

Package ‘TTMap’

January 11, 2025

Type Package

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

Version 1.29.0

Date 2017-07-12

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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.

License GPL-2

Suggests BiocStyle, airway

Depends rgl, colorRamps

Imports grDevices,graphics,stats,utils, methods, SummarizedExperiment, Biobase

biocViews Software, Microarray, DifferentialExpression, MultipleComparison, Clustering, Classification

git_url <https://git.bioconductor.org/packages/TTMap>

git_branch devel

git_last_commit f7d844b

git_last_commit_date 2024-10-29

Repository Bioconductor 3.21

Date/Publication 2025-01-10

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| | |
|---------------|--|
| TTMap-package | <i>Two-Tier Mapper: a clustering tool based on topological data analysis</i> |
|---------------|--|

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]{tmap_sgn_genes}}
```

| | |
|----------|--|
| calcul_e | <i>Calculation of the value of epsilon</i> |
|----------|--|

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 <code>generate_mismatch_distance</code> |
| 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](#), [tmap_sgn_genes](#), [generate_mismatch_distance](#)

Examples

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

```
tumor.pcl = the_experiment$TEST,
normalname = "The_healthy_controls",
dataname = "Effect_of_cancer",
org.directory = tempdir(), e = 0, P = 1.1, B = 0);
Kprime <- 4;
TMAP_part1_hda <-
TMap::hyperrectangle_deviation_assessment(x =
TMAP_part1prime,
k = Kprime, dataname = "Effect_of_cancer",
normalname = "The_healthy_controls");
annot <- c(paste(colnames(
the_experiment$TEST[-(seq_len(3))]), "Dis", sep = "."),
paste(colnames(the_experiment$CTRL[
-seq_len(3)]), "Dis", sep = "."))
dd5_sgn_only <- TMap::generate_mismatch_distance(
TMAP_part1_hda,
select=rownames(TMAP_part1_hda$Dc.Dmat), alpha = ALPHA)
e <- TMap::calcul_e(dd5_sgn_only, 0.95, TMAP_part1prime, 1)
```

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. |
| e | 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 |
| P | if more than P percent of features are outliers the feature is removed, by default all are kept |
| B | Batch vector a vector for normal and test samples with a same number corresponding to a same batch |

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 `tmap_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 numbers 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 beginning

`U1` The different batches in `Normal.mat`

`U2` The different batches in `Disease.mat`

Author(s)

Rachel Jeitziner

See Also

[hyperrectangle_deviation_assessment](#), [tmap](#) [tmap_sgn_genes](#)

Examples

```
##--
library(airway)
data(airway)
airway <- airway[rowSums(assay(airway))>80,]
assay(airway) <- log(assay(airway)+1,2)
ALPHA <- 1
the_experiment <- TMap::make_matrices(airway,
seq_len(4), seq_len(4) + 4,
rownames(airway), rownames(airway))
TTMAP_part1prime <-TMap::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);
```

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$Dc.Dmat) <- c("A", "B", "C")
dd <- TMap::generate_mismatch_distance(ttmap_part1_hda, select =
rownames(ttmap_part1_hda$Dc.Dmat))
dd <- TMap::generate_euclidean(ttmap_part1_hda, select =
rownames(ttmap_part1_hda$Dc.Dmat))
```

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

| | |
|----------------------------|---|
| <code>x</code> | output object given back by control_adjustment , list |
| <code>k</code> | A factor if not all the lines in the control group should be kept |
| <code>dataname</code> | the name of the project |
| <code>normalname</code> | A name for the corrected control files |
| <code>Org.directory</code> | 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](#), [tmap_sgn_genes](#)

Examples

```
##a full example can be found in tmap_sgn_genes
##--
library(airway)
data(airway)
airway <- airway[rowSums(assay(airway))>80,]
assay(airway) <- log(assay(airway)+1,2)
ALPHA <- 1
the_experiment <- TMap::make_matrices(airway,
seq_len(4), seq_len(4) + 4,
rownames(airway), rownames(airway))
TTMAP_part1prime <-TMap::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);
Kprime <- 4;
TTMAP_part1_hda <-
TMap::hyperrectangle_deviation_assessment(x =
TTMAP_part1prime,
k = Kprime, dataname = "Effect_of_cancer",
normalname = "The_healthy_controls");
```

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](#), [tmap_sgn_genes](#), "[RangedSummarizedExperiment](#)"

Examples

```

##--
##--
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 <- 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)
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,
mean = a1, sd = sqrt(b1)))
RB1_c <- do.call(rbind, RB1_c)
RB2_c <- lapply(seq_len(C0), function(i) rnorm(B2,
mean = a2, sd = sqrt(b2)))
RB2_c <- do.call(rbind, RB2_c)
norm1 <- rbind(RA, RA_c)
dis <- cbind(rbind(RB1, RB1_c), rbind(RB2, RB2_c))
colnames(norm1) <- paste("N", seq_len(Aa), sep = "")
rownames(norm1) <- c(paste("norm", seq_len(D0 - C0), sep = ""),
paste("diff", seq_len(C0), sep = ""))
colnames(dis) <- c(paste("B1", seq_len(B1), sep=""),
paste("B2", seq_len(B2), sep = ""))
rownames(dis)<-c(paste("norm",
seq_len(D0 - C0), sep = ""),
paste("diff", seq_len(C0), sep = ""))
the_experiment <- TMap::make_matrices(cbind(norm1, dis),
col_ctrl = colnames(norm1),
col_test = colnames(dis), NAME = rownames(norm1),

