Package 'Mercator'

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Title Clustering and Visualizing Distance Matrices
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Description Defines the classes used to explore, cluster and visualize distance matrices, especially those arising from binary data. See Abrams and colleagues, 2021, <doi:10.1093 bioinformatics="" btab037="">.</doi:10.1093>
Depends R (>= 3.5), Thresher (>= 1.1)
Imports methods, stats, utils, graphics, grDevices, KernSmooth, cluster, Rtsne, ClassDiscovery, Polychrome, dendextend, igraph, flexmix, umap, kohonen
VignetteBuilder knitr
Suggests knitr, rmarkdown
License Apache License (== 2.0)
biocViews Clustering
<pre>URL http://oompa.r-forge.r-project.org/</pre>
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Description

The binaryDistance function defines various similarity or distance measures between binary vectors, which represent the first step in the algorithm underlying the Mercator visualizations.

Usage

binaryDistance(X, metric)

Arguments

X An object of class matrix.

metric An object of class character limited to the names of 10 selected distance met-

rics: jaccard, sokalMichener, hamming, russellRao, pearson, goodmanKruskal,

manhattan, canberra, binary, or euclid.

Details

Similarity or difference between binary vectors can be calculated using a variety of distance measures. In the main reference (below), Choi and colleagues reviewed 76 different measures of similarity of distance between binary vectors. They also produced a hierarchical clustering of these measures, based on the correlation between their distance values on multiple simulated data sets. For metrics that are highly similar, we chose a single representative.

Cluster 1, represented by the jaccard distance, contains Dice & Sorenson, Ochiai, Kulcyznski, Bray & Curtis, Baroni-Urbani & Buser, and Jaccard.

Cluster 2, represented by the sokalMichener distance, contains Sokal & Sneath, Gilbert & Wells, Gower & Legendre, Pearson & Heron, Hamming, and Sokal & Michener. Also within this cluster are 4 distances represented independently within this function: hamming, manhattan, canberra, and euclidean distances

Cluster 3, represented by the russellRao distance, contains Driver & Kroeber, Forbes, Fossum, and Russell & Rao.

The remaining metrics are more isolated, without strong clustering. We considered a few examples, including the Pearson distance (pearson) and the Goodman & Kruskal distance (goodmanKruskal). The binary distance is also included.

Value

Returns an object of class dist corresponding to the distance metric provided.

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Note

Although the distance metrics provided in the binaryDistance function are explicitly offered for use on matrices of binary vectors, some metrics may return useful distances when applied to non-binary matrices.

Author(s)

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References

Choi SS, Cha SH, Tappert CC, A Survey of Binary Similarity and Distance Measures. Systemics, Cybernetics, and Informatics. 2010; 8(1):43-48.

See Also

This set includes all of the metrics from the dist function.

Examples

```
my.matrix <- matrix(rbinom(50*100, 1, 0.15), ncol=50)
my.dist <- binaryDistance(my.matrix, "jaccard")</pre>
```

BinaryMatrix-class

Class "BinaryMatrix"

Description

The BinaryMatrix object class underlies the threshLGF and Mercator methods and visualizations of the Mercator package. The BinaryMatrix function returns a new object of BinaryMatrix class.

Usage

BinaryMatrix(binmat, columnInfo, rowInfo)

Arguments

binmat A binary matrix of class numeric or integer with values 0 and 1.

columnInfo A data. frame of at least one column containing column names. If no colnames

are specified, the column names associated with the data matrix will be used.

rowInfo A dataframe of at least one column containing row names. If no rownames are

specified, the row names associated with the data matrix will be used.

Value

The BinaryMatrix function returns a new object of binaryMatrix class.

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Objects from the Class

Objects should be defined using the BinaryMatrix constructor. In the simplest case, you simply pass in the binary data matrix that you want to visualize, and the BinaryMatrix is constructed using the matrix's existing column and row names.

Slots

binmat: Object of class matrix; the binary data used for visualization.

columnInfo: Object of class data. frame; names and definitions of columns.

rowInfo: Object of class data. frame; names and definitions of rows.

info: Object of class list; identifies \$notUsed and \$redundant features.

history: Object of class "character"; returns a history of manipulations by Mercator functions to the BinaryMatrix object, including "Newly created," "Subsetted," "Transposed," "Duplicate features removed," and "Threshed."

