Package 'BinMat'

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Type Package

Title Processes Binary Data Obtained from Fragment Analysis (Such as AFLPs, ISSRs, and RFLPs)

Version 0.1.6

Description A molecular genetics tool that processes binary data from fragment analysis. It consolidates replicate sample pairs, outputs summary statistics, and produces hierarchical clustering trees and nMDS plots. This package was developed from the publication available here: <doi:10.1016/j.biocontrol.2020.104426>. The GUI version of this package is available on the R Shiny online server at: <https://clarkevansteenderen.shinyapps.io/BINMAT/> or it is accessible via GitHub by typing: shiny::runGitHub(``BinMat'', ``clarkevansteenderen'') into the console in R. Two real-world datasets accompany the package: an AFLP dataset of Bunias orientalis samples from Tewes et. al. (2017) <doi:10.1111/1365-2745.12869>, and an ISSR dataset of Nymphaea specimens from Reid et. al. (2021) <doi:10.1016/j.aquabot.2021.103372>. The authors of these publications are thanked for allowing the use of their data.

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Encoding UTF-8

LazyData true

RoxygenNote 7.3.1

Depends R (>= 3.0)

Imports pvclust (>= 2.0), MASS (>= 7.3), stats (>= 3.4.0), graphics (>= 3.4.0), base (>= 3.4.0), ggpubr (>= 0.4.0), tibble (>= 3.1.4)

Suggests knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

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Example input data containing a consolidated binary matrix with groups

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Description

Example input data containing a consolidated binary matrix with groups

Usage

```
data(BinMatInput_ordination)
```

Format

A dataframe with columns for loci, and rows of replicate pairs. Grouping information is in the second column.

Examples

```
data(BinMatInput_ordination)
mat = BinMatInput_ordination
group.names(mat)
scree(mat)
shepard(mat)
clrs = c("red", "green", "black")
nmds(mat, colours = clrs, labs = TRUE)
```

BinMatInput_reps	*Example input data containing a binary matrix comprising replicate pairs*

Description

Example input data containing a binary matrix comprising replicate pairs

Usage

```
data(BinMatInput_reps)
```

Format

A dataframe with columns for loci, and rows of replicate pairs.

Examples

```
data(BinMatInput_reps)
mat = BinMatInput_reps
check.data(mat)
cons = consolidate(mat)
pks = peaks.consolidated(cons)
err = errors(cons)
rem = peak.remove(cons, 4)
clust = upgma(cons)
```

---

bunias_orientalis	*Example input file of Bunias orientalis AFLP data, taken from Tewes et. al. (2017). This dataset has already been consolidated, and can be used as input for the generation of an nMDS plot. The paper can be found here: <doi:10.1111/1365-2745.12869>*

Description

Example input file of Bunias orientalis AFLP data, taken from Tewes et. al. (2017). This dataset has already been consolidated, and can be used as input for the generation of an nMDS plot. The paper can be found here: <doi:10.1111/1365-2745.12869>

Usage

```
data(bunias_orientalis)
```

Format

A dataframe with columns for loci, and rows of replicate pairs. Grouping information is in the second column.

Examples

```
bunias = bunias_orientalis
group.names(bunias)
nmds(bunias, labs = FALSE, include_ellipse = TRUE, legend_pos = "right")
```

---

check.data   *Checks binary matrix for unwanted characters.*

Description

Checks for unwanted values (other than 1, 0, and ?).

Usage

```
check.data(x)
```

Arguments

x   A CSV file containing replicate pairs of binary data.

Value

Index positions where unwanted values occur (row, column).

Examples

```
data(BinMatInput_reps)
mat = BinMatInput_reps
check.data(mat)
```

---

consolidate   *Consolidates replicate pairs in a binary matrix.*

Description

Reads in a binary matrix comprising replicate pairs and consolidates each pair into a consensus read. For each replicate pair at each locus, 1 & 1 -> 1 (shared presence), 0 & 0 -> 0 (shared absence), 0 & 1 -> ? (ambiguity).

Usage

```
consolidate(x)
```

Arguments

x   A CSV file containing replicate pairs of binary data. See the example input file
                         "BinMatInput_reps".

Value

Consolidated binary matrix.

