# Package 'rexposome'

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Title Exposome exploration and outcome data analysis

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**Description** Package that allows to explore the exposume and to perform association analyses between exposures and health outcomes.

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### **Description**

Method to get the classification of the samples from an ExposomeClust.

# Usage

```
classification(object)
```

# **Arguments**

object

An ExposomeClust to get the samples' classification.

### Value

A labelled vector with the classification of each exposure.

#### See Also

clustering as a constructor for ExposomeClust, plotClassification to plot the groups

# **Examples**

```
data("eclust")
tt <- classification(expo_c)
table(tt)</pre>
```

clustering

Method to perform clustering on the samples of an ExposomeSet

# Description

This method allows to create an ExposomeClust object from an ExposomeSet object by clustering samples through the exposure levels. The method is flexible to accept any clustering method (method) that allows to obtain a classification (cmethod) of the samples. The function assigned to argument method must have an argument called data, waiting for the matrix of exposures (samples as rows, exposures as columns). If the result object of the method has no accessor \$classification, then a cmethod is required and will be applied on the result of method to obtain a labelled vector with the samples' classification.

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#### Usage

```
clustering(object, method, cmethod, ..., warnings = TRUE)
```

# **Arguments**

object	ExposomeSet containing the exposures used for the clustering process
method	Function applied to the exposures of object. This function must has an argument named as data that will receive the matrix of exposures.
cmethod	(optional) Function to obtain the classification from the object generated with method.
	Passed to content of method.
warnings	(default TRUE) If set to FALSE warnings will not be displayed.

#### Value

ExposomeClust with the original exposures and the classification of each exposure.

#### Note

The function assigned to cmethod will be directy applied to the result of the method as: cmethod(model); being model the result of method.

### See Also

classification to see how to obtain the classification of the samples from an ExposomeClust, plot-Classification to plot the groups

```
data("exposome")
# EXAMPLE 1: Clustering with mclust
library(mclust)
c <- clustering(expo[12:32, ], method = Mclust, G = 2)</pre>
table(classification(c)) # This works since the result of Mclust has an accessor
                    # $classification
# EXAMPLE 2: Cluseting with flexmix
library(flexmix)
# First we carete a function to apply flexmix to the ExposomeSet
flexmix_clust <- function(data, ...) {</pre>
  data <- as.matrix(data)</pre>
  flexmix(formula = data~1, ...)
\mbox{\tt\#} Then if we apply the method to the <code>ExposomeSet</code> it will crash:
# c <- clustering(expo[12:32, ], method = flexmix_clust, k = 2, model = FLXMCmvnorm())</pre>
# Because the method does not know how to obtain the classification for the result
# since flexmix has not an accessor called $classiciation
# We create a function to get the classification
flexmix_clas <- function(model, ...) {</pre>
  return(clusters(model))
```

correlation 5

```
# We put it to the ExposomeClust
c <- clustering(expo[12:32, ], method = flexmix_clust, cmethod = flexmix_clas,
    k = 2, model = FLXMCmvnorm())
classification(c) # This works because the ExposomeClust has a way to get
    # the classification</pre>
```

correlation

Creation of an ExposomeCorr from an ExposomeSet.

#### **Description**

Method to calculate the correlation between the exposures of an ExposomeSet. The correlation method takes into account the nature of each pair of exposures: continuous vs. continuous uses cor function from R base, categorical vs. categorical uses cramerV function from lsr R package and categorical vs. continuous exposures correlation is calculated as the square root of the adjusted r-square obtained from fitting a lineal model with the categorical exposures as dependent variable and the continuous exposure as independent variable. The function creates and returns an ExposomeCorr object.

# Usage

```
correlation(object, ..., warnings = TRUE)
```

# **Arguments**

object ExposomeSet which exposures will be used to calculate their correlation

Other arguments passed to cor, cramersV or to lm.

warnings (default TRUE) If set to FALSE warnings will not be displayed.

### Value

ExposomeCorr with the correlation between the selected exposures and their description

### See Also

plotCorrelation to plot the correlations of an ExposomeCorr, clustering to see how the exposures can cluster samples, pca to compute PCA on exposures

```
data("exposome")
expo.c <- correlation(expo)
expo.c
expo.c.table <- extract(expo.c)</pre>
```

6 expos

expo

ExposomeSet for testing purpouses

# Description

ExposomeSet with full set of 104 exposures, 1200 simulated samples and 4 phenotypes (asthma status, BMI measure, sex, and age).

#### Usage

```
data("exposome")
```

#### **Format**

An object of class ExposomeSet of dimension 104 x 1200 x 4.

#### Value

An ExposomeSet object.

# **Examples**

```
data("exposome")
dim(expo)
exposureNames(expo)
familyNames(expo)
sampleNames(expo)
phenotypeNames(expo)
```

expos

Returns the exposures matrix of an ExposomeSet.

# Description

Given an ExposomeSet it returns the inner matrix of exposures, having the exposures as columns and the samples as rows.

# Usage

```
expos(object)
```

# Arguments

object

An ExposomeSet.

#### Value

A matrix of exposures

```
data("exposome")
expos(expo)[1:3, 1:3]
```

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ExposomeClust	Class ExposomeClust
---------------	---------------------

# **Description**

Class ExposomeClust obtained from clustering on an ExposomeSet object, represents the groups of samples created applying a clustering method on the ExposomeSet' exposures.

# Usage

```
## S4 method for signature 'ExposomeClust,ANY'
plot(x, y, ...)

## S4 method for signature 'ExposomeClust'
classification(object)

## S4 method for signature 'ExposomeClust'
plotClassification(object, type = "heatmap", ...)

## S4 method for signature 'ExposomeClust'
sampleNames(object)
```

#### **Arguments**

X	Object of class ExposomeClust
у	NOT USED
	Argument given to heatmap. 2
object	An object of class ExposomeClust
type	(default "heatmap") Type of plot.

#### Value

An object of class ExposomeClust

# Methods (by generic)

- plot(x = ExposomeClust, y = ANY): Wrapper for plotClassification method.
- classification(ExposomeClust): Return classe asigned to each sample
- plotClassification(ExposomeClust): Draws a heatmap for the samples' classification.
- sampleNames(ExposomeClust): Method to obtain samples' names

# **Slots**

```
model Result obtained on applying method on the exposures.

method Function used to perform the clustering of the exposures.

call Call used to create this object.

samples Name of the exposures after the clustering process.
```

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#### See Also

clustering to apply a clustering on an ExposomeSet and create an ExposomeClust.

ExposomeCorr

Class ExposomeCorr

# **Description**

Class ExposomeCorr contains a matrix of correlations between continuos exposures calculated using cor. It also contains the description of each exposures (fData of the original ExposomeSet) in order to maintain a coherence with the original source. It extends eSet-class.

# Usage

```
## S4 method for signature 'ExposomeCorr,ANY'
plot(x, y, ...)

## S4 method for signature 'ExposomeCorr'
dim(x)

## S4 method for signature 'ExposomeCorr'
extract(object, sort, ...)

## S4 method for signature 'ExposomeCorr'
plotCorrelation(object, type = c("circos", "matrix"), ...)
```

#### **Arguments**

x	Object of class ExposomeCorr
У	NOT USED
	Arguments passed to corrplot when type="matrix".
object	An ExposomeCorr object.
sort	NOT USED
type	To choose between "circos" and "matrix".

#### Value

An object of class ExposomeCorr

# Methods (by generic)

- plot(x = ExposomeCorr, y = ANY): Wrapper for plotClassification method.
- dim(ExposomeCorr): Return the dimension of the internat matrix of correlation.
- extract(ExposomeCorr): Return the raw correlation matrix
- plotCorrelation(ExposomeCorr): Draws both a matrix of circos plot of correlations

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#### **Slots**

assayData Contains the correlation matrix (see eSet, AssayData).

featureData Contains the description of the exposures including the family where they belong (see eSet, AnnotatedDataFrame).

# See Also

pca to study the behavioud between samples and exposures in an ExposomeSet

ExposomePCA

Class ExposomePCA

#### **Description**

Class ExposomePCA contains a matrix of exposures used to compute the PCA, also a table of phenotypes and a set congtaing the multiple results of computing the PCA.

