Package 'TTMap'

October 16, 2025

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Type	Package
	Two-Tier Mapper: a clustering tool based on topological data analysis
Versio	n 1.30.0
Date 2	2017-07-12
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	ption ITMap is a clustering method that groups together samples with the same deviation in comparison to a control group. It is specially useful when the data is small. It is parameter free.
Licens	se GPL-2
Sugge	sts BiocStyle, airway
Depen	ds rgl, colorRamps
	ts grDevices, graphics, stats, utils, methods, Summarized Experiment, Biobase
	iews Software, Microarray, DifferentialExpression, MultipleComparison, Clustering, Classification
git_ur	https://git.bioconductor.org/packages/TTMap
git_br	anch RELEASE_3_21
git_las	st_commit 2d14c49
git_las	st_commit_date 2025-04-15
Repos	itory Bioconductor 3.21
Date/F	Publication 2025-10-15
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TTMap-package

Two-Tier Mapper: a clustering tool based on topological data analysis

Description

TTMap is a clustering method that groups together samples with the same deviation in comparison to a control group. It is specially useful when the data is small. It is parameter free.

Details

The DESCRIPTION file: TTMap/DESCRIPTION Version 1.0

Author(s)

Rachel Jeitziner Maintainer: Rachel Jeitziner <rachel.jeitziner@epfl.ch>

References

R. Jeitziner et al., TTMap, 2018, DOI:arXiv:1801.01841

See Also

rgl, colorRamps

Examples

#to be found in \code{\link[TTMap]{ttmap_sgn_genes}}

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calcul_e

Calculation of the value of epsilon

Description

Calculation of the value of epsilon

Usage

```
calcul_e(dd5, pvalcutoff = 0.95, tt1, alpha = 1, S =
colnames(tt1$Normal.mat))
calcul_e_single(dd5, pvalcutoff = 0.95, tt1, alpha = 1, S =
colnames(tt1$Normal.mat))
```

Arguments

dd5 distance matrix as created by generate_mismatch_distance

pvalcutoff cutoff of 0.05 percent (default) or less
tt1 output of control_adjustment

alpha a cutoff value for the FC between the group of control and the disease group

S subset of columns to be considered

Value

al number representing the cutoff to choose for the relatedness with dd5

Author(s)

Rachel Jeitziner

See Also

control_adjustment, hyperrectangle_deviation_assessment, ttmap_sgn_genes, generate_mismatch_distance

```
##--
library(airway)
data(airway)
airway <- airway[rowSums(assay(airway))>80,]
assay(airway) <- log(assay(airway)+1,2)
ALPHA <- 1
the_experiment <- TTMap::make_matrices(airway,
seq_len(4), seq_len(4) + 4,
rownames(airway), rownames(airway))
TTMAP_part1prime <-TTMap::control_adjustment(
normal.pcl = the_experiment$CTRL,</pre>
```

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```
tumor.pcl = the_experiment$TEST,
normalname = "The_healthy_controls",
dataname = "Effect_of_cancer",
org.directory = tempdir(), e = 0, P = 1.1, B = 0);
Kprime <- 4;</pre>
TTMAP_part1_hda <-
TTMap::hyperrectangle_deviation_assessment(x =
TTMAP_part1prime,
k = Kprime,dataname = "Effect_of_cancer",
normalname = "The_healthy_controls");
annot <- c(paste(colnames(</pre>
the_experiment$TEST[,-(seq_len(3))]), "Dis", sep = "."),
paste(colnames(the_experiment$CTRL[,
-seq_len(3)]), "Dis", sep = "."))
dd5_sgn_only <-TTMap::generate_mismatch_distance(</pre>
TTMAP_part1_hda,
select=rownames(TTMAP_part1_hda$Dc.Dmat), alpha = ALPHA)
e <- TTMap::calcul_e(dd5_sgn_only, 0.95, TTMAP_part1prime, 1)</pre>
```

control_adjustment

Calculates a corrected control group, discovers outliers in it.

Description

control_adjustment function finds outliers in the control group and removes them

Usage

