fixed_wells = NULL,
  spatial_constraint = "none",
  max_iteration = 20
)
```
**Arguments**

- **user_df**
  - dataframe containing user data obtained with the `convertCSV()` or `convertESet()` functions.

- **plate_dims**
  - list, containing 2 values: the first is the number of plate's lines and second is the number of plate's columns.

- **nb_plates**
  - numeric, corresponds to the number of plates to fill

- **forbidden_wells**
  - character, the wells that will not be used at all for the experiment. This argument needs to be a character string giving the wells coordinates of the form "Letter-Number" (e.g. "A1" for the well positionned in the first row/first column of the plate).

- **buffer_wells**
  - character, the wells that will be used during experiment but without biological sample in it. Same input structure as for forbidden_wells parameter.

- **fixed_wells**
  - character, the wells that will be used for Quality Control samples or standards during the Experiment. Same input structure as for forbidden_wells parameter.

- **spatial_constraint**
  - character, is the spatial constraint used to place the samples on the plate. It can also be called neighborhood constraint. Currently, the possible values are "none", "NS" (for North-South), "WE" (for West-East) and "NEWS" (North-South-East-West).

- **max_iteration**
  - numeric, maximal number of attempts for wpm to find a valid solution.

**Value**

- a dataframe if wpm finds a solution.

**Examples**

```r
# create a MSnSet toy example
sample_names <- c("s1","s2","s3","s4","s5")
M <- matrix(NA, nrow = 4, ncol = 5)
colnames(M) <- sample_names
rownames(M) <- paste0("id", LETTERS[1:4])
pd <- data.frame(Environment = rep_len(LETTERS[1:3], 5),
                  Category = rep_len(1:2, 5), row.names = sample_names)
rownames(pd) <- colnames(M)
x <- MSnbase::MSnSet(exprs = M, pData = pd)
# convert it to a valid dataframe for wpm
df <- convertESet(x, "Environment")
# run wpm on the toy example
wrapperWPM(user_df = df, plate_dims = list(8,12), nb_plates = 1,
            forbidden_wells = "A1,A2,A3", fixed_wells = "B1,B2",
            spatial_constraint = "NS")
```
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