# Usage

```
## S4 method for signature 'ExposomePCA, ANY'
plot(x, y, ...)
## S4 method for signature 'ExposomePCA'
exposureNames(object)
## S4 method for signature 'ExposomePCA'
extract(object, table = "exposures", ...)
## S4 method for signature 'ExposomePCA'
ndim(object)
## S4 method for signature 'ExposomePCA'
phenotypeNames(object)
## S4 method for signature 'ExposomePCA'
plot3PCA(
  object,
  cmpX,
  cmpY,
  cmpZ,
  phenotype,
  main,
  angle = 35,
  pch = 16,
  legend = TRUE,
  plines = TRUE
## S4 method for signature 'ExposomePCA'
plotEXP(object, exposure)
```

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```
## S4 method for signature 'ExposomePCA'
plotPCA(
  object,
  set,
  cmpX = 1,
  cmpY = 2,
  show.exposures = FALSE,
  show.samples = FALSE,
  phenotype
)

## S4 method for signature 'ExposomePCA'
plotPHE(object, phenotype, exp2fac = 5)
```

#### **Arguments**

x Object of class ExposomePCA

y NOT USED
... NOT USED

object An ExposomePCA object

table Can takes values "exposures" or "individuals".

cmpX PC to place in X-axis
cmpY PC to place in Y-axis

cmpZ PC to place in Z-axis

phenotype (when set="samples") A phenotype can be selected so the samples are coloured

by its value.

main Title

angle Point of view pch Size of the dots

legend Boolean to show or hide the legend

plines Boolean to show of hide the dotted lines that helps to place the dots in the X/Y

axes

exposure Vector of exposures to be shown in the plot

set Can take values "exposures", "samples" or "all" show. exposures When set to TRUE, labels for exposures are shown show. samples When set to TRUE, labels for samples are shown

exp2fac Number of different values to considere an exposures continuous

#### Value

An object of class ExposomePCA

### Methods (by generic)

- plot(x = ExposomePCA, y = ANY): Wrapper for plotPCA method.
- exposureNames (ExposomePCA): Getter to obtain the exposures's names.
- extract(ExposomePCA): Method to extract the raw results of the PCA.
- ndim(ExposomePCA): Number of principal components in an ExposomePCA.
- phenotypeNames (ExposomePCA): Getter to obtain the phenotype's names.
- plot3PCA(ExposomePCA): Methdo to draw a 3D plot for PCA
- plotEXP(ExposomePCA): Plot correlation between exposures and PCA
- plotPCA(ExposomePCA): Methdo to draw a 2D plot for PCA
- plotPHE(ExposomePCA): Plot association score between phentoypes and PCA

### **Slots**

pca list containing all elements of the PCA phenoData Contains the phenotypes or variables experimenter-supplied (see eSet, AnnotatedDataFrame). featureData Contains the description of the exposures including the family where they belong

#### See Also

correlation to study the correlation between exposures in a ExposomeSet

(see eSet, AnnotatedDataFrame).

 ${\tt ExposomeSet}$ 

Class ExposomeSet

#### **Description**

Class ExposomeSet contains the exposure levels, the exposure's description and the samples phenotype. It is the starting object for rexposome package and extends eSet.

# Usage

```
## S4 method for signature 'ExposomeSet,ANY'
plot(x, y, ...)

## S4 method for signature 'ExposomeSet'
clustering(object, method, cmethod, ..., warnings = TRUE)

## S4 method for signature 'ExposomeSet'
correlation(object, ..., warnings = TRUE)

## S4 method for signature 'ExposomeSet'
dim(x)

## S4 method for signature 'ExposomeSet'
expos(object)

## S4 method for signature 'ExposomeSet'
```

```
exposureNames(object)
## S4 method for signature 'ExposomeSet'
exwas(
  object,
  formula,
  filter,
  family,
  . . . ,
  baselevels,
  tef = TRUE,
  verbose = FALSE,
  warnings = TRUE,
  robust = FALSE
)
## S4 method for signature 'ExposomeSet'
familyNames(object, by.exposure = FALSE)
## S4 method for signature 'ExposomeSet'
highAndLow(
  object,
  ngroups = 3,
  intervals = c("standard", "extreme"),
  select,
  drop = FALSE,
  warnings = TRUE
)
## S4 method for signature 'ExposomeSet'
ilod(
  object,
  seed = 1234,
  lod.col = "LOD",
  pNA = 0.2,
  tLog = FALSE,
  method = "QRILC",
  warnings = TRUE,
)
## S4 method for signature 'ExposomeSet'
imputation(object, select, ..., messages = FALSE)
## S4 method for signature 'ExposomeSet'
invExWAS(object, formula, filter, tef = TRUE, verbose = FALSE, warnings = TRUE)
## S4 method for signature 'ExposomeSet'
mexwas(object, phenotype, family, warnings = TRUE)
## S4 method for signature 'ExposomeSet'
normalityTest(
```

```
object,
 exposure,
  th = 0.05,
 min.val = 5,
 na.rm = TRUE,
 warnings = TRUE
## S4 method for signature 'ExposomeSet'
pca(object, npc = 10, pca = FALSE, ...)
## S4 method for signature 'ExposomeSet'
phenotypeNames(object)
## S4 method for signature 'ExposomeSet'
plotFamily(x, family, group, group2, scatter = TRUE, na.omit = TRUE)
## S4 method for signature 'ExposomeSet'
plotHistogram(x, select, density = TRUE, show.trans = FALSE)
## S4 method for signature 'ExposomeSet'
plotLOD(object, lod.col = "LOD", x.max = 100, sort = TRUE)
## S4 method for signature 'ExposomeSet'
plotMissings(
 object,
  set = c("exposures", "phenotypes"),
 x.max = 100,
  sort = TRUE
)
## S4 method for signature 'ExposomeSet'
standardize(object, select, method = "normal", na.rm = TRUE, warnings = TRUE)
## S4 method for signature 'ExposomeSet'
Summary(x, set = c("exposures", "phenotypes"), select, ..., na.rm = FALSE)
## S4 method for signature 'ExposomeSet'
tableLOD(object, output = "n", lod.col = "LOD", sort = TRUE)
## S4 method for signature 'ExposomeSet'
tableMissings(
 object,
  set = c("exposures", "phenotypes"),
 output = "n",
  sort = TRUE
## S4 method for signature 'ExposomeSet'
trans(object, fun, select, by.exposure = FALSE, ...)
```

#### **Arguments**

x An ExposomeSet object.

y NOT USED

. . . Arguments to be passed to imputeFAMD

object An ExposomeSet object.
method Method to be used.

cmethod Function implementing a systsme to retrieve classification from clustering out-

put

warnings If set to TRUE it prints the warning messsages.

formula Formula, not including exposures, to be tested. No need to provide response

(left term)

filter Expression to be used to filter ExposomeSet

family Family descriving the nature of the health outcome

baselevels Labeled vector with the default base level for categorical exposures.

tef If TRUE it computed the threshold for effective tests. verbose If set to TRUE is shows messages on progression.

ngroups Number of intervals to be used

intervals If "standard" all levels are kept, if "extreme" intermetiate levels are set to NA.

select Vector selecting thee xposures to be used.
drop If set to TRUE exposures are replaced

seed Numeric seed

lod.col Indicator of the column where the LOD is located pNA Maximum percentage allowed of values under LOD

tLog If set to TRUE it transforms all the exposures to lod before the imputation.

messages If set to TRUE messages from mice's function will be displayed.

phenotype Health outcome to be used as dependent variable.

exposure Vecror of exposures to be used.

th Threshold of P-Value used to considere normalit min.val Minimum number of observations to perform test

na.rm If set to TRUE removes NA values

npc Number of PC to be kept

pca Perform PCA (only numerical variables) or FAMD (numerical and categorical)

group Phenotype to group exposures group2 Phenotype to group exposures

scatter If set to true it shows the samples value in the plot

na.omit If set to TRUE, NA values are discarded

density If set to TRUE a desntiry plot is draw on the histogram

show. trans If set to TRUE, three extra plots are drawn with usual transformations

 $\begin{array}{ll} \text{x.max} & \text{Threshold for x axis (in \%)} \\ \text{sort} & \text{If set to TRUE, results are ordered} \end{array}$ 

set Cantake values "exposures" or "phentoypes".

output Can take values "n" (count) ot "p" (percentage)

fun Function to bt used in the transformation process

#### Value

An object of class ExposomeSet

#### Methods (by generic)

- plot(x = ExposomeSet, y = ANY): Wrapper for plotFamily method.
- clustering(ExposomeSet): Performs clustering on samples based on exposure levels.
- correlation(ExposomeSet): Computes correlation on exposures.
- dim(ExposomeSet): Returns the number of exsures, samples and phenotypes.
- expos(ExposomeSet): Returns a data.frame with exposures.
- exposureNames(ExposomeSet): Getter to obtain the exposures's names.
- exwas(ExposomeSet): Performs an EXposome-Wide Association Study
- familyNames(ExposomeSet): Getter to obtain the families's names of the family of each exposure.
- highAndLow(ExposomeSet): Performs a discretization of continuous exposures.
- ilod(ExposomeSet): Imputation of under-LOD values of exposures.
- imputation(ExposomeSet): Imputation of missing values of exposures.
- invExWAS(ExposomeSet): Performs an EXposome-Wide Association Study (modelling the exposures as response)
- mexwas(ExposomeSet): Performs a Multiple-EXposure-Wide Association Study.
- normalityTest(ExposomeSet): Test the normality of each exposure.
- pca(ExposomeSet): Performs a PCA
- phenotypeNames(ExposomeSet): Getter to obtain the phenotypes's names.
- plotFamily(ExposomeSet): Draws a boxplot or accumulated-bar plot for each exposure in a given family.
- plotHistogram(ExposomeSet): Draws an histogram of a given continuous exposure or a pie chart if a given categorycal exposure.
- plotLOD(ExposomeSet): Draws a barchart with the amount of under-LOD values.
- plotMissings(ExposomeSet): Draws a bar-plot with the amount of missing values.
- standardize(ExposomeSet): Standardization of exposures.
- Summary (ExposomeSet): Summary of both continuous and categorical exposures
- tableLOD(ExposomeSet): Returns a vector with the number of under-LOD values per exposure.
- tableMissings(ExposomeSet): Returns a vector with the number of missing values per exposure.
- trans(ExposomeSet): Transformation of exposures.

### **Slots**

assayData Contains the exposures matrix with column number equal to nrow(phenoData) (see eSet, AssayData).

featureData Contains the description of the exposures including the family where they belong (see eSet, AnnotatedDataFrame).

phenoData Contains the phenotypes or variables experimenter-supplied (see eSet, AnnotatedDataFrame).

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#### See Also

readExposome to create an ExposomeSet from files, loadExposome to create an ExposomeSet from data.frames

exposureNames

Getter to obtain the exposures's names of an ExposomeSet or ExposomePCA

# Description

Getter to obtain the exposures's names of an ExposomeSet or ExposomePCA

# Usage

exposureNames(object)

# **Arguments**

object

ExposomeSet that will be queried for the exposures's names.

# Value

The name of the exposures as a character vector.

# Warning

exposureNames collides with featureNames of eSet. Although in rexposome 1.0.0 both function can be used as synonyms, this usage is discouraged and it is not assured.

# See Also

phenotypeNames to get the phenotypes, familyNames to get the families of exposures