Methods

[]: Subsetting by [] returns a subsetted binary matrix, including subsetted row and column names. Calling @history will return the history "Subsetted."

dim: returns the dimensions of the @binmat component of the binaryMatrix object.

print: Shows the first ten rows and columns of the @binmat component.

show: Shows the first ten rows and columns of the @binmat component.

summary: For a given BinaryMatrix, returns object class, dimensions of the @binmat component, and @history.

t: Transposes the @binmat and its associated rowInfo and columnInfo. Calling @history will return the history "Subsetted."

Note

Attempting to construct or manipulate a BinaryMatrix containing NAs, missing values, or columns containing exclusively 0 values may introduce error.

Author(s)

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See Also

The removeDuplicateFeatures function can be used to remove duplicate columns from the binaryMatrix class before threshing or visualization. The threshLGF can be used to identify and remove uninformative features before visualization or further analysis.

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Examples

```
my.matrix <- matrix(rbinom(50*100, 1, 0.15), ncol=50)
my.rows <- as.data.frame(paste("R", 1:100, sep=""))
my.cols <- as.data.frame(paste("C", 1:50, sep=""))
my.binmat <- BinaryMatrix(my.matrix, my.cols, my.rows)
summary(my.binmat)
my.binmat <- my.binmat[1:50, 1:30]
my.binmat <- t(my.binmat)
dim(my.binmat)
my.binmat@history
my.binmat</pre>
```

downsample

Downsampling a Distance Visualization to Facilitate iGraph

Description

The downsample function implements a structured reduction of data points with a parent Mercator distance visualization to improve visualization and computational time, especially for the implementation of the iGraph visualization.

Usage

```
downsample(target, distanceMat, cutoff)
```

Arguments

target An integer number of points to which the user wishes to reduce the parent

Mercator object.

distanceMat An object of class matrix containing the distance matrix component of the par-

ent Mercator object.

cutoff An inclusion cutoff for selected points based on the local density within the

parent data.

Details

Mercator can be used to visualize complex networks using iGraph. To improve clarity of the visualization and computational time, we implement the downsample function to reduce the number of data points to be linked and visualized. The conceptual grounding for downsample draws on Peng Qiu's implementation of the SPADE clustering algorithm for mass cytometry data. The downsample function under-samples the densest regions of the data space to make it more likely that rarer clusters will still be adequately sampled.

Value

downsample returns an object of class Mercator containing a structured subset of items from the parent Mercator object.

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Author(s)

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References

Qiu, P., et. al. (2011). Extracting a cellular hierarchy from high-dimensional cytometry data with SPADE. Nature biotechnology, 29(10), 886.

Examples

```
#Form a BinaryMatrix
data("iris")
my.data <- as.matrix(iris[,c(1:4)])</pre>
my.rows <- as.data.frame(c(1:length(my.data[,1])))</pre>
my.binmat <- BinaryMatrix(my.data, , my.rows)</pre>
my.binmat <- t(my.binmat)</pre>
summary(my.binmat)
# Form and plot Mercator object
# Set K to the known number of species in the dataset
my.vis <- Mercator(my.binmat, "euclid", "tsne", K=3)</pre>
summary(my.vis)
plot(my.vis, view = "tsne", main="t-SNE plot of all data points")
#Downsample the Mercator object
M <- as.matrix(my.vis@distance)</pre>
set.seed(21340)
DS <- downsample(50, M, 0.1)
red.vis <- my.vis[DS]</pre>
#Visualize the down sampled t-SNE plot
plot(red.vis, view = "tsne", main="Down sampled t-SNE Plot")
```

Mercator-class

The Mercator Distance Visualization Object

Description

The Mercator object represents a distance matrix together with clustering assignments and a set of visualizations. It implements four visualizations for clusters of large-scale, multi-dimensional data: hierarchical clustering, multi-dimensional scaling, t-Stochastic Neighbor Embedding (t-SNE), and iGraph. The default Mercator constructor applies one of ten metrics of binaryDistance to an object of the BinaryMatrix class.

Usage

```
Mercator(X, metric, method, K, ...)
addVisualization(DV, method, ...)
getClusters(DV)
```

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Arguments

X Either a BinaryMatrix or a dist object.

metric A binaryDistance currently limited to the names of 10 selected distance met-

rics: jaccard, sokalMichener, hamming, russellRao, pearson, goodmanKruskal,

manhattan, canberra, binary, or euclid.

method A visualization method, currently limited to hclust, mds, tsne, graph, umap,

and som.

K An integer specifying the number of desired clusters.

DV A distance visualization produced as the output of the Mercator function.