```
control_adjustment(normal.pcl, tumor.pcl, normalname, dataname, org.directory = "", A = 1, e = 0, meth = 0, P = 1.1, B = 0)
```

Arguments

normal.pcl	the control matrix with annotation as obtained by \$CTRL from make_matrices
tumor.pcl	the disease/test data matrix with annotation as obtained by \$TEST from make_matrices
normalname	A name for the corrected control files
dataname	the name of the project
org.directory	where the outputs should be saved
A	integer if A=0 then the difference to the median is calculated otherwise the difference to the mean.
е	integer giving how far to the median an outlier is at least
meth	value or method that defines how to replace outliers, default is set to replace by the median
Р	if more than P percent of features are outliers the feature is removed, by default all are kept
В	Batch vector a vector for normal and test samples with a same number corresponding to a same batch

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Details

control_adjustment calculates a corrected control group, discovers outliers in it.

Value

Several files are created

paste(org.directory, normalname, ".normMesh", sep = "")

The normal matrix with only common features with the test matrix. This file is only created if the two have different rows

paste(org.directory, dataname, ".normMesh", sep = "")

The test matrix with only common features with the normal matrix. This file is only created if the two have different rows.

mean_vs_variance.pdf

A pdf showing a plot of the mean (X axis) against the variances (Y axis) of each feature

mean_vs_variance_after_correction.pdf

A pdf showing a plot of the mean (X axis) against the variances (Y axis) of each feature after correction of the control group

na_numbers_per_row.txt

number of outliers per row

na_numbers_per_col.txt

number of outliers per column

And values of ttmap_part1_ctrl_adj

e Selected criteria for what is an outlier

tag.pcl Annotation of features, ID of features and weight

Normal.mat The control matrix without annotation and only with the common rows with

Disease.mat

Disease .mat The test/disease matrix without annotation and only with the common rows with

Disease.mat

flat.Nmat A list \$mat being the corrected control matrix \$m a record of the different num-

bers of removed genes per sample

record numbers recording the number of columns in Disease.mat and Normal.mat

B The batch vector B introduced in the begining

U1 The different batches in Normal.mat
U2 The different batches in Disease.mat

Author(s)

Rachel Jeitziner

See Also

hyperrectangle_deviation_assessment, ttmap ttmap_sgn_genes

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Examples

```
##--
library(airway)
data(airway)
airway <- airway[rowSums(assay(airway))>80,]
assay(airway) <- log(assay(airway)+1,2)
ALPHA <- 1
the_experiment <- TTMap::make_matrices(airway,
seq_len(4), seq_len(4) + 4,
rownames(airway), rownames(airway))
TTMAP_part1prime <-TTMap::control_adjustment(
normal.pcl = the_experiment$CTRL,
tumor.pcl = the_experiment$TEST,
normalname = "The_healthy_controls",
dataname = "Effect_of_cancer",
org.directory = tempdir(), e = 0, P = 1.1, B = 0);</pre>
```

generate_correlation Generates different distance matrices

Description

Single cell complete mismatch distance, single cell complete mismatch distance with a parameter of cutoff, mismatch distance, correlation distance, p-value of correlation test distance and euclidean distance.

Usage

```
generate_single_cell_complete_mismatch(ttmap_part1_hda,
select, alpha = 1)
generate_single_cell_mismatch_with_parameter(ttmap_part1_hda,
select, alpha = 1)
generate_correlation(ttmap_part1_hda, select)
generate_euclidean(ttmap_part1_hda, select)
generate_mismatch_distance(ttmap_part1_hda, select, alpha = 1)
generate_p_val_correlation(ttmap_part1_hda, select)
```

Arguments

```
ttmap_part1_hda
an object given back by hyperrectangle_deviation_assessment
select A sublist of rownames of ttmap_part1_hda$Dc.Dmat
alpha A real number corresponding to a cutoff
```

Details

If one is interested only in clustering samples according to a list of genes belonging to a certain pathway, then this list is provided to the parameter select. Alpha is a cutoff for deviations that should be considered as noise, for gene expression data such as normalised RNA-seq or microarrays for instance a cutoff of 1, corresponding to a two fold change is being chosen.

Value

Distance matrix

Author(s)

Rachel Jeitziner

Examples