```

```

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 <- TMap::make_matrices(airway,
seq_len(4), seq_len(4) + 4,
rownames(airway), rownames(airway))

```

make_matrices-methods *Prepares the matrices for [control_adjustment](#)*

Description

make_matrices generates the control (output \$CTRL) and the test (output \$TEST) matrices 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)

```

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 |
| n | 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

See Also

[control_adjustment](#), [hyperrectangle_deviation_assessment](#), [tmap_sgn_genes](#)

Examples

```
##--
library(airway)
data(airway)
airway <- airway[rowSums(assay(airway))>80,]
assay(airway) <- log(assay(airway)+1,2)
ALPHA <- 1
the_experiment <- TMap::make_matrices(airway,
seq_len(4), seq_len(4) + 4,
rownames(airway), rownames(airway))
TMAP_part1prime <-TMap::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);
Kprime <- 4;
TMAP_part1_hda <-
TMap::hyperrectangle_deviation_assessment(x =
TMAP_part1prime,
k = Kprime,dataname = "Effect_of_cancer",
normalname = "The_healthy_controls");
annot <- c(paste(colnames(
the_experiment$TEST[-(seq_len(3))]),"Dis", sep = "."),
paste(colnames(the_experiment$CTRL[,
-seq_len(3)]), "Dis", sep = "."))
annot <- cbind(annot, annot)
rownames(annot)<-annot[, 1]
dd5_sgn_only <-TMap::generate_mismatch_distance(
TMAP_part1_hda,
select=rownames(TMAP_part1_hda$Dc.Dmat), alpha = ALPHA)
TMAP_part2 <-
TMap::tmap(TMAP_part1_hda, TMAP_part1_hda$m,
select = rownames(TMAP_part1_hda$Dc.Dmat), annot,
e = TMap::calcul_e(dd5_sgn_only, 0.95, TMAP_part1prime, 1),
filename = "first_comparison", n = 1, dd = dd5_sgn_only)
```

tmap_sgn_genes

Gives a list of associated genes per cluster

Description

[tmap_sgn_genes](#) function

Usage

```
tmap_sgn_genes(tmap_part2_gtlmap, tmap_part1_hda,
tmap_part1_ctrl_adj, c, n = 2, a = 0,
filename = "TEST2", annot = tmap_part1_ctrl_adj$tag.pcl,
col = "NAME", path = getwd(), Relaxed = 1)
tmap_sgn_genes_inter2(q, tmap_part1_hda, alpha = 0)
tmap_sgn_genes_inter(q, tmap_part1_hda, alpha = 0)
```

Arguments

| | |
|---------------------|--|
| tmap_part2_gtlmap | output of tmap |
| tmap_part1_hda | output of hyperrectangle_deviation_assessment |
| tmap_part1_ctrl_adj | output of control_adjustment |
| c | annotation file of the samples |
| n | column to give the name to the cluster |
| a | cutoff to be considered different than noise |
| filename | Name of the files |
| annot | annotation file |
| col | which column should be considered to annotate the features |
| 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 |
| q | The sample in one cluster |
| alpha | cutoff to be considered different than noise inherited by a |

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

Examples

```
##--
library(airway)
data(airway)
airway <- airway[rowSums(assay(airway))>80,]
assay(airway) <- log(assay(airway)+1,2)
ALPHA <- 1
the_experiment <- TMap::make_matrices(airway,
seq_len(4), seq_len(4) + 4,
rownames(airway), rownames(airway))
TTMAP_part1prime <-TMap::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);
Kprime <- 4;
TTMAP_part1_hda <-
TMap::hyperrectangle_deviation_assessment(x =
TTMAP_part1prime,
k = Kprime,dataname = "Effect_of_cancer",
normalname = "The_healthy_controls");
annot <- c(paste(colnames(
the_experiment$TEST[-(seq_len(3))]),"Dis", sep = "."),
paste(colnames(the_experiment$CTRL[,
-seq_len(3)]), "Dis", sep = "."))
annot <- cbind(annot, annot)
rownames(annot)<-annot[, 1]
dd5_sgn_only <-TMap::generate_mismatch_distance(
TTMAP_part1_hda,
select=rownames(TTMAP_part1_hda$Dc.Dmat), alpha = ALPHA)
TTMAP_part2 <-
TMap::tmap(TTMAP_part1_hda, TTMAP_part1_hda$m,
select = rownames(TTMAP_part1_hda$Dc.Dmat), annot,
e = TMap::calcul_e(dd5_sgn_only, 0.95, TTMAP_part1prime, 1),
filename = "first_comparison", n = 1, dd = dd5_sgn_only)
TMap::tmap_sgn_genes(TTMAP_part2, TTMAP_part1_hda,
TTMAP_part1prime, annot,
n = 2, a = 1, filename = "first_list_of_genes",
annot = TTMAP_part1prime$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](#))

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 below. 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 meaningful 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](#)

Examples

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

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