... Additional arguments passed on to the functions that implement different meth-

ods for addVisualization (possibly passed here through the Mercator func-

tion). These include

any Any arguments to the cmdscale function for an mds visualization. Most commonly, this is likely to include k, the number of dimensions to compute.

any $\ensuremath{\mathsf{Any}}$ arguments to the Rtsne function for a tsne visualization. Common

examples include dims and perplexity.

any Any arguments to the som function to construct or view a self-organizing map. Most commonly, this is likely to include somgrid, to specify the size and layout of the grid, or type to specify which data to show in the plot.

Q A quantile cutoff for the creation of the IGraph visualization. By default, the value is set at the 10th percentile.

Value

The Mercator function constructs and returns a distance visualization object of the Mercator class, including a distance matrix calculated on a given metric and given visualizations. It is also possible (though not advisable) to construct a Mercator object directly using the new function. Default clustering in Mercator is now performed on the distance matrix using hierarchical clustering (hclust) with the wardD2 linkage method.

The addVisualizations function can be used to add additional visualizations to an existing Mercator object.

The getClusters function returns a vector of cluster assignments.

Slots

metric: Object of class "character"; the name of the binaryDistance applied to create this object.

distance: Object of class "dist"; the distance matrix used and represented by this object.

view: Object of class "list"; contains the results of calculations to generate each visualize the object.

clusters: A numeric vector of cluster assignments.

symbols: A numeric vector of valid plotting characters, as used by par(pch).

palette: A character vector of color names.

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Methods

plot(x, view = NULL, ask = NULL, ...): Produce a plot of one or more visualizations within a Mercator object. The default view, when omitted, is the first one contained in the object. You can request multiple views at once; if the current plot layout doesn't have enough space in an interactive session, the ask parameters determines whether the system will ask you before advancing to the next plot. When plotting a graph view, you can use an optional layout parameter to select a specific layout by name.

barplot(height, main = ", sub = NULL, border = NA, space = 0, ...) Produce a (colored) barplot of the silhouette widths for elements clustered in this class. Arguments are as described in te base function barplot.

scatter(object, view = NULL, ask = NULL, colramp = NULL, ...): Produce a smooth scatter plot of one or more visualizations within a Mercator object. The default view, when omitted, is the first one contained in the object. You can request multiple views at once; if the current plot layout doesn't have enough space in an interactive session, the ask parameters determines whether the system will ask you before advancing to the next plot. When plotting a graph view, you can use an optional layout parameter to select a specific layout by name. Arguments are otherwise the same as the smoothScatter function, execpt that the default color ramp is topo.colors.

hist(x, breaks=123, ...): Produce a histogram of distances calculated in the dissimilarity matrix generated in the Mercator object.

summary(object, ...): Returns the chosen distance metric, dimensions of the distance matrix, and available, calculated visualizations in this object.

dim(x): Returns the dimensions of the distance matrix of this object.

[: Subsets the distance matrix of this object.

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See Also

```
silhouette, smoothScatter, topo.colors, som, umap.
```

Examples

```
# Form a BinaryMatrix
data("iris")
my.data <- as.matrix(iris[,c(1:4)])
my.rows <- as.data.frame(c(1:length(my.data[,1])))
my.binmat <- BinaryMatrix(my.data, , my.rows)
my.binmat <- t(my.binmat)
summary(my.binmat)

# Form a Mercator object
# Set K to the known number of species in the dataset
my.vis <- Mercator(my.binmat, "euclid", "hclust", K=3)
summary(my.vis)
hist(my.vis)</pre>
```

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```
barplot(my.vis)
my.vis <- addVisualization(my.vis, "mds")
plot(my.vis, view = "hclust")
plot(my.vis, view = "mds")

scatter(my.vis, view ="mds")

# change the color palette
slot(my.vis, "palette") <- c("purple", "red", "orange", "green")
scatter(my.vis, view ="mds")

# Recover cluster identities
# What species comprise cluster 1?
my.clust <- getClusters(my.vis)
my.species <- iris$Species[my.clust == 1]
my.species</pre>
```

mercator-data

CML Cytogenetic Data

Description

These data sets contain binary versions of subsets of cytogenetic karyotype data from patients with chronic myelogenous leukemia (CML).

Usage