Examples

```
data(BinMatInput_reps)
mat = BinMatInput_reps
cons = consolidate(mat)
```

---

errors   *Calculates Jaccard and Euclidean error rates.*

Description

Calculates the Jaccard and Euclidean error rates for the dataset. Jaccard's error does not take shared
absences of bands as being biologically meaningful. JE = (f10 + f01)/(f10 + f01 + f11) and EE
= (f10 + f01)/(f10 + f01 + f11 + f00). At each locus, f01 and f10 indicates a case where a 0 was
present in one replicate, and a 1 in the other. f11 indicates the shared presence of a band in both
replicates, and f00 indicates a shared absence. For example, if a replicate pair comprises Rep1 =
00101 and Rep2 = 01100, JE = (1+1)/(1+1+1) = 2/3 = 0.67, EE = (1+1)/(1+1+1+2) = 2/5 = 0.4.

Usage

```
errors(x)
```

Arguments

x   Consolidated binary matrix.

Value

JE (Jaccard Error), EE (Euclidean Error), and standard deviations.

Examples

```
data(BinMatInput_reps)
mat = BinMatInput_reps
cons = consolidate(mat)
errors(cons)
```

---

group.names   *Outputs group names specified in the input file for the creation of an*
                                      nMDS plot.

Description

Returns group names in the uploaded consolidated binary data. This will help in knowing which colours are assigned to which group name.

Usage

```
group.names(x)
```

Arguments

x   Consolidated binary matrix with grouping information in column 2.

Value

Scree plot.

Examples

```
mat = BinMatInput_ordination
group.names(mat)
```

---

nmds   *Creates a non-metric multidimensional scaling plot (nMDS).*

Description

Creates an nMDS plot from a consolidated binary matrix with grouping information. Colours and shapes of plotted points need to be specified. For example, if there are two groups, then: clrs = c("red", "blue"), sh = c(16, 16). This assigns red to the first group name, and blue to the second. Both will have a pch shape of 16 (round dot). These two vectors are then passed to the function nmds() as: colours = clrs, shapes = sh.

Usage

```
nmds(
  x,
  dist_meth = "binary",
  k_val = 2,
  pt_size = 1,
 colours = c("dodgerblue", "black", "red", "green3", "orange", "darkblue", "gold2",
```

```
     "darkgreen", "darkred", "grey", "darkgrey", "magenta", "darkorchid", "purple",
     "brown", "coral3", "turquoise", "deeppink", "lawngreen", "deepskyblue", "tomato",
     "yellow", "yellowgreen", "royalblue", "olivedrab", "midnightblue", "indianred1",
       "darkturquoise"),
    labs = FALSE,
    legend_pos = "right",
    include_ellipse = FALSE,
    ellipse_type = "norm",
    dimension1 = 1,
    dimension2 = 2
)
```

Arguments

x	Consolidated binary matrix with grouping information in the second column.
dist_meth	Distance method. Set to "binary" by default. Other options are "euclidean", "maximum", "manhattan", "canberra", or "minkowski".
k_val	Number of dimensions for the nMDS plot. Set to 2 by default.
pt_size	Point size for symbols on the plot. Set to 1 by default.
colours	Vector containing colours to be assigned to groups. This can be changed to the options available in the RColorBrewer palette set (e.g. "Set1"). See <http://applied-r.com/rcolorbrewer-palettes/> for more palette options. Alternatively, the colours can be set manually using, for example, c("red", "green", "blue"), thereby setting a colour for each group in your dataset. There are 28 default colours that will be set automatically to your groups.
labs	Indicate whether labels should appear on the graph or not (TRUE or FALSE). Default = FALSE.
legend_pos	Indicate the position of the legend. Default = "right", but other options are "left", "bottom", "top", or "none"
include_ellipse	
	Indicate whether ellipses should be included around groups. Default = FALSE.
ellipse_type	Select the type of ellipses to include around groups. Options are "convex", "confidence", "t", "norm", and "euclid". See the ggpubr::ggscatter() function documentation for more details.
dimension1	Indicate the first dimension to plot (1, 2, or 3) for the x axis. If k = 2, the first two dimensions will automatically be plotted. If k = 3, select between the three.
dimension2	Indicate the second dimension to plot (1, 2, or 3) for the y axis

Value

nMDS plot.

