

Package ‘oposSOM’

April 7, 2023

Title Comprehensive analysis of transcriptome data

Version 2.16.0

Description This package translates microarray expression data into metadata of reduced dimension. It provides various sample-centered and group-centered visualizations, sample similarity analyses and functional enrichment analyses. The underlying SOM algorithm combines feature clustering, multidimensional scaling and dimension reduction, along with strong visualization capabilities. It enables extraction and description of functional expression modules inherent in the data.

Depends R (>= 4.0.0), igraph (>= 1.0.0)

Imports fastICA, tsne, scatterplot3d, pixmap, fdrtool, ape, biomaRt, Biobase, RcppParallel, Rcpp, methods, graph, XML, png, RCurl

LinkingTo RcppParallel, Rcpp

License GPL (>=2)

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biocViews GeneExpression, DifferentialExpression, GeneSetEnrichment, DataRepresentation, Visualization

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

git_branch RELEASE_3_16

git_last_commit 15105f8

git_last_commit_date 2022-11-01

Date/Publication 2023-04-07

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oposSOM-package	<i>Comprehensive analysis of transcriptome data</i>
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Description

This package translates microarray expression data into metadata of reduced dimension. It provides various sample-centered and group-centered visualizations, sample similarity analyses and functional enrichment analyses. The underlying SOM algorithm combines feature clustering, multidimensional scaling and dimension reduction, along with strong visualization capabilities. It enables extraction and description of functional expression modules inherent in the data. The results are given within a separate folder and can be browsed using the summary HTML file.

Details

Package: oposSOM
Type: Package
Version: 2.11.1

Date: 2021-31-07
License: GPL (>= 2)

Author(s)

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References

Wirth, Loeffler, v.Bergen, Binder: Expression cartography of human tissues using self organizing maps. (BMC Bioinformatics 2011)

Wirth, v.Bergen, Binder: Mining SOM expression portraits: feature selection and integrating concepts of molecular function. (BioData Mining 2012)

Loeffler-Wirth, Kalcher, Binder: oposSOM: R-package for high-dimensional portraying of genome-wide expression landscapes on Bioconductor. (Bioinformatics 2015)

Examples

```
# Example with artificial data
env <- opossom.new(list(dataset.name="Example",
                        dim.1stLvlSom=20))

env$indata <- matrix(rnorm(10000), 1000, 10)

env$group.labels <- "auto"

opossom.run(env)

# Real Example - This will take several minutes
#env <- opossom.new(list(dataset.name="Tissues",
#                        dim.1stLvlSom=30,
#                        geneset.analysis=TRUE,
#                        pairwise.comparison.list=list(
#                            list("Homeostasis"=c(1, 2), "Imune System"=c(9, 10)),
#                            list("Homeostasis"=c(1, 2), "Muscle"=c(8))
#                        )))
#
#data(opossom.tissues)
#env$indata <- opossom.tissues
#
#env$group.labels <- c(rep("Homeostasis", 2),
#                      "Endocrine",
#                      "Digestion",
#                      "Exocrine",
#                      "Epithelium",
#                      "Reproduction",
#                      "Muscle",
#                      rep("Imune System", 2),
#                      rep("Nervous System", 2))
#
#opossom.run(env)
```

opossom.genesets

Additional literature genesets

Description

Genesets collected from publications and independent analyses.

Usage

```
data(opossom.genesets)
```

Format

The data set is stored in RData (binary) format. Each element of the list represents one distinct gene set and contains the Ensembl-IDs of the member genes.

Details

The oposSOM package allows for analysing the biological background of the samples using predefined sets of genes of known biological context. A large and diverse collection of such gene sets is automatically derived from the Gene Ontology (GO) annotation database using biomaRt interface. `opossom.genesets` contains more than 4,500 additional gene sets collected from Biocarta, KEGG and Reactome databases, from literature on chemical and genetic perturbations, from literature on cancer types and subtypes, and from previous analyses using the oposSOM pipeline.

`opossom.new`

Initialize the oposSOM pipeline.

Description

This function initializes the oposSOM environment and sets the preferences.

Usage

```
opossom.new(preferences)
```

Arguments

`preferences`

list with the following optional values:

- `indata`: input data matrix containing the expression values or an `Biobase::ExpressionSet` object (see 'Details' and 'Examples')
- `group.labels`: sample assignment to a distinct group, subtype or class (character; "auto" or one label for each sample; may be given with `indata ExpressionSet`)
- `group.colors`: colors of the samples for diverse visualizations (character; one color for each sample; may be given with `indata ExpressionSet`)
- `dataset.name`: name of the dataset; used to name results folder and environment image (character).
- `note`: a short note shown in html summary file to give some keywords about the data or analysis parameters (character).
- `dim.1stLvlSom`: dimension of primary SOM; use "auto" to apply automatic size estimation (integer, >5)
- `dim.2ndLvlSom`: dimensions of second level SOM (integer, >5)
- `training.extension`: factor to extend the number of iterations in SOM training (numerical, >0)
- `rotate.SOM.portraits`: number of rotations of the primary SOM in counter-clockwise fashion (integer {0,1,2,3})
- `flip.SOM.portraits`: mirroring the primary SOM along the bottom-left to top-right diagonal (boolean)
- `database.dataset`: type of ensemble dataset addressed with biomaRt interface; use "auto" to detect parameter automatically (character)