```
data("exposome")
exposureNames(expo)
```

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expo\_c

ExposomeClust for testing purpouses

# Description

ExposomeClust created from an ExposomeSet with full set of 104 exposures, 1200 simulated samples and 4 phenotypes (asthma status, BMI measure, sex, and age). The clustering was done using hclust and cutree with k = 3.

# Usage

```
data("eclust")
```

#### **Format**

An object of class ExposomeClust of dimension 99 x 1200 x 5.

#### Value

An ExposomeSet object.

#### **Examples**

```
data("eclust")
dim(expo_c)
table(classification(expo_c))
```

extract

Raw data from ExWAS, ExposomeClust and ExposomeCorr.

# **Description**

Returns internal table of results of objects of class ExWAS, ExposomeClust and ExposomeCorr.

# Usage

```
extract(object, ...)
```

### **Arguments**

object Object of class ExWAS, ExposomeClust or ExposomeCorr
... NO USED

# Value

A data. frame containing the raw result from PsyGeNET or a data. frame with the result Jaccard Index for each disease.

ExWAS

EXWAS Class ExWAS

# **Description**

Class ExWAS obtained from exwas method of an ExposomeSet object, contains the result of testing the association of exposures of an ExposomeSet to its phenotypes. "ExWAS" is the acronym of "Exposome-Wide Association Study". The function can be applied to one of to many phenotypes in the ExposomeSet object.

# Usage

```
## S4 method for signature 'ExWAS, ANY'
plot(x, y, ...)
## S4 method for signature 'ExWAS'
extract(object, sort = TRUE, ...)
## S4 method for signature 'ExWAS'
get_robust_sd(object, sort = TRUE, ...)
## S4 method for signature 'ExWAS'
names(x)
## S4 method for signature 'ExWAS'
plotEffect(x, y, select, labels, xlab, ylab)
## S4 method for signature 'ExWAS'
plotExwas(
  object,
  ...,
  subtitles,
  color,
  exp.order,
  labels,
  show.effective = TRUE
## S4 method for signature 'ExWAS'
plotVolcano(x, p.value = -log10(0.001), labels, show.effect = FALSE)
## S4 method for signature 'ExWAS'
tef(object)
```

### **Arguments**

```
    x An ExWAS object
    y An ExWAS object
    ... NOT USED
    object An object of class ExWAS, mExWAS or nlExWAS.
```

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sort If TRUE, the results are ordered by pvalue. (optional) Vector with the selected exposures select (optional) Character vector with the labels for each exposure. It must be labeled labels xlab (optional) Label for x-axis ylab (optional) Label for y-axis Character vector with the "subtitle" for each plot when given more than one subtitles ExWAS. color (optional) A vector of colors. The vector must have length equal to the number of families. The vector must be names with the name of the families. exp.order (optional) Order of the exposures. show.effective (default TRUE) draws a brown line on the threshold given by the effective number of tests. (default -log10(0.001)) Is the threshold from where the exposures can be taken p.value as significants.

#### Value

An object of class ExWAS

# Methods (by generic)

show.effect

- plot(x = ExWAS, y = ANY): Wrapper for plotExwas method.
- extract(ExWAS): Method to obtain the matrix of association scores
- get\_robust\_sd(ExWAS): Method to obtain the matrix of association scores

(default false) Apply exp to obtained beta.

- names (ExWAS): Method to obtain the Threshold for effective tests (TEF)
- plotEffect(ExWAS): Draws a plot with the confidence interval of each exposure. Alows to compare two ExWAS instances.
- plotExwas(ExWAS): Method to plot a manhatan plot for association between exposures and phenitypes
- plotVolcano(ExWAS): Method to plot a volcano plot for association between exposures and phenotypes
- tef(ExWAS): Method to obtain the Threshold for effective tests (TEF)

# Slots

effective Number containing the effective number of tests.

formula Tested formula.

comparison Result of performing the test to find association between levels of exposures and phenotype.

description Description of the exposures used in the ExWAS. (in description file).

### See Also

exwas to perform an Exposome-Wide Association Study and to create an ExWAS, mexwas to perform a Multivariate Exposome-Wide Association Study and to create a mExWAS

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exwas	Testing the association between an exposure and a phenotype of an ExposomeSet

#### **Description**

The exwas method performs an "Exposome-Wide Association Study" (ExWAS) using the exposures in ExposomeSet and one of its phenotype.

# Usage

```
exwas(
  object,
  formula,
  filter,
  family,
   ...,
  baselevels,
  tef = TRUE,
  verbose = FALSE,
  warnings = TRUE,
  robust = FALSE
)
```

# **Arguments**

object	ExposomeSet that will be used for the ExWAS.
formula	formula indicating the test to be done. If any exposure is included it will be used as covariate. exwas metho will perform the test for each exposure.
filter	expression to be used to filter the individuals included into the test.
family	Family of the distribution followed by the health outcome to be tested (gaussian, bionomal, check glm).
	NOT USED
baselevels	(optional) If set, must be a labeled vector with the default base level for categorical exposures.
tef	(default TRUE) If TRUE it computed the effective number of tests and the threhold for the effective number of tests. Usually it needs imputed data.
verbose	(default FALSE) If set o true messages along the tests are shown.
warnings	(default TRUE) If set to FALSE warnings will not be displayed.

#### Value

An codeExWAS object with the result of the association study

# References

An Environment-Wide Association Study (ExWAS) on Type 2 Diabetes Mellitus. Chirag J. Patel, Jayanta Bhattacharya, Atul J. Butte. May 20, 2010 Plos One

Evaluating the effective numbers of independent tests and significant p-value thresholds in commercial genotyping arrays and public imputation reference datasets. Miao-Xin Li, Juilian M. Y. Yeung, Stacey S. Cherny and Pak C. Sham. May 2012 Hum Genet.

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#### See Also

extract to obtain a table with the result of the ExWAS, plotExwas to plot the results of the ExWAS

# **Examples**

```
data(exposome)
w1 <- exwas(expo[1:5, ], asthma~1, family = "binomial")
w2 <- exwas(expo[1:5, ], asthma~sex+age, family = "binomial")
w3 <- exwas(expo[1:5, ], asthma~age, family = "binomial", filter = sex=="boy")</pre>
```

ex\_imp

imExposomeSet for testing purpouses

# **Description**

imExposomeSet created from the raw data included in the package. The creation process is ilustrated in the vignette.

# Usage

```
data("ex_imp")
```

# **Format**

An object of class imExposomeSet of dimension 47 x 109 x 10.

# Value

An imExposomeSet object.

# **Examples**

```
data("ex_imp")
ex_imp
```

familyNames

Getter to obtain the exposures's names of an ExposomeSet.

#### **Description**

This method returns the name of the families in an ExposomeSet, but it can return a vector, labeled with the exposures in the ExposomeSet, containing the family belonging to each exposure.

# Usage

```
familyNames(object, by.exposure = FALSE)
```

get\_robust\_sd

# **Arguments**

object ExposomeSet that will be queried for the exposures's family-names.

by exposure (default FALSE) If TRUE a vector labeled with each exposure name will be re-

turned with the family of each exposures. If FALSE a vector with the (unique)

name of the families of exposures will be returned.

### Value

The families of the exposures into the ExposomeSet, or the family of each exposure into the ExposomeSet.

#### See Also

exposureNames to get the name of the exposures, phenotypeNames to get the phenotypes

# **Examples**

```
data("exposome")
# Get families
familyNames(expo)
# Get the family of each exposure
familyNames(expo, by.exposure = TRUE)
```

get\_robust\_sd

Raw data from ExWAS

# Description

Returns internal table of robust SD of objects of class ExWAS

# Usage

```
get_robust_sd(object, ...)
```

# Arguments

object Object of class ExWAS

... NO USED

# Value

A data.frame containing the raw result from robust  $SD\,$ 

highAndLow 23

hi			

Function to convert continuous exposures to categorical exposures

# **Description**

This method allows to convert continuous exposures of an ExposomeSet to categorical exposures using the n-percentile groups, defined by ngroups argument. By default, all levels are kept but if intervals is set to "extrem", the levels between the extrems (aka. lowes and highest) are discarted and their values set to NA.

# Usage

```
highAndLow(
  object,
  ngroups = 3,
  intervals = "standard",
  select,
  drop = FALSE,
  warnings = TRUE
)
```

#### **Arguments**

object An object of class ExposomeSet.

ngroups (default 3) Number of intervals to be created.

intervals (default "standard") If set to "sctandard" all levels are set. If set to "extreme"

obly lowes and highest levels are kept (others are set to NA).

select (optional) Subset of exposures where the discretization is applied. If missing,

all exposures are used.

drop (default FALSE) If set to FALSE original exposures are kept and discretized ex-

posures are add to ExposomeSet. If set to TRUE, original exposures are replaced

by categorical exposures.

warnings (defaulr TRUE) If set to FALSE warnings are not shown.

#### Value

A new  ${\tt ExposomeSet}$  with categorical exposures.

# See Also

trans to transform exposures, standardize to standardize exposures.