```
ttmap_part1_hda <- list()
ttmap_part1_hda$Dc.Dmat <- matrix(c(-1, 2, 0, -4, 5, 6), nrow = 2)
rownames(ttmap_part1_hda$Dc.Dmat) <- c("Gene1", "Gene2")
colnames(ttmap_part1_hda$Dc.Dmat) <- c("A", "B", "C")
dd <- TTMap::generate_mismatch_distance(ttmap_part1_hda, select =
rownames(ttmap_part1_hda$Dc.Dmat))
dd <- TTMap::generate_euclidean(ttmap_part1_hda, select =
rownames(ttmap_part1_hda$Dc.Dmat))</pre>
```

hyperrectangle_deviation_assessment

Calculation of deviation components

Description

hyperrectangle_deviation_assessment function calculates the hyperrectangle deviation assessment (HDA) that calculates the deviation components using normal_hda2 which calculates the normal component of the test sample and deviation_hda2 which calculates the deviation component.

Usage

```
hyperrectangle_deviation_assessment(x,
k = dim(x$Normal.mat)[2], dataname,
normalname,Org.directory = getwd())
```

Arguments

x output object given back by control_adjustment, listk A factor if not all the lines in the control group should be kept

dataname the name of the project

normalname A name for the corrected control files
Org.directory where the outputs should be saved

Details

The function performs the hyperrectangle deviation assessment (HDA)

Value

Outputs

Tdis.pcl The matrix of the deviation components for each test sample

Tnorm.pcl The matrix of the normal components for each test sample

NormalModel.pcl

The normal model used

Values

Dc. Dmat the deviation component matrix composed of the deviation components of all

the samples in the test group

m the values of the filter function per sample in the test group

Author(s)

Rachel Jeitziner

See Also

```
control_adjustment, hyperrectangle_deviation_assessment, ttmap_sgn_genes
```

```
##a full example can be found in ttmap_sgn_genes
##--
library(airway)
data(airway)
airway <- airway[rowSums(assay(airway))>80,]
assay(airway) <- log(assay(airway)+1,2)</pre>
ALPHA <- 1
the_experiment <- TTMap::make_matrices(airway,</pre>
seq_len(4), seq_len(4) + 4,
rownames(airway), rownames(airway))
TTMAP_part1prime <-TTMap::control_adjustment(</pre>
normal.pcl = the_experiment$CTRL,
tumor.pcl = the_experiment$TEST,
normalname = "The_healthy_controls",
dataname = "Effect_of_cancer",
org.directory = tempdir(), e = 0, P = 1.1, B = 0);
Kprime <- 4;</pre>
TTMAP_part1_hda <-
TTMap::hyperrectangle_deviation_assessment(x =
TTMAP_part1prime,
k = Kprime, dataname = "Effect_of_cancer",
normalname = "The_healthy_controls");
```

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make_matrices	Prepares the matrices for control_adjustment	
---------------	--	--

Description

make_matrices generates the control and the test matrice in the right format

Usage

