Package 'wpm'

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Type Package

Version 1.21.0

Title Well Plate Maker

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 **Encoding** UTF-8 LazyData false RoxygenNote 7.1.1 Suggests MSnbase, testthat, BiocStyle, knitr, rmarkdown VignetteBuilder knitr NeedsCompilation no URL https://github.com/HelBor/wpm, https://bioconductor.org/packages/release/bioc/html/wpm.html BugReports https://github.com/HelBor/wpm/issues git_url https://git.bioconductor.org/packages/wpm git_branch devel

Description The Well-Plate Maker (WPM) is a shiny application deployed as an R

2 backtracking

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Contents

backtracking	2
balancedGrpDistrib	3
checkConstraints	4
checkWpmInputs	5
convertCSV	5
convertESet	6
convertSE	7
convertVector2Df	8
data_test	8
defineBufferCoords	
drawMap	10
findNEWSneighbors	11
findNSneighbors	11
findWEneighbors	12
generateMap	12
joinDataframes	13
randomWalk	14
resample	15
solveCell	15
wpm	16
wrapperWPM	16
	18
	10

backtracking Backtracking Function

Description

Index

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

balancedGrpDistrib 3

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) numeric, number of columns on the plate(s) numeric, number of plates

constraint character, spatial mode

prog progress bar used for shiny app only

Value

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

balancedGrpDistrib

Makes a balanced distribution of the elements between several plates.

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.

```
balancedGrpDistrib(d, nb_p, df_max_size)
```

4 checkConstraints

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.

 ${\sf checkConstraints}$

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 5

checkWpmInputs

Check the inputs for the wrapper function

Description

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

Usage

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

Arguments

Value

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

convertCSV

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.

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

6 convertESet

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

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 7

Value

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

Examples

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

8 data_test

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.

```
data(data_test)
```

defineBufferCoords 9

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.

10 drawMap

drawMap

Generate a ggplot object of a plate plan

Description

Function to plot the input dataframe containing the Sample names, the Row, Column coordinates, the group and the status

Usage

```
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)),</pre>
                         "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("A2", "B3", "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(1,2,3,2,1,1,1,2,3,2,3,3),
                         "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")))</pre>
drawMap(df = user_data, sample_gps = 3, gp_levels = gp_lvl, plate_lines = 3,
        plate_cols = 4, project_title = p)
```

findNEWSneighbors 11

findNEWSneighbors

Find the 4 cardinal neighbors of an element of a matrix

Description

Function for spatial contraints: 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

12 generateMap

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

```
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.

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

joinDataframes 13

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 reeched 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.

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

14 randomWalk

Arguments

forbidden_w dataframe, the forbidden wells buffer_w datarame, 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 15

resam	pΙα	е

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

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.

16 wrapperWPM

wpm

Run the Shiny Application of Well Plate Maker

Description

Run the Shiny Application of Well Plate Maker

Usage

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

Arguments

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

Value

a shiny application object with golem options

Examples

```
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.

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

wrapperWPM 17

Arguments

user_df dataframe containing user data obtained with the 'convertCSV()' or 'convertE-

Set()' 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" (eg. "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 attemps for wpm to find a valid solution.

Value

a dataframe if wpm finds a solution.

Examples

Index

```
\ast datasets
     data_test, 8
{\tt backtracking, 2}
{\tt balancedGrpDistrib}, {\tt 3}
{\it checkConstraints}, 4
checkWpmInputs, 5
convertCSV, 5
convertESet, 6
convertSE, 7
convertVector2Df, 8
{\tt data\_test}, {\color{red} 8}
{\tt defineBufferCoords}, 9
drawMap, 10
{\it findNEWSneighbors}, {\it 11}
findNSneighbors, 11
findWEneighbors, 12
generateMap, 12
joinDataframes, 13
randomWalk, 14
resample, 15
solveCell, 15
wpm, 16
wrapperWPM, 16
```