```
# No drop
data("exposome")
exp.hl <- highAndLow(expo, intervals = "standard", select = "ldde_lip")
dim(exp.hl)
# exposures samples phenotyes
# 105 1200 4
dim(expo)</pre>
```

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```
# exposures samples phenotyes
# 104
                1200
# exps.hl has 107 exposures: the original 104 plus the new
         3 factored exposures
# Drop
exp.hl <- highAndLow(expo, intervals = "standard",</pre>
   select = "ldde_lip", drop = TRUE)
dim(exp.hl)
# exposures samples phenotyes
      104
dim(expo)
            samples phenotyes
# exposures
     104
             1200
```

ilod

Function to impute under-LOD values from an ExposomeSet

# **Description**

This function is a wrapper of the functions impute.MinProb from the package imputeLCMD.

# Usage

```
ilod(
  object,
  seed = 1234,
  lod.col = "LOD",
  pNA = 0.2,
  tLog = FALSE,
  method = "QRILC",
  warnings = TRUE,
  ...
)
```

#### **Arguments**

object	ExposomeSet which exposures will be imputed.
seed	(default 1234) Seed to make the imputation reproducible.
lod.col	(default "LOD") Name of the column in fData with the threshold of the LOD.
pNA	(default 0.2) Maximum percentage allowed of values under LOD
tLog	(default FALSE) If set to TRUE it transforms all the exposures to lod before the imputation.
method	(default "QRILC") Method to be used to impute the under-LOD values. Two allowed: QRILC method (value "QRILC") and stochastic minimal value approach (value "MinProb").
warnings	(default TRUE) If set to FALSE warnings will not be displayed.
	Arguments passed to impute.QRILC or impute.MinProb from imputeLCMD.

#### Value

A new ExposomeSet with the imputed exposures.

#### See Also

plotMissings to plot the missing data of an ExposomeSet, tableMissings to get a table with the missing data of an ExposomeSet

### **Examples**

```
## Not run:
#Being x an ExposomeSet
x <- ilod(x)
## End(Not run)</pre>
```

imExposomeSet

Class imExposomeSet

# **Description**

Class imExposomeSet was designed to store the exposures obtained after a multiple imputation process done using mice. The data.frame obtained from mice has the particulative to contain the columns .imp and .id joint to phenotypes and exposures. The slots assayData, featureData, and phenoData are coordinated.

# Usage

```
## S4 method for signature 'imExposomeSet, ANY'
plot(x, y, ...)
## S4 method for signature 'imExposomeSet'
dim(x)
## S4 method for signature 'imExposomeSet'
expos(object)
## S4 method for signature 'imExposomeSet'
exposureNames(object)
## S4 method for signature 'imExposomeSet'
extract(object, rid = -1, ...)
## S4 method for signature 'imExposomeSet'
exwas(
  object,
  formula,
  filter,
  family,
  baselevels,
```

```
tef = TRUE,
  verbose = FALSE,
  warnings = TRUE,
  robust = FALSE
## S4 method for signature 'imExposomeSet'
familyNames(object, by.exposure = FALSE)
## S4 method for signature 'imExposomeSet'
phenotypeNames(object)
## S4 method for signature 'imExposomeSet'
plotFamily(x, family, group, group2, scatter = FALSE, na.omit = TRUE)
## S4 method for signature 'imExposomeSet'
sampleNames(object)
## S4 method for signature 'imExposomeSet'
x[[i]]
## S4 method for signature 'imExposomeSet, ANY, ANY, ANY'
x[i, j, k, ..., drop = FALSE]
## S4 method for signature 'imExposomeSet'
toES(object, rid = 1)
```

# **Arguments**

warnings

X An imexposomeset object.	X	An imExposomeSet o	biect.
----------------------------	---	--------------------	--------

y NOT USED

... Other used arguments

object An object of class imExposomeSet

rid Number of the imputation to be extracted formula Formula, not including exposures, to be tested. filter Expression to be used to filter ExposomeSet

family Family descriving the nature of the health outcome

baselevels Labeled vector with the base-level of the categorical exposures tef If set to TRUE the threshold for effective test is computed.

If set to TRUE it shows warnings on progession.

verbose If set to TRUE it shows messages on progression.

by . exposure If set to TRUE ir returns the family which each exposure belongs

group Phenotype to group exposures

group2 NOT USED

scatter If set to true it shows the samples value in the plot

na.omit NOT USED

i Character coresponding to selected exposures.

•	C1 .	1.	1 . 1	1
7	Character corre	enonding to	selected s	ample names
	Character cont	sponding to	sciccica s	ampic mames.
<i>3</i>		1 0		1

k Character corresponding to selected phenotypes.

drop NOT USED

#### Value

An object of class imExposomeSet

# Methods (by generic)

- plot(x = imExposomeSet, y = ANY): Wrapper for plotFamily method.
- dim(imExposomeSet): Returns the number of exsures, samples and phenotypes.
- expos(imExposomeSet): Returns a data.frame with exposures.
- exposureNames(imExposomeSet): Method to obtain samples' names
- extract(imExposomeSet): Method to extract exposures for a single imputation
- exwas(imExposomeSet): Performs an EXposome-Wide Association Study
- familyNames(imExposomeSet): Getter to obtain the families's names of the family of each exposure.
- phenotypeNames(imExposomeSet): Getter to obtain the families's names of the family of each exposure.
- plotFamily(imExposomeSet): Draws a boxplot or accumulated-bar plot for each exposure in the all imputed sets.
- sampleNames(imExposomeSet): Method to obtain samples' names
- [[: Get an ExposomeSet with the selected imputation
- x[i: Subset an imExposomeSet
- toES(imExposomeSet): Returns an ExposomeSet with ethe given imputation.

# **Slots**

```
nimputation Number of imputations done with mice.
assayData data.frame containing .imp, .id and the exposures.
featureData data.frame containing the description of the exposures.
phenoData data.frame containing .imp, .id and the phenotypes.
```

# Note

Sample order is not guarantee

#### See Also

loadImputed to create an imExposomeSet from data.frames

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im	putation
T !!!	putation

Function to impute missing values from an ExposomeSet

# Description

This function is a wrapper of the functions mice and complete from the package mice. Also to the impute from the package Hmisc. The function is designed to use those functions to impute missing values on exposures (not in phenotypes).

# Usage

```
imputation(object, select, ..., messages = FALSE)
```

# **Arguments**

object ExposomeSet which exposures will be imputed.

select Exposures to be imputed. If missing, all exposes will be imputed.

... Argument given to function mice of pakcage mice (printFlag is set from messages).

messages

(default FALSE) If set to TRUE messages from mice's function will be displayed.

# Value

A new ExposomeSet with the imputed exposures.

# See Also

plotMissings to plot the missing data of an ExposomeSet, tableMissings to get a table with the missing data of an ExposomeSet

# **Examples**

```
## Not run:
#Being x an ExposomeSet
x <- imputation(x)
## End(Not run)</pre>
```

imputeLOD

Function to impute values under limit of detection

# Description

Homologous function to the ilod method of ExposomeSet for a given data. frame of exposures and a vector of threshold. The use of this function is related to HELIX Project.

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#### Usage

```
imputeLOD(
    x,
    lod,
    description = NULL,
    pNA = 0.2,
    pLOD = 0,
    log = TRUE,
    seed = NULL
)
```

# **Arguments**

x data.frame containing the exposures as columns and the samples as rows.

lod vectro containing the

description 1 means values under LOD while 2 means quantifiable value, 3

pNA (default: 0.2) maximum percentage of allowed missing data

pLOD (default: 0) minimum percentave of values under LOD

log (default: NA) log transformation to normalize data

seed (default: NULL)

#### Value

A new data. frame with the imputed exposures.

# **Examples**

invExWAS

Testing the association between an exposure and a phenotype of an ExposomeSet (modelling the exposures as response)

# Description

The invExWAS method performs an "Exposome-Wide Association Study" (ExWAS) using the exposures in ExposomeSet and one of its phenotype. (modelling the exposures as response)

# Usage

```
invExWAS(object, formula, filter, tef = TRUE, verbose = FALSE, warnings = TRUE)
```

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# **Arguments**

object	ExposomeSet that will be used for the ExWAS.
formula	formula indicating the test to be done. If any exposure is included it will be used as covariate. exwas metho will perform the test for each exposure.
filter	expression to be used to filter the individuals included into the test.
tef	(default TRUE) If TRUE it computed the effective number of tests and the threhold for the effective number of tests. Usually it needs imputed data.
verbose	(default FALSE) If set o true messages along the tests are shown.
warnings	(default TRUE) If set to FALSE warnings will not be displayed.