```
make_matrices(mat, col_ctrl, col_test, NAME, CLID,
GWEIGHT = rep(1, dim(mat)[1]), EWEIGHT = 0)
```

Arguments

mat	the gene expressions can be matrix , data.frame , "RangedSummarizedExperiment", "ExpressionSet" format
col_ctrl	the columns in the matrix "mat" of the control samples
col_test	the columns in the matrix "mat" of the test samples
NAME	Name of genes, or annotation, e.g. WNT4
CLID	Identities of genes, e.g. ENSMUSG00000000001
GWEIGHT	the weight for each gene
EWEIGHT	the weight for each experiment

Details

make_matrices generates the test matrix and the control matrix in the format accepted by control_adjustment from a matrix object

Value

junk A list containing \$CTRL and \$TEST the matrices to impute in control_adjustment

Author(s)

Rachel Jeitziner

See Also

control_adjustment, hyperrectangle_deviation_assessment, ttmap_sgn_genes, "RangedSummarizedExperiment"

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```
##--
##--
Aa = 6
B1 = 3
B2 = 3
C0 = 100
D0 = 10000
a0 = 4
b0 = 0.1
a1 = 6
b1 = 0.1
a2 = 2
b2 = 0.5
ALPHA = 1
E = 1
Pw = 1.1
Bw = 0
RA \leftarrow matrix(rep(0, Aa * D0), nrow = D0)
RB1 <- matrix(rep(0, B1 * D0), nrow = D0)
RB2 <- matrix(rep(0, B2 * D0), nrow = D0)
RA <- lapply(seq_len(D0 - C0), function(i) rnorm(Aa,
mean = a0, sd = sqrt(b0))
RA<-do.call(rbind, RA)
RB1<- lapply(seq_len(D0 - C0), function(i) rnorm(B1,
mean = a0, sd = sqrt(b0))
RB1 <- do.call(rbind, RB1)</pre>
RB2 <- lapply(seq_len(D0 - C0), function(i) rnorm(B2,
mean = a0, sd = sqrt(b0))
RB2 <- do.call(rbind, RB2)
RA_c <- lapply(seq_len(C0), function(i) rnorm(Aa,
mean = a0, sd = sqrt(b0))
RA_c <- do.call(rbind, RA_c)
RB1_c <- lapply(seq_len(C0), function(i) rnorm(B1,</pre>
mean = a1, sd = sqrt(b1))
RB1_c <- do.call(rbind, RB1_c)</pre>
RB2_c <- lapply(seq_len(C0), function(i) rnorm(B2,</pre>
mean = a2, sd = sqrt(b2))
RB2_c <- do.call(rbind, RB2_c)</pre>
norm1 <- rbind(RA, RA_c)</pre>
dis <- cbind(rbind(RB1, RB1_c), rbind(RB2, RB2_c))</pre>
colnames(norm1) <- paste("N", seq_len(Aa), sep = "")</pre>
rownames(norm1) <- c(paste("norm", seq_len(D0 - C0), sep = ""),</pre>
paste("diff", seq_len(C0), sep = ""))
colnames(dis) <- c(paste("B1", seq_len(B1), sep=""),</pre>
paste("B2", seq_len(B2), sep =""))
rownames(dis)<-c(paste("norm",</pre>
seq_len(D0 - C0), sep = ""),
paste("diff", seq_len(C0), sep = ""))
the_experiment <- TTMap::make_matrices(cbind(norm1, dis),</pre>
col_ctrl = colnames(norm1),
col_test = colnames(dis), NAME = rownames(norm1),
```

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```
CLID = rownames(norm1))
###other example using SummarizedExperiment
library(airway)
data(airway)
airway <- airway[rowSums(assay(airway))>80,]
assay(airway) <- log(assay(airway)+1,2)
the_experiment <- TTMap::make_matrices(airway,
seq_len(4), seq_len(4) + 4,
rownames(airway), rownames(airway))</pre>
```

make_matrices-methods Prepares the matrices for control_adjustment

Description

make_matrices generates the control (output \$CTRL) and the test (output \$TEST) matrice in the right format for control_adjustment

Methods

```
signature(mat = "data.frame") Method make_matrice for data.frame object.
signature(mat = "matrix") Method make_matrice for matrix object.
signature(mat = "SummarizedExperiment") Method make_matrice for SummarizedExperiment object.
signature(mat = "RangedSummarizedExperiment") Method make_matrice for RangedSummarizedExperiment object.
signature(mat = "ExpressionSet") Method make_matrice for ExpressionSet object.
```

ttmap

Visualisation of the clustering

Description

Enables a quick view on the groups in the dataset (globally) and how locally they differ.

Usage