- `database.id.type`: type of rowname identifier in biomaRt database; obsolete if `database.dataset="auto"` (character)
- `activated.modules` (list): activates/deactivates pipeline functionalities:
 - `reporting` (boolean): enables or disables output of pdf and csv results and html summaries (default: TRUE). When deactivated, only R workspace will be stored after analysis.
 - `primary.analysis` (boolean): enables or disables data preprocessing and SOM training (default: TRUE). When deactivated, prior SOM training results are required to be contained in the workspace environment.
 - `sample.similarity.analysis` (boolean): enables or disables diversity analyses such as clustering heatmaps, correlation networks and ICA (default: TRUE).
 - `geneset.analysis` (boolean): enables or disables geneset analysis (default: TRUE).
 - `psf.analysis` (boolean): enables or disables pathway signal flow (PSF) analysis (default: TRUE). Human gene expression data is required as input data.
 - `group.analysis` (boolean): enables or disables group centered analyses such as group portraits and functional mining (default: TRUE).
 - `difference.analysis` (boolean): enables or disables pairwise comparisons of the groups and of pairs provided by `pairwise.comparison.list` as described below (default: TRUE).
- `standard.spot.modules`: spot modules utilized in diverse downstream analyses (character, one of {"overexpression", "group.overexpression", "underexpression", "kmeans", "correlation", "dmap"})
- `spot.coresize.modules`: spot detection in summary maps, minimum size (numerical, >0)
- `spot.threshold.modules`: spot detection in summary maps, expression threshold (numerical, between 0 and 1)
- `spot.coresize.groupmap`: spot detection in group-specific summary maps, minimum size (numerical, >0)
- `spot.threshold.groupmap`: spot detection in group-specific summary maps, expression threshold (numerical, between 0 and 1)
- `feature.centralization`: enables centralization of the features (boolean)
- `sample.quantile.normalization`: enables quantile normalization of the samples (boolean)
- `pairwise.comparison.list`: group list for pairwise analyses (list of group lists, see 'Examples') or NULL otherwise

Details

The package accepts the `indata` parameter in two formats:
 Firstly a simple two-dimensional numerical matrix, where the columns and rows represent the samples and genes, respectively. The expression values are usually obtained by calibration and summarization algorithms (e.g. MAS5, VSN or RMA), and transformed into logarithmic scale prior to utilizing them in the pipeline. Secondly the input data can also be given as `Biobase::ExpressionSet` object. Please check the vignette for more details on the parameters.

Value

A new oposSOM environment which is passed to `opossom.run`.

Examples

```
env <- opossom.new(list(dataset.name="Example",
note="a test with 10 random samples",
                        dim.1stLvlSom="auto",
                        dim.2ndLvlSom=10,
                        training.extension=1,
                        rotate.SOM.portraits=0,
                        flip.SOM.portraits=FALSE,
                        database.dataset="auto",
                        activated.modules = list(
"reporting" = TRUE,
                        "primary.analysis" = TRUE,
                        "sample.similarity.analysis" = TRUE,
                        "geneset.analysis" = TRUE,
                        "psf.analysis" = TRUE,
                        "group.analysis" = TRUE,
                        "difference.analysis" = TRUE ),
                        standard.spot.modules="dmap",
                        spot.coresize.modules=4,
                        spot.threshold.modules=0.9,
                        spot.coresize.groupmap=4,
                        spot.threshold.groupmap=0.7,
                        feature.centralization=TRUE,
                        sample.quantile.normalization=TRUE,
                        pairwise.comparison.list=list(
                          list("groupA"=c("sample1", "sample2"),
                              "groupB"=c("sample3", "sample4")))))

# definition of indata, group.labels and group.colors
env$indata = matrix( runif(1000), 100, 10 )
env$group.labels = c( rep("class 1", 5), rep("class 2", 4), "class 3" )
env$group.colors = c( rep("red", 5), rep("blue", 4), "green" )

# alternative definition of indata, group.labels and group.colors using Biobase::ExpressionSet
library(Biobase)

env$indata = ExpressionSet( assayData=matrix(runif(1000), 100, 10),
                           phenoData=AnnotatedDataFrame(data.frame(
                             group.labels = c( rep("class 1", 5), rep("class 2", 4), "class 3" ),
                             group.colors = c( rep("red", 5), rep("blue", 4), "green" ) ))
                           )
```

opossom.run

Execute the oposSOM pipeline.

Description

This function realizes the complete pipeline functionality: single gene expression values are clustered to metagenes using a self-organizing map. Based on these metagenes, visualizations (e.g. expression portraits), downstreaming sample similarity analyses (e.g. hierarchical clustering, ICA) and functional enrichment analyses are performed. The results are given within a separate folder and can be browsed using the summary HTML file.

Usage

```
opossom.run(env)
```

Arguments

env	the opossom environment created with opossom.new according to the users' preferences
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Examples

```
# Example with artificial data
env <- opossom.new(list(dataset.name="Example",
                        dim.1stLvlSom=20))

env$indata <- matrix(rnorm(1000), 100, 10)

opossom.run(env)
```

opossom.tissues	<i>Example data set.</i>
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Description

A data set comprising of 12 selected human tissues.

Usage

```
data(opossom.tissues)
```

Format

The data set is stored in RData (binary) format.

Details

The data set was downloaded from Gene Expression Omnibus repository (<http://www.ncbi.nlm.nih.gov/geo>, GEO accession no. GSE7307). About 20,000 genes in more than 650 samples were measured using the Affymetrix HGU133-Plus2 microarray. A subset of 12 selected tissues from different categories is used as example data set for the oposSOM-package.

Source

<http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSE7307>

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