#### Value

An codeExWAS object with the result of the association study

#### See Also

extract to obtain a table with the result of the ExWAS, plotExwas to plot the results of the association

# **Examples**

```
data(exposome)
w1 <- invExWAS(expo, ~BMI)
w2 <- invExWAS(expo, ~BMI + sex)
plotExwas(w1, w2)</pre>
```

 ${\tt loadExposome}$ 

Creation of an ExposomeSet from data.frames

# Description

Given three data. frames that defines the exposome (measures of exposome, exposome description and individuals phentype) it loads them and creates an object of type ExposomeSet.

# Usage

```
loadExposome(
  exposures,
  description,
  phenotype,
  description.famCol = "family",
  exposures.asFactor = 5,
  warnings = TRUE
)
```

loadExposome 31

#### **Arguments**

exposures data.frame of exposures.

description data. frame with the description of the exposures (relation between exposures

and exposure-family).

phenotype data. frame with the phenotypes of interest.

description.famCol

(default "family") Index where the family's name (per exposures) if found in

file "description". It can be both numeric or character.

exposures.asFactor

(default 5) The exposures with more than this number of unique items will be considered as "continuous" while the exposures with less or equal number of

items will be considered as "factor".

warnings (default TRUE) If TRUE shows useful information/warnings from the process of

loading the exposome.

#### **Details**

The rows of the exposure's data.frames, that corresponds to samples' names, must be the same than the phenotype's data.frames. In the same way, the columns in exposure's data.frames must be the same in description data.frame.

#### Value

An object of class ExposomeSet.

### Note

ExposomeSet's fData will contain some inner columns called .std, .trn, .fct and .type in order to trace the transformations an exposure suffers and to know, at eny moment, if an exposure is categorical or continuous. The "description" file can contains a column called type with values "factor" and "numeric" to speficy how an exposure needs to be understood. If given, this column will be renamed to .type. If not given, it will be created using exposures.asFactor value.

#### See Also

ExposomeSet for class description, readExposome for constructor from txt/csv files.

```
path <- file.path(path.package("rexposome"), "extdata")
description <- file.path(path, "description.csv")
phenotype <- file.path(path, "phenotypes.csv")
exposures <- file.path(path, "exposures.csv")
dd <- read.csv(description, header=TRUE)
ee <- read.csv(exposures, header=TRUE)
pp <- read.csv(phenotype, header=TRUE)
rownames(dd) <- dd[, 2]
dd <- dd[, -2]
rownames(ee) <- ee[ , 1]
ee <- ee[ , -1]
rownames(pp) <- pp[ , 1]
pp <- pp[ , -1]
exp <- loadExposome(</pre>
```

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```
exposures = ee,
description = dd,
phenotype = pp,
description.famCol = "Family"
)
```

loadExposome\_plain

Creation of an ExposomeSet from single data.frame

# Description

Creation of an ExposomeSet from single data.frame

# Usage

```
loadExposome_plain(
  data,
  data_id,
  sep = ",",
  pheno_cols,
  na.strings = c("NA", "-", "?", " ", ""),
  families = NULL,
  exposures.asFactor = 5,
  warnings = TRUE
)
```

# Arguments

warnings

data	data.frame With the exposures and phenotypes (in no particular order!) or string with the path to a file (.csv, .tsv, .txt) with the table of exposures and phenotypes	
data_id	character Name of the column on the selected table that contains the ID	
sep	character (default ",") Separator used by read. table to load the files "exposures", "description" and "phenotype". Only applies when providing a path on the data argument	
pheno_cols	character Character vector of the phenotype columns (all the other columns are considered exposures)	
na.strings	character (default c("NA", "-", "?", "", "")) Character defining the NA values in expsome's files.	
families	list (default NULL) List to specify the families of the exposures, construct it as: list(Family1 = c("exposure_1_1", "exposure_1_2", "exposure_1_n"), Family2 = c("exposure_2_1", "exposure_2_2", "exposure_2_n"), FamilyM = c("exposure_M_1", "exposure_M_2", "exposure_M_n")). All the exposures on the data table have to be on this provided list with their respective families. The family classification is optional, input NULL to bypass the family classifier	
exposures.asFactor		
	numeric (default 5) The exposures with more than this number of unique items	

will be considered as "continuous" while the exposures with less or equal num-

(default TRUE) If TRUE shows useful information/warnings from the process of

ber of items will be considered as "factor".

loading the exposome.

loadImputed 33

#### Value

An object of class ExposomeSet.

#### **Examples**

```
path <- file.path(path.package("rexposome"), "extdata")
phenotype <- file.path(path, "phenotypes.csv")
exposures <- file.path(path, "exposures.csv")
ee <- read.csv(exposures, header=TRUE)
pp <- read.csv(phenotype, header=TRUE)
# Create fake dataset with exposures and phenotypes combined
data <- cbind(ee, pp)

loadExposome_plain <- function(data, data_id = "idnum",
pheno_cols = c("rhinitis", "wheezing", "sex", "age", "cbmi", "blood_pre", "whistling_chest", "flu"))</pre>
```

loadImputed

Creation of an imExposomeSet from data.frames

# **Description**

Given a data.frame from code with the multiple imputations of both exposures and phenotypes, join with a data.frame with exposures' description, and object of class imExposomeSet is created.

### Usage

```
loadImputed(
  data,
  description,
  description.famCol = "family",
  description.expCol = "exposure",
  exposures.asFactor = 5,
  warnings = TRUE
)
```

#### **Arguments**

data The data.frame of both exposures and phentoypes obtained from mice.

description data.frame with the description of the exposures (relation between exposures

and exposure-family).

description.famCol

(default "family") Index where the family's name (per exposures) if found in file "description". It can be both numeric or character.

description.expCol

(default "exposures") Index where the exposure's name if found in file "description". It can be both numeric or character.

exposures.asFactor

(default 5) The exposures with more than this number of unique items will be considered as "continuous" while the exposures with less or equal number of items will be considered as "factor".

warnings (defaul

(default TRUE) If TRUE shows useful information/warnings from the process of loading the exposome.

me me

#### **Details**

The coordination of the information is based in the columns .imp and .id from the data.frame obtained from mice. The division of exposures and phenotypes is based in description data.frame, that are the exposures. Hence, the elements in the main data.frame that are not in the description, are the phentoypes.

#### Value

An object of class imExposomeSet.

#### See Also

imExposomeSet for class description

### **Examples**

```
data("me") # me is an imputed matrix of exposure and phenotyes
path <- file.path(path.package("rexposome"), "extdata")
description <- file.path(path, "description.csv")
dd <- read.csv(description, header=TRUE, stringsAsFactors=FALSE)
dd <- dd[dd$Exposure %in% colnames(me), ]
ex_imp <- loadImputed(data = me, description = dd,
description.famCol = "Family",
description.expCol = "Exposure")</pre>
```

me

data.frame for testing purpouses

# Description

data.frame created with mice used to test and ilustrate the creation of imExposomeSet.

# Usage

```
data("me")
```

# **Format**

An object of class data. frame with 654 rows and 57 columns.

# Value

```
A data.frame.
```

```
data("me")
dim(me)
colnames(me)
```

mExWAS 35

mExWAS Class mExWAS

# **Description**

Class mExWAS obtained from mexwas method of an ExposomeSet object, contains the result of testing the multiple models of exposures of an ExposomeSet to a set of given phenotypes. "mExWAS" is the #' acronym of "Multivariate Exposome-Wide Association Study".

# Usage

```
## S4 method for signature 'mExWAS,ANY'
plot(x, y, ...)

## S4 method for signature 'mExWAS'
extract(object, type = "test", sort = TRUE)

## S4 method for signature 'mExWAS'
plotExwas(
  object,
    ...,
  subtitles,
  color,
  exp.order,
  labels,
  show.effective = TRUE
)
```

# **Arguments**

X	Object of class mExWAS
У	NOT USED
	Other used arguments.
object	object of class mExWAS.
type	(default "test"). Can take "test" or "raw" to obtain a data. frame of glmnet result.
sort	NOT USED
subtitles	NOT USED
color	NOT USED
exp.order	NOT USED
labels	NOT USED
show.effective	NOT USED

# Value

An object of class mExWAS

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# Methods (by generic)

- plot(x = mExWAS, y = ANY): Wrapper for plotExwas method.
- extract(mExWAS): Method to obtain the generated model
- plotExwas(mExWAS): Method to plot a heap-map with the coeficient of each exposure

#### **Slots**

```
result klist with the fitted model and result.

phenotype Name of the phenotype used in the analysys.

description feature data from original ExposomeSet.
```

# See Also

mexwas to perform a Multivariate Exposome-Wide Association Study and to create a mExWAS, exwas to perform an Exposome-Wide Association Study and to create an ExWAS

mexwas	Testing the association between an exposure and a phenotype of an
	ExposomeSet using a multivariate aproach.

### **Description**

The mexwas method performs an "Multi Exposome-Wide Association Study" (m-ExWAS) using the exposures in ExposomeSet and one of its phenotype. It uses the packages glmnet and partDSA.

#### Usage