```
ttmap(ttmap_part1_hda, m1,
select = row.names(ttmap_part1_hda$Dc.Dmat),
ddd, e, filename = "TEST", n = 3, ad = 0, bd = 0, piq = 1,
dd = generate_mismatch_distance(ttmap_part1_hda = ttmap_part1_hda,
select = select), mean_value_m1 = "N", ni = 2)
```

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Arguments

ttmap_part1_hda

list output of hyperrectangle_deviation_assessment

m1 either a user imputed vector whose names are the names of the samples with

addition of .Dis. or by default it is the amount of deviation

select Should all the features (default) or only a sublist be considered to calculate the

distance

ddd Annotation matrix with rownames the different sample names with addition of

.Dis. There can be as many columns as wanted, but only the column n will be

selected to annotated the clusters

e integer parameter defining under which value two samples are considered to be

close

filename Name for the description file annotating the clusters

The column to be considered to annotate the clusters

ad if ad!=0 then the clusters on the output picture will not be annotated

bd if different than 0 (default), the output will be without outliers of the test data

set (clusters composed of only "piq" element)

piq parameter used to determine what small clusters are, see bd

dd the distance matrix to be used

mean_value_m1 if == "N" the average of the values in m1 divided by the number of the samples

are put into the legend (by default represents the average of the samples in a cluster of the mean-deviation of the features) otherwise it will show the average value of the values in m1 (is useful for instance if m1 represents the age of the

samples)

ni The column to consider to annotate the samples (is put into parenthesis) for the

description file

Details

Is the Two-tiers Mapper function. The output is an interactive image of the clusters in the different layers.

Value

all	the clusters in the overall group
low	the clusters in the lower quartile group
mid1	the clusters in the first middle quartile group
mid2	the clusters in the second middle quartile group
high	the clusters in the higher quartile group

Author(s)

Rachel Jeitziner

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See Also

control_adjustment, hyperrectangle_deviation_assessment, ttmap_sgn_genes

Examples

```
##--
library(airway)
data(airway)
airway <- airway[rowSums(assay(airway))>80,]
assay(airway) <- log(assay(airway)+1,2)</pre>
ALPHA <- 1
the_experiment <- TTMap::make_matrices(airway,</pre>
seq_len(4), seq_len(4) + 4,
rownames(airway), rownames(airway))
TTMAP_part1prime <-TTMap::control_adjustment(</pre>
normal.pcl = the_experiment$CTRL,
tumor.pcl = the_experiment$TEST,
normalname = "The_healthy_controls",
dataname = "Effect_of_cancer",
org.directory = tempdir(), e = 0, P = 1.1, B = 0);
Kprime <- 4;</pre>
TTMAP_part1_hda <-
TTMap::hyperrectangle_deviation_assessment(x =
TTMAP_part1prime,
k = Kprime,dataname = "Effect_of_cancer",
normalname = "The_healthy_controls");
annot <- c(paste(colnames(</pre>
the_experiment$TEST[,-(seq_len(3))]),"Dis", sep = "."),
paste(colnames(the_experiment$CTRL[,
-seq_len(3)]), "Dis", sep = "."))
annot <- cbind(annot, annot)</pre>
rownames(annot)<-annot[, 1]</pre>
dd5_sgn_only <-TTMap::generate_mismatch_distance(</pre>
TTMAP_part1_hda,
select=rownames(TTMAP_part1_hda$Dc.Dmat), alpha = ALPHA)
TTMAP_part2 <-
TTMap::ttmap(TTMAP_part1_hda, TTMAP_part1_hda$m,
select = rownames(TTMAP_part1_hda$Dc.Dmat), annot,
e = TTMap::calcul_e(dd5_sgn_only, 0.95, TTMAP_part1prime, 1),
filename = "first_comparison", n = 1, dd = dd5_sgn_only)
```

ttmap_sgn_genes

Gives a list of associated genes per cluster

Description

ttmap_sgn_genes function

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Usage

```
ttmap_sgn_genes(ttmap_part2_gtlmap, ttmap_part1_hda,
ttmap_part1_ctrl_adj, c, n = 2, a = 0,
filename = "TEST2", annot = ttmap_part1_ctrl_adj$tag.pcl,
col = "NAME", path = getwd(), Relaxed = 1)
ttmap_sgn_genes_inter2(q, ttmap_part1_hda, alpha = 0)
ttmap_sgn_genes_inter(q, ttmap_part1_hda, alpha = 0)
```

Arguments

```
ttmap_part2_gtlmap
                  output of ttmap
ttmap_part1_hda
                  output of hyperrectangle_deviation_assessment
ttmap_part1_ctrl_adj
                  output of control_adjustment
                  annotation file of the samples
С
                  column to give the name to the cluster
n
                  cutoff to be considered different than noise
filename
                  Name of the files
                  annotation file
annot
                  which column should be considered to annotate the features
col
path
                  where to put the output files
Relaxed
                  If Relaxed then one allows sample to be as the control and for all the others in
                  one cluster to be going in the same direction (more than alpha) otherwise all the
                  features must be deviating to be considered a significant feature
                  The sample in one cluster
q
                  cutoff to be considered different than noise inherited by a
alpha
```

Details

Is giving per cluster the features that vary in the same direction

Value

generates a file per cluster of significant features with an annotation

Author(s)

Rachel Jeitziner

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Examples