Examples

```
 mat = BinMatInput_ordination
group.names(mat)
```

```
clrs = c("red", "green", "black")
nmds(mat, colours = clrs, labs = TRUE, include_ellipse = TRUE)
```

| nymphaea | *Example input file of Nymphaea ISSR data, taken from Reid et. al. (2021). This dataset has already been consolidated, and can be used as input for the generation of an nMDS plot. The paper can be found here: <doi:10.1016/j.aquabot.2021.103372>* |

Description

Example input file of Nymphaea ISSR data, taken from Reid et. al. (2021). This dataset has already been consolidated, and can be used as input for the generation of an nMDS plot. The paper can be found here: <doi:10.1016/j.aquabot.2021.103372>

Usage

```
data(nymphaea)
```

Format

A dataframe with columns for loci, and rows of replicate pairs. Grouping information is in the second column

Examples

```
nymph = nymphaea
group.names(nymph)
colrs = c("dodgerblue", "black", "red", "green3", "orange", "darkblue",
"gold2", "darkgreen", "darkred", "grey", "darkgrey", "magenta",
"darkorchid", "purple", "brown", "coral3", "turquoise", "deeppink",
"lawngreen", "deepskyblue", "tomato")
nmds(nymph, labs = FALSE, include_ellipse = FALSE, colours = colrs,
legend_pos = "right", pt_size = 2)
```

| peak.remove | *Removes samples with peaks equal to or less than a specified threshold value.* |

Description

Removes samples with a peak number less than a specified value.

Usage

```
peak.remove(x, thresh)
```

Arguments

x	Binary matrix - consolidated or original.
thresh	Peak threshold value for removal.

Value

Filtered dataset, and either the row name/s or row number/s of samples that were removed.

Examples

```
mat = BinMatInput_ordination
new = peak.remove(mat, 4)
```

---

peaks.consolidated	*Calculates peak numbers for a consolidated data set (total, maximum, and minimum).*

Description

Returns total, maximum, and minimum number of peaks in the binary matrix.

Usage

```
peaks.consolidated(x)
```

Arguments

x	Binary matrix comprising replicate pairs.

Value

Peak information.

Examples

```
data(BinMatInput_reps)
mat = BinMatInput_reps
cons = consolidate(mat)
peaks.consolidated(cons)
```

peaks.original	*Calculates peak numbers for the data set with all replicates (total, maximum, and minimum).*

Description

Returns total, maximum, and minimum number of peaks in the binary matrix.

Usage

```
peaks.original(x)
```

Arguments

x   Binary matrix comprising replicate pairs.

Value

Peak information.

Examples

```
data(BinMatInput_reps)
mat = BinMatInput_reps
peaks.original(mat)
```

scree	*Draws a scree plot.*

Description

Creates a scree plot for the nMDS. This indicates the optimum number of dimensions to use to minimise the stress value. The stress value is indicated by a red dotted line at 0.15. Values equal to or below this are considered acceptable.

Usage

```
scree(x, dimensions = 4, dist_meth = "binary")
```

Arguments

x   Consolidated binary matrix with grouping information in column 2.

dimensions   Number of dimensions to plot. Set to 4 by default.

dist_meth   Distance method. Set to "binary" by default. Other options are "euclidean", "maximum", "manhattan", "canberra", or "minkowski".

Value

Scree plot.

Examples

```
mat = BinMatInput_ordination
scree(mat)
```

---

shepard   *Creates a shepard plot.*

Description

Creates a Shepard plot for the nMDS. This indicates the 'goodness of fit' of the original distance matrix vs the ordination representation. A high R-squared value is favourable.

Usage

```
shepard(x, k_val = 2, dist_meth = "binary")
```

Arguments

x	Consolidated binary matrix.
k_val	Number of dimensions. Set to 2 by default.
dist_meth	Distance method. Set to "binary" by default. Other options are "euclidean", "maximum", "manhattan", "canberra", or "minkowski".

Value

Shepard plot.

Examples

```
mat = BinMatInput_ordination
shepard(mat)
```

---

upgma   *Draws a hierarchical clustering tree (UPGMA).*

Description

Creates a UPGMA hierarchical clustering tree, with a specified number of bootstrap repetitions.

Usage

```
upgma(
  x,
  bts = 10,
  size = 0.55,
  lab_size = 0.55,
  method = "binary",
  hclust = "average",
  fromFile = FALSE
)
```

Arguments

x	Consolidated binarx matrix.
bts	Bootstrap replications. Set to 10 by default.
size	Size of plot. Set to 0.55 by default.
lab_size	Size of label text. Set to 0.55 by default.
method	Distance method. Set to 'binary' (=Jaccard distance) by default.
hclust	Clustering method. Set to 'average' (=UPGMA) by default
fromFile	Indicates whether the binary data used by the function has been consolidated by BinMat, or whether it comes from the user's own file. Set to FALSE by default (in the assumption that the data has been consolidated by BinMat, and that that object is being passed to the function).

Value

UPGMA tree

Examples

```
data(BinMatInput_reps)
mat = BinMatInput_reps
cons = consolidate(mat)
clust = upgma(cons)
```

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