```
mexwas(object, phenotype, family, warnings = TRUE)
```

#### **Arguments**

object	ExposomeSet that will be used for the ExWAS.
phenotype	Target phenotype used for the study. If missing all the phenotypes in the ExposomeSet will be used.
family	It must decrive the nature of the outcome. Can take values "gaussian", "binomial", "poisson", "multinomial", "cox" or "mgaussian".

warnings (default TRUE) If set to FALSE warnings will not be displayed.

# Value

Returns an object of class mExWAS

#### See Also

extract to obtain a table with the result of the ExWAS, plotExwas to plot the results of the ExWAS

```
data("exposome")
wt <- mexwas(expo[3:7, 1:100], phenotype = "asthma", family = "binomial")</pre>
```

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ndim

Number of principal components in an ExposomePCA.

## **Description**

Number of principal components in an ExposomePCA.

## Usage

```
ndim(object)
```

#### **Arguments**

object

ExposomePCA to obtain the number of components.

## Value

The number of components in the ExposomePCA.

#### See Also

plotPCA to plot the PCA values of an ExposomePCA, clustering to see how the exposures can cluster samples, correlation to compute the correlation between exposures

# **Examples**

```
data("exposome")
epca <- pca(expo[3:7, 1:100])
ndim(epca)</pre>
```

 ${\tt normalityTest}$ 

It creates a data. frame of boolean indicating if the exposures follows a normal distribution or not.

# Description

This functions uses shapiro.test to test the normality of the exposures and returns a data.frame with a boolean value and a p-value for each exposure.

```
normalityTest(
  object,
  exposure,
  th = 0.05,
  min.val = 5,
  na.rm = TRUE,
  warnings = TRUE
```

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# Arguments

object	ExposomeSet with the exposome to be tested.
exposure	Name of the exposure to be tested, if missing all the exposures will be tested.
th	(by default $0.05$ ) Threshold to considere an exposure to follow a normal distribution.
min.val	(by default 5) Minimum number of values not missings to test the exposures.
na.rm	(by default TRUE) Removes the NA values to test the normality on the exposure.
warnings	(by default: TRUE) Show warnings if required.

#### Value

A data.frame with three columns: exposure, normality and p.value. "exposure" column contains the name of each exposure. "normalty" column contains a logical value indicating if the obtained p-value is under the given threshold. "p.value" column contains the obtained p-value from shapiro.test.

#### See Also

plotHistogram to draw the shape of an exposure, plotMissings to draw a plot with the missing data an ExposomeSet, imputation to impute missing data on the exposures of an ExposomeSet

# **Examples**

```
data("exposome")
normalityTest(expo)
```

рса

Creation of an ExposomePCA from an ExposomeSet.

#### **Description**

Method to calculate a PCA based on the exposures of an ExposomeSet. Only numerical-exposures (non categorical) will be computed. The function resurns an ExposomePCA object. This PCA is performed by using FactoMineR package.

## Usage

```
pca(object, npc = 10, pca = FALSE, ...)
```

# Arguments

object	ExposomeSet which exposures will be used for the PCA
npc	(by default 10) number of dimensions kept in the results
рса	(default FALSE) Set to TRUE to Perform PCA (only numerical variables) or FALSE to perform FAMD (numerical and categorical)
	Arguments to be passed to imputeFAMD

## Value

An ExposomePCA with the values of the PCA.

phenotypeNames 39

#### See Also

plotPCA to plot the PCA values of an ExposomePCA, clustering to see how the exposures can cluster samples, correlation to compute the correlation between exposures

# **Examples**

```
data("exposome")
epca <- pca(expo[12:20, ])</pre>
```

phenotypeNames

Getter to obtain the phenotype's names of an ExposomeSet or ExposomePCA.

## **Description**

Getter to obtain the phenotype's names of an ExposomeSet or ExposomePCA.

## Usage

```
phenotypeNames(object)
```

# Arguments

object

ExposomeSet that will be queried for the phenotype's names.

## Value

The name of the phenotypes as a a character vector.

## See Also

exposureNames to get the name of the exposures, familyNames to get the families of exposures

```
data("exposome")
phenotypeNames(expo)
```

40 plot3PCA

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Ploting PCA in a 3D space

#### **Description**

Methdo to draw a plot for samples using three PC contained in an ExposomePCA

# Usage

```
plot3PCA(
  object,
  cmpX,
  cmpY,
  cmpZ,
  phenotype,
  main,
  angle = 35,
  pch = 16,
  legend = TRUE,
  plines = TRUE
)
```

## **Arguments**

object	An onbject of class ExposomePCA
cmpX	Component to be placed at X axis
cmpY	Component to be placed at Y axis
cmpZ	Component to be placed at Z axis
phenotype	Used to color samples by phentoype
main	Title for the plot

angle (default 35) angle between x and y axis.

pch (default 16) plotting "character", i.e. symbol to use.

legend (default TRUE) If TRUE shows the legend.

plines (default TRUE) If TRUE it draws the lines from each dot to the base plane.

# Value

A list with different graphics option from scatterplot3d.

## See Also

```
pca to compite PCA on an ExposomeSet, plotPCA to plot the PCA, ExposomePCA as main class data("exposome") epca <- pca(expo[3:7, 1:100]) plot3PCA(epca, cmpX = 1, cmpY = 2, cmpZ = 3, phenotype = "sex")
```

plotClassification 41

plotClassification	Draw the profile of the levels exposures after a classification with a
	clustering method

# Description

Draw the profile of the levels exposures after a classification with a clustering method

## Usage

```
plotClassification(object, type = "heatmap", ...)
```

## **Arguments**

```
object Object of class Exposomeclust
type Two types are available: "heatmap" or "valuemap".
... NOT USED
```

## Value

A list with different graphics parameters.

#### See Also

clustering as a constructor for ExposomeClust, classification to see how to obtain the classification of the samples from an ExposomeClust

# **Examples**

```
## Not run:
data("eclust")
plotClassification(expo_c)
## End(Not run)
```

plotCorrelation

It draws both circos or matrix plot for the correlation in ExposomeCorr

# Description

While the circos plot can be used to see the general behaviours intra and extra families of exposures, the matrix plot allows for a detailed view of the correlations within an ExposomeCorr object.

```
plotCorrelation(object, type = "circos", ...)
```

42 plotEffect

## **Arguments**

object ExposomeCorr which correlations will be plotted.

type (default "circos") Can take both "circos" or "matrix".

... Arguments given to corrplot of package corrplot if a matrix is draw. Moreover

extra arguments are can be passed to inner functions to draw both the matrix and

the circos of correlations.

#### Value

A list with different graphics parameters.

#### See Also

correlation as a constructor for ExposomeCorr objects, pca to compute PCA on exposures

## **Examples**

```
data("exposome")
expo.c <- correlation(expo)
plotCorrelation(expo.c, type="circos")
plotCorrelation(expo.c, type="matrix")</pre>
```

plotEffect

Function to draw a plot of the pvalues stored in an ExWAS object

# Description

This function draws a sort of manhattan plots using the p-value of the association of the exposures with phenotypes of an ExWAS object.

## Usage

```
plotEffect(x, y, select, labels, xlab, ylab)
```

## **Arguments**

x An ExWAS object which effect will be ploted
---

y (optional) Another ExWAS object. If provded its effects will be ploted in Y-axis.

select (optional) Character with exposures to be shown.

labels (optional) Character vector with the labels for each exposure. It must be labeled

vector.

xlab (optional) Label for X-axis. ylab (optional) Label for Y-axis.

## Value

An object of class ggplot.

plotEXP 43

#### See Also

exwas as a constructor for ExWAS objects, extract to obtain a table with the result of the ExWAS

## **Examples**

```
data(exposome)
w1 <- exwas(expo[1:5, ], asthma~1, family = "binomial")
w2 <- exwas(expo[1:5, ], asthma~sex+age, family = "binomial")
plotEffect(w1, w2)</pre>
```

plotEXP

Plot correlation between exposures and PCA

# Description

Function used to plot the correlation between the exposures in an ExposomePCA and the values for each component of the PCA in the same ExposomePCA

## Usage

```
plotEXP(object, exposure)
```

# **Arguments**

object An object of class ExposomePCA

exposure (optional) to select a set of exposures to be ploted. If not given all are used.

## Value

An object of class ggplot.

# See Also

pca to compute PCA on an ExposomeSet, plotPHE to plot the P-Value of association between phenotypes ans PCA, ExposomePCA as main class

```
data("exposome")
epca <- pca(expo[3:7, 1:100])
plotEXP(epca)</pre>
```

44 plotExwas

Function to draw a plot of the pvalues stored in an ExWAS object

# Description

This function draws a sort of manhattan plots using the p-value of the association of the exposures with phenotypes of an ExWAS object.

# Usage

```
plotExwas(
  object,
  ...,
  subtitles,
  color,
  exp.order,
  labels,
  show.effective = TRUE
)
```

# Arguments

object	An ExWAS object which p-values will be plotted.
	Other objects of class ExWAS.
subtitles	(optional) Characters used as "substitle" when more than one ExWAS is given.
color	(optional) Character vector of HTML colors, labeled with family's names. Used to colore the exposures.
exp.order	(optional) Character vector of exposures used to order and subset the plot.
labels	(optional) Character vector with the labels for each exposure. It must be labeled vector.
show.effective	$(default\ TRUE)\ If\ set\ to\ FALSE,\ line\ showing\ effective\ test\ threshold\ is\ not\ shown.$

# Value

An object of class ggplot.

## See Also

exwas as a constructor for ExWAS objects, extract to obtain a table with the result of the ExWAS