```
data("lgfFeatures")
data("CML500")
data("CML1000")
data("fakedata") # includes "fakeclin"
```

Format

- lgfFeatures A data matrix with 2748 rows and 6 columns listing the cytogentic bands produced as output of the CytoGPS algorithm that converts text-based karyotypes into a binary Loss-Gain-Fusion (LGF) model. The columns include the Label (the Type and Band, joined by an underscore), Type (Loss, Gain, or Fusion), Band (standard name of the cytogenetic band), Chr (chromosome), Arm (the chromsome arm, of the form #p or #q), and Index (an integer that can be used for sorting or indexing).
- CML500 A BinaryMatrix object with 770 rows (subset of LGF features) and 511 columns (patients). The patients were selected using the downsample function from the full set of more than 3000 CML karyotypes. The rows were selected by removing redundant and non-informative features when considering the full data set.
- CML1000 A BinaryMatrix object with 770 rows (subset of LGF features) and 1057 columns (patients). The patients were selected using the downsample function from the full set of more than 3000 CML karyotypes. The rows were selected by removing redundant and non-informative features when considering the full data set.

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fakedata A matrix with 776 rows ("features") and 300 columns ("samples") containing synthetic continuos data.

fakeclin A data frame with 300 rows ("samples") and 4 columns of synthetic clincal data related to the fakedata.

Author(s)

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Source

The cytogenetic data were obtained from the public Mitelman Database of Chromosomal Aberrations and Gene Fusions in Cancer on 4 April 2019. The database is currently located at https://cgap.nci.nih.gov/Chromosomes as part of hte Cancer Genome Anatomy Project (CGAP). The CGAP web site is expected to close on 1 October 2019 at which point the Mitelman database will move to an as-yet-undisclosed location. The data were then converted from text-based karyotrypes into binary vectors using CytoGPS http://cytogps.org/.

References

Abrams ZB, Zhang L, Abruzzo LV, Heerema NA, Li S, Dillon T, Rodriguez R, Coombes KR, Payne PRO. CytoGPS: A Web-Enabled Karyotype Analysis Tool for Cytogenetics. Bioinformatics. 2019 Jul 2. pii: btz520. doi: 10.1093/bioinformatics/btz520. [Epub ahead of print]

removeDuplicates

Remove Duplicate Features or Samples from a Binary Matrix Object

Description

The removeDuplicates function removes duplicate columns from a binaryMatrix object in the Mercator package.

Usage

```
removeDuplicates(object)
removeDuplicateFeatures(object)
```

Arguments

object

An object of class binaryMatrix.

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Details

In some analyses, it may be desirable to remove duplicate features to collapse a group of identical, related events to a single feature, to prevent overweighting when clustering. Historically, this funciton was called removeDuplicateFeatures. That name is still retained for backwards compatibility, but it may be deprecated in future versions in favor of removeDuplicates. In the same way, for some clustering applications, it may be usedful to remove duplicate samples, or those that have an identical feature set.

Removal of duplicates is not required for performance of the binaryMatrix or Mercator objects and associated functions.

The history slot of the binaryMatrix object documents the removal of duplicates.

Future versions of this package may include functionality to store the identities of any duplicates that were removed.

Value

Returns an object of class binaryMatrix with duplicate columns removed.

Note

Transposing the binaryMatrix can allow the removeDuplicates function to be applied to both features and observations, if desired.

Features containing exclusively 0s or 1s may interfere with performance of removeDuplicates.

Author(s)

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Examples

setClusters

Changing Cluster and Color Assignments in Mercator

Description

Cluster assignments from unsupervised analyses typically assign arbitrary integers to the classes. When comparing the results of different algorithms or different distance metrics, it is helpful to match the integers in order to use colors and symbols that are as consistent as possible. These functions help achieve that goal.

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Usage

```
setClusters(DV, clusters)
recolor(DV, clusters)
remapColors(fix, vary)
recluster(DV, K)
```

Arguments

DV An object of the Mercator class.

clusters An integer vector specifiny the cluster membership of each element.

fix An object of the Mercator class, used as the source of color and cluster assign-

ments.

vary An object of the Mercator class, used as the target of color and cluster assign-

ments.

K An integer, the number of clusters.

Details

In the most general sense, clustering can be viewed as a function from the space of "objects" of interest into a space of "class labels". In less mathematical terms, this simply means that each object gets assigned an (arbitrary) class label. This is all well-and-good until you try to compare the results of running two different clustering algorithms that use different labels (or even worse, use the same labels – typically the integers $1, 2, \ldots, K$ – with different meanings). When that happens, you need a way to decide which labels from the different sets are closest to meaning the "same thing".

The functions setClusters and remapColors solve this problem in the context of Mercator objects. They accaomplish this task using the greedy algorithm implemented and described in the remap function in the Thresher package.

Value

Both setClusters and remapColors return an object of class Mercator in which only the cluster labels and associated color and symbol representations (but not the distance metric used, the number of clusters, the cluster assignments, nor the views) have been updated.

The recolor function is currently an alias for setClusters. However, using recolor is deprecated, and the alias will likely be removed in the next version of the package.

Author(s)

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See Also

remap

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Examples