```
library(airway)
data(airway)
airway <- airway[rowSums(assay(airway))>80,]
assay(airway) <- log(assay(airway)+1,2)</pre>
ALPHA <- 1
the_experiment <- TTMap::make_matrices(airway,</pre>
seq_len(4), seq_len(4) + 4,
rownames(airway), rownames(airway))
TTMAP_part1prime <-TTMap::control_adjustment(</pre>
normal.pcl = the_experiment$CTRL,
tumor.pcl = the_experiment$TEST,
normalname = "The_healthy_controls",
dataname = "Effect_of_cancer",
org.directory = tempdir(), e = 0, P = 1.1, B = 0);
Kprime <- 4;</pre>
TTMAP_part1_hda <-
TTMap::hyperrectangle_deviation_assessment(x =
TTMAP_part1prime,
k = Kprime,dataname = "Effect_of_cancer",
normalname = "The_healthy_controls");
annot <- c(paste(colnames(</pre>
the_experiment$TEST[,-(seq_len(3))]),"Dis", sep = "."),
paste(colnames(the_experiment$CTRL[,
-seq_len(3)]), "Dis", sep = "."))
annot <- cbind(annot, annot)</pre>
rownames(annot)<-annot[, 1]</pre>
dd5_sgn_only <-TTMap::generate_mismatch_distance(</pre>
TTMAP_part1_hda,
select=rownames(TTMAP_part1_hda$Dc.Dmat), alpha = ALPHA)
TTMAP_part2 <-
TTMap::ttmap(TTMAP_part1_hda, TTMAP_part1_hda$m,
select = rownames(TTMAP_part1_hda$Dc.Dmat), annot,
e = TTMap::calcul_e(dd5_sgn_only, 0.95, TTMAP_part1prime, 1),
filename = "first_comparison", n = 1, dd = dd5_sgn_only)
TTMap::ttmap_sgn_genes(TTMAP_part1, TTMAP_part1_hda,
TTMAP_part1prime, annot,
n = 2, a = 1, filename = "first_list_of_genes",
annot = TTMAP_part1prime$tag.pcl, col = "NAME",
path = getwd(), Relaxed = 1)
```

write_pcl

Reading, writing and annotation files

Description

Reading (read_pcl), writing (write_pcl) files and annotating matrices (mat2pcl)

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Usage

```
mat2pcl(mat, tag)
write_pcl(df, dataname, fileaddress = "")
read_pcl(filename, na.type = "", Nrows = -1,
Comment.char = "", ...)
```

Arguments

df PCL object to be saved

dataname Name of the file

fileaddress Where to save the file

filename File name to be loaded on R

na. type feels the parameter na. strings of read.table

Nrows Number of rows to be ignored (nrows of read.table)

Comment.char comment.char of read.table other read.table arguments

mat matrix to be changed in annotated

tag annotation

Details

The file (called filename) MUST contain 3 columns before the actual values, which are called CLID, NAME and GWEIGHT, described bellow. The first row must be the header of the columns (starting with CLID,NAME and GWEIGHT) and the second row must be EWEIGHT. Representing how much weight each column has: if some columns are n replicates they can have each a weight of 1/n.

Value

Data frame composed of

CLID Column called CLID which is the ID of the features, which will then be the

rownames of the dataframe

NAME A possibly longer name, more meaningfull than CLID, text format

GWEIGHT A weight for each gene or feature. If some genes are less important than others

or only a pathway should be selected than the file (called filename) should have

this information

Matrix The matrix with numbers of the different observations

Author(s)

Rachel Jeitziner

See Also

```
control_adjustment
```

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```
library(airway)
data(airway)
airway <- airway[rowSums(assay(airway))>80,]
assay(airway) <- log(assay(airway)+1,2)
ALPHA <- 1
to_be_saved <- TTMap::make_matrices(airway,
seq_len(4), seq_len(4) + 4,
rownames(airway), rownames(airway))
TTMap::write_pcl(to_be_saved, "tempfile()", getwd())</pre>
```

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