```
data(exposome)
w1 <- exwas(expo[1:5, ], asthma~1, family = "binomial")
plotExwas(w1)</pre>
```

plotFamily 45

plotFamily	It draws the profile of the exposome in an ExposomeSet	

# Description

This function draw a profile of the full exposome into an ExposomeSet or the profile of the exposures in a specific family. For continuous families, box-plots are drawn; while for categorical families accumulative bar-charts.

# Usage

```
plotFamily(x, family, group, group2, scatter = TRUE, na.omit = TRUE)
```

## **Arguments**

x	ExposomeSet which exposome will be plotted.
family	Name of the familty that will be drawn. 'all' is allowed to draw a grid with all the families.
group	If set it displays the family grouped by the given phenotype.
group2	If set it displays the family grouped by the given phenotype.
scatter	(default TRUE) If the family to be plotted is continuous, the samples will be shown.
na.omit	(default TRUE) Do not show NA values.

#### Value

A ggplot object if a family was selected. invisible() if argument family was set to "all".

# See Also

plotHistogram to draw the shape of an exposure, plotMissings to plot the missing data from an ExposomeSet

```
data("exposome")
plt <- plotFamily(expo, family = "Metals")
plt <- plt + ggplot2::ggtitle("Metals")
plt
plt <- plotFamily(expo, family = "Indoor air")
plt <- plt + ggplot2::ggtitle("Indoor air")
plt</pre>
```

46 plotLOD

plotHistogram	It draws a histogram for each exposure in an ExposomeSet	
plotHistogram	It draws a histogram for each exposure in an ExposomeSet	

## **Description**

It draws a grid with an histogram per exposure in an ExposomeSet.

# Usage

```
plotHistogram(x, select, density = TRUE, show.trans = FALSE)
```

# **Arguments**

x ExposomeSet which exposome will be plotted.

select Name fo the exposure to be plotted. If missing, all exposures will be used. density (default TRUE) If TRUE a density plot is drawn overlapping the histogram.

show.trans (default FALSE) If set to TRUE it will draw a panel of auxiliar plots with the

continuous exposure transformed with log and sqrt.

#### Value

A ggplot object.

## See Also

plotFamily to draw the profile of a family of exposures, plotMissings to plot the missing data from an ExposomeSet

# Examples

```
data("exposome")
plotHistogram(expo[1:3, ], select = "ldde_lip")
```

plotLOD	It draws a chart with the percentage of under-LOD values in an Expo-
	someSet

## **Description**

This function can be used to draw the amount of under-LOD values in the exposures of an ExposomeSet.

```
plotLOD(object, lod.col = "LOD", x.max = 100, sort = TRUE)
```

plotMissings 47

#### **Arguments**

object ExposomeSet which exposome will be plotted.

lod.col (default "LOD") Name of the column in fData containing the LOD thresholds.

x.max (default 100) Fix the maxium value of the X-axis.

sort (default TRUE) If TRUE the chart will be ordered from the features with less miss-

ing data to the ones with more under-LOD values.

#### Value

A ggplot object.

#### See Also

plotFamily to draw the profile of a family of exposures, plotHistogram to draw the shape of an exposure, tableMissings to get a table with the missing data of an ExposomeSet, imputation to impute missing data on the exposures of an ExposomeSet

## **Examples**

```
data("exposome")
# The included has no missing data
plotLOD(expo)
```

plotMissings

It draws a chart with the percentage of missing in an ExposomeSet

## **Description**

This function can be used to draw the number of missing data in exposures and in phenotypes of an ExposomeSet.

# Usage

```
plotMissings(object, set, x.max = 100, sort = TRUE)
```

# **Arguments**

object ExposomeSet which exposome will be plotted.

set Can be set to "exposures" or to "phenotypes".

x.max (default 100) Fix the maxium value of the X-axis.

sort (default TRUE) If TRUE the chart will be ordered from the features with less miss-

ing data to the ones with more missing data.

## Value

A ggplot object.

48 plotPCA

#### See Also

plotFamily to draw the profile of a family of exposures, plotHistogram to draw the shape of an exposure, tableMissings to get a table with the missing data of an ExposomeSet, imputation to impute missing data on the exposures of an ExposomeSet

## **Examples**

```
data("exposome")
# The included has no missing data
plotMissings(expo, set = "exposures")
plotMissings(expo, set = "phenotypes")
```

plotPCA

Ploting PCA

## **Description**

Methdo to draw a plot for PCA contained in an ExposomePCA

# Usage

```
plotPCA(
  object,
  set,
  cmpX = 1,
  cmpY = 2,
  show.exposures = FALSE,
  show.samples = FALSE,
  phenotype
)
```

#### **Arguments**

```
object An onbject of class ExposomePCA
```

set Group ("all", "samples" or "exposures") taht will be ploted.

cmpX (default: 1) component to be placed at X axis cmpY (default: 2) component to be placed at Y axis

show.exposures (default: FALSE) If set to true, labels indicating the exposures are shown.

show.samples (default: FALSE) If set to true, labels indicating the samples are shown.

phenotype If set is set to "samples" can be used to color samples by phenotype

## Value

An object of class ggplot or an object of class gtable if argument set was set to "all".

# See Also

pca to compite PCA on an ExposomeSet, plotPCA to plot the PCA, ExposomePCA as main class

plotPHE 49

#### **Examples**

```
data("exposome")
epca <- pca(expo[3:7, 1:100])
# A grid with exposures space, samples space and explained variance
plotPCA(epca, set = "all")
# Only exposures space
plotPCA(epca, set = "exposures") + ggplot2::theme(legend.position = "bottom")
# Only samples space
plotPCA(epca, set = "samples")
# Only samples space but coloured by phenotype
plotPCA(epca, set = "samples", phenotype = "sex") +
ggplot2::theme(legend.position = "bottom")</pre>
```

plotPHE

Plot association score between phentoypes and PCA

## **Description**

Function used to plot the association between the phentoypes in an ExposomePCA and the values for each component of the PCA in the same ExposomePCA

## Usage

```
plotPHE(object, phenotype, exp2fac = 5)
```

# **Arguments**

object An object oc class ExposomePCA

phenotype (optional) to select a set of phenotypes to be ploted. If not given all are used.

exp2fac (default, 5) Threshold to considere a phentoype categorical (less or equal to) or

continuous (more than).

## Value

An object of class ggplot.

## See Also

pca to compute PCA on an ExposomeSet, plotEXP to plot the correlation between exposures ans PCA, ExposomePCA as main class

```
data("exposome")
epca <- pca(expo[3:7, 1:100])
plotPHE(epca)</pre>
```

50 readExposome

plotVolcano Function to draw a plot of the pvalues stored in an ExWAS object
--

# Description

This function draws a sort of manhattan plots using the p-value of the association of the exposures with phenotypes of an ExWAS object.

## Usage

```
plotVolcano(x, p.value = -log10(0.001), labels, show.effect = FALSE)
```

## **Arguments**

X	An ExWAS object which effect will be ploted.
p.value	(default "-log10(0.001)") Threshold for P-Value.
labels	(optional) Character vector with the labels for each exposure. It must be labeled vector.
show.effect	(default FALSE) Applyes an exponential transformation on the effects of the exposures.

#### Value

An object of class ggplot.

#### See Also

exwas as a constructor for ExWAS objects, extract to obtain a table with the result of the ExWAS, plotEffect to see or compare effects of one or two models.

readExposome	Creation of an ExposomeSet from files

# Description

Given the files that defines the exposome (measures of exposome, exposome description and individuals phentype) it loads them and creates an object of type ExposomeSet.

```
readExposome(
  exposures,
  description,
  phenotype,
  sep = ",",
  na.strings = c("NA", "-", "?", " ", ""),
  exposures.samCol = "sample",
  description.expCol = "exposure",
  description.famCol = "family",
```

readExposome 51

```
phenotype.samCol = "sample",
  exposures.asFactor = 5,
  warnings = TRUE
)
```

## **Arguments**

exposures String with the path to the file with the matrix of exposures.

description String with the path to the file with the description of the exposures (relation

between exposures and exposure-family).

phenotype String with the path to the file with the phenotypes of interest.

sep (default ", ") Separator used by read.table to load the files "exposures", "de-

scription" and "phenotype".

na.strings (default c("NA", "-", "?", "", "")) Character defining the NA values in exp-

some's files.

exposures.samCol

(default "sample") Index where the samples' name are found in file "expo-

sures". It can be both character or numeric.

description.expCol

(default "exposure") Index where the exposures' name are found in file "de-

scription". It can be both numeric or character.

description.famCol

(default "family") Index where the family's name (per exposures) if found in

file "description". It can be both numeric or character.

phenotype.samCol

(default "sample") Index where the sample's name are found in file "pheno-

type". It can be both numeric or character.

exposures.asFactor

(default 5) The exposures with more than this number of unique items will be considered as "continuous" while the exposures with less or equal number of

items will be considered as "factor".

warnings (default TRUE) If TRUE shows useful information/warnings from the process of

loading the exposome.

#### **Details**

The rows of the exposure's file, that corresponds to samples' names, must be the same than the phenotype's file. In the same way, the columns in exposure's file must be the same found as rows in description file.

#### Value

An object of class ExposomeSet.

#### Note

ExposomeSet's fData will contain some inner columns called .std, .trn, .fct and .type in order to trace the transformations an exposure suffers and to know, at eny moment, if an exposure is categorical or continuous. The "description" file can contains a column called type with values "factor" and "numeric" to speficy how an exposure needs to be understood. If given, this column will be renamed to .type. If not given, it will be created using exposures.asFactor value.

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#### See Also

ExposomeSet for class description, loadExposome for constructor from loaded data. frames

#### **Examples**