```
#Form a BinaryMatrix
data("iris")
my.data <- t(as.matrix(iris[,c(1:4)]))</pre>
colnames(my.data) <- 1:ncol(my.data)</pre>
my.binmat <- BinaryMatrix(my.data)</pre>
# Form a Mercator object; Set K to the number of known species
my.vis <- Mercator(my.binmat, "euclid", "tsne", K=3)</pre>
table(getClusters(my.vis), iris$Species)
summary(my.vis)
# Recolor the Mercator object with known species
DS <- recolor(my.vis, as.numeric(iris$Species))</pre>
table(getClusters(DS), iris$Species)
# Use a different metric
my.vis2 <- Mercator(my.binmat, "manhattan", "tsne", K=3)</pre>
table(getClusters(my.vis2), iris$Species)
table(Pearson = getClusters(my.vis2), Euclid = getClusters(my.vis))
# remap colors so the two methods match as well as possible
my.vis2 <- remapColors(my.vis, my.vis2)</pre>
table(Pearson = getClusters(my.vis2), Euclid = getClusters(my.vis))
# recluster with K=4
my.vis3 <- recluster(my.vis, K = 4)</pre>
# view the results
opar <- par(mfrow=c(1,2))</pre>
plot(my.vis, view = "tsne", main="t-SNE plot, Euclid")
plot(my.vis2, view = "tsne", main="t-SNE plot, Pearson")
par(opar)
```

threshLGF

Threshing and Reaping the BinaryMatrix

Description

The threshLGF function produces an object of class ThreshedBinaryMatrix from threshing on an object of class BinaryMatrix.

The function threshLGF and the ThreshedBinaryMatrix object can be used to access the functionality of the Thresher R-package within Mercator.

Usage

```
threshLGF(object, cutoff = 0)
```

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Arguments

object An object of class BinaryMatrix

cutoff The value of delta set to demarcate an uninformative feature. Features with a

value greater than the cutoff will be kept.

Details

The Thresher R-package provides a variety of functionalities for data filtering and the identification of and reduction to "informative" features. It performs clustering using a combination of outlier detection, principal component analysis, and von Mises Fisher mixture models. By identifying significant features, Thresher performs feature reduction through the identification and removal of noninformative features and the nonbiased calculation of the number of groups (K) for down-stream use.

Value

threshLGF returns an object of class ThreshedBinaryMatrix. The ThreshedBinaryMatrix object retains all the functionality, slots, and methods of the BinaryMatrix object class with added features. After threshing, the ThreshedBinaryMatrix records the history, "Threshed."

Additional Slots

thresher: Returns the functions of the Thresher object class of the Thresher R-package.

reaper: Returns the functions of the Reaper object class of the Thresher R-package.

Note

The Thresher R-package applies the Auer-Gervini statistic for principal component analysis, outlier detection, and identification of uninformative features on a matrix of class integer or numeric.

An initial delta of 0.3 is recommended.

Author(s)

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References

Wang, M., Abrams, Z. B., Kornblau, S. M., & Coombes, K. R. (2018). Thresher: determining the number of clusters while removing outliers. BMC bioinformatics, 19(1), 9.

See Also

The threshLGF function creates a new object of class ThreshedBinaryMatrix from an object of class BinaryMatrix.

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Examples

```
#Create a BinaryMatrix
set.seed(52134)
my.matrix <- matrix(rbinom(50*100, 1, 0.15), ncol=50)</pre>
my.rows <- as.data.frame(paste("R", 1:100, sep=""))</pre>
my.cols <- as.data.frame(paste("C", 1:50, sep=""))</pre>
my.binmat <- BinaryMatrix(my.matrix, my.cols, my.rows)</pre>
summary(my.binmat)
#Identify delta cutoff and thresh
my.binmat <- threshLGF(my.binmat)</pre>
Delta <- my.binmat@thresher@delta</pre>
sort(Delta)
hist(Delta, breaks=15, main="", xlab="Weight")
abline(v=0.3, col='red')
my.binmat <- threshLGF(my.binmat, cutoff = 0.3)</pre>
summary(my.binmat)
#Principal Component Analysis
my.binmat@reaper@pcdim
my.binmat@reaper@nGroups
plot(my.binmat@reaper@ag)
abline(h=1, col="red")
screeplot(my.binmat@reaper)
abline(v=6, col="forestgreen", lwd=2)
```

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