```
## Locate the data-files
path <- file.path(path.package("rexposome"), "extdata")
description <- file.path(path, "description.csv")
phenotype <- file.path(path, "phenotypes.csv")
exposures <- file.path(path, "exposures.csv")

## Create ExposomeSet from files
exp <- readExposome(
    exposures = exposures,
    description = description,
    phenotype = phenotype,
    exposures.samCol = 1,
    description.famCol = 2,
    description.famCol = 1,
    phenotype.samCol = 1
)</pre>
```

rexposome

rexposome: Package for exposome exploration and outcome data analysis

#### **Description**

#' @section exposures loading and exposures management: rexposome offers two methods to bring exposome data to R and Bioconductor. readExposome allows to read three txt-like files (.csv, .tsv, ...) while loadExposome is sued with matrix and data.frames. The class obtained is an ExposomeSet, a class based in eSet for exposome data management.

#### exposures processing

The packages offers a wide set of functions to preprocess exposome data. Method trans allow to transforms the exposures, method normalityTest allows to check for normality in exposome, standardize allows to standardize the exposures, among others. Finally, impute and ilod allow tu use mice, Hmisc and imputeLCMD for exposure missing data and exposure under-lod data imputation.

#### exposures analyses

the two methods exwas and mexwas allows to test the association between exposures and health outcomes (phenotpe data).

## exposures plotting

The methods plotFamily allows to see how the exposures behaves within families. plotCorrelation helps to understand how exposures are related between themselves. plotClassification allos to visually detect cuslters of samples that share the same pattern of levels of exposures.

standardize 53

standardize

#' Summary of an ExposomeSet. #' #' Given an ExposomeSet is shows a summary for its exposures or #' its phenotypes. #' #' @name Summary #' @rdname Summary-methods #' @aliases Summary #' @param object codeExposomeSet with 'set' will be summarized. #' @param set Set to be sumarized ("exposures" or "phenotypes"). #' @param select Subseting of exposures of phenotypes. #' @return A basic description of the exposures in the ExposomeSet #' @examples #' data("exposome") #' Summary(expo, set = "exposures") #' @export Summary setGeneric("Summary", function(object, set=c("exposures", "phenotypes"), select) standardGeneric("Summary") ) Standardize of an ExposomeSet.

#### **Description**

Given an ExposomeSet it standardizes the exposures by using mean/sd if method is "normal" or by using median/mad if method is "robust".

#### Usage

```
standardize(object, select, method = "normal", na.rm = TRUE, warnings = TRUE)
```

## **Arguments**

object	ExposomeSet with exposures to be standardized.
select	Subseting of exposures of phenotypes.
method	(default "normal") Character selecting the method to be applied ("normal" "iqr" or "robust").
na.rm	(by default TRUE) Removes NA data to perform standardization.
warnings	(defaulr TRUE) If set to FALSE warnings are not shown.

## Value

An ExposomeSet with the selected exposures standardized and keeping the others exposures as the original input object.

#### See Also

highAndLow to transform the continuous exposures to levelled factors, trans to transform the exposures

```
data("exposome")
exp.sn <- standardize(expo, method = "normal", select = "lbde100_lip")
exp.rs <- standardize(expo, method = "iqr", select = "lbde100_lip")
exp.rs <- standardize(expo, method = "robust", select = "lbde100_lip")</pre>
```

54 tableMissings

tableLOD	It creates a vector with the amount of under-LOD exposures in an ExposomeSet

## **Description**

This function can be used to obtain a table with the under-LOD data in exposures of an Exposome-Set.

## Usage

```
tableLOD(object, output = "n", lod.col = "LOD", sort = TRUE)
```

## **Arguments**

object	ExposomeSet which exposome will be plotted.
output	(default "n") Can be "n" for number of values, and "p" for percentage.
lod.col	(default "LOD") Name of the column in fData containing the LOD thresholds.
sort	(default TRUE) If TRUE the chart will be ordered from the features with less missing data to the ones with more under-LOD values.

#### Value

A numeric vector with number of udner-LOD values per exposure. The vector is labeled with the exposure's names.

#### See Also

plotFamily to draw the profile of a family of exposures, plotHistogram to draw the shape of an exposure, plotMissings to draw a plot with the missing data an ExposomeSet, imputation to impute missing data on the exposures of an ExposomeSet

# **Examples**

```
data("exposome")
# The included has no missing data
tableLOD(expo, output = "n")
```

tableMissings

It creates a vector with the amount of missing in an ExposomeSet

# Description

This function can be used to obtain a table with the missing data in exposures and in phenotypes of an ExposomeSet.

```
tableMissings(object, set, output = "n", sort = TRUE)
```

tef 55

## **Arguments**

object ExposomeSet which exposome will be plotted.

set Can be set to "exposures" or to "phenotypes".

output (default "n") Can be "n" for number of values, and "p" for percentage.

sort (default TRUE) If TRUE the chart will be ordered from the features with less miss-

ing data to the ones with more missing data.

#### Value

A numeric vector with number of missing values per exposure. The vector is labeled with the exposure's names.

#### See Also

plotFamily to draw the profile of a family of exposures, plotHistogram to draw the shape of an exposure, plotMissings to draw a plot with the missing data an ExposomeSet, imputation to impute missing data on the exposures of an ExposomeSet

## **Examples**

```
data("exposome")
# The included has no missing data
tableMissings(expo, set = "exposures")
tableMissings(expo, set = "phenotypes")
```

tef

Function to get the Threshold for effective tests (TEF)

#### **Description**

Function to get the Threshold for effective tests (TEF)

# Usage

```
tef(object)
```

## **Arguments**

object An ExWAS object

#### Value

A number indicating the efective threshold.

## References

Evaluating the effective numbers of independent tests and significant p-value thresholds in commercial genotyping arrays and public imputation reference datasets. Miao-Xin Li, Juilian M. Y. Yeung, Stacey S. Cherny and Pak C. Sham. May 2012 Hum Genet.

56 trans

#### See Also

exwas as a constructor for ExWAS objects

## **Examples**

```
data(exposome)
w1 <- exwas(expo[1:5, ], asthma~1, family = "binomial")
w2 <- exwas(expo[1:5, ], asthma~sex+age, family = "binomial")
tef(w1)
tef(w2)</pre>
```

toES

Method to convert an imExposomeSet to an ExposomeSet

## Description

This methods allows to select an imputed-set and use it to create an ExposomeSet from an imExposomeSet.

## Usage

```
toES(object, rid = 1)
```

## **Arguments**

object An object of class imExposomeSet

rid (default 1) Number of the imputation to be extracted

## Value

An object of class ExposomeSet-

# **Examples**

```
data("ex_imp")
toES(ex_imp, rid = 1)
```

trans

Function to apply a transformation to the exposures of an Exposome-Set

## **Description**

The exposures in an ExposomeSet can be transformed using this function. transform apples a function fun to the selected exposures.

```
trans(object, fun, select, by.exposure = FALSE, ...)
```

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## **Arguments**

object ExposomeSet which exposures will be transformed.

fun Function to be applied on the exposures.

select If not set, receive the name of all exposures. It can takes a character vector to

select specific exposures.

by exposure (default FALSE) If TRUE applies fun to each exposure (given as a vector ). If

FALSE the matrix of exposures is fiven to fun.

... Argument given to fun.

#### Value

A new ExposomeSet with selected exposures transformed with fun.

#### See Also

highAndLow to transform the continuous exposures to levelled factors, standardize to standardize by normal or robust methods the exposures

## **Examples**

```
data("exposome")
exp.t <- trans(expo, fun = log, select = "ldde_lip")</pre>
```

volcano\_plot

Function to draw a Volcano Plot

#### **Description**

Function that takes two numeric vectors (P-Value and fold change) and draws a volcano plot using ggplot2

# Usage

```
volcano_plot(
  pval,
  fc,
  names,
  size = 2,
  tFC = 2,
  tPV = -log10(0.001),
  show.effect = FALSE
)
```

## **Arguments**

pval numeric vector of P.Values

fc numeric vector of fold change

names character vector with the feature's names.

size (default 2) Sice of the labels in case they are placed.

58 volcano\_plot

tFC (default 2) fold change threshold. It can be set to NULL to do not filter.

tPV (default -log10(0.001)) P-Value threshold. It can be set to NULL to not filter.

show.effect (default FALSE) If set to TRUE, the X-axis will should 2^logFC instead to teh

default logFC.

# Value

A ggplot object

```
data(exposome)
w1 <- extract(exwas(expo[1:20, ], asthma~1, family = "binomial"))
volcano_plot(w1$pvalue, w1$effect, rownames(w1))</pre>
```

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