Package 'micompr'

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Title Multivariate Independent Comparison of Observations

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Description A procedure for comparing multivariate samples associated with different groups. It uses principal component analysis to convert multivariate observations into a set of linearly uncorrelated statistical measures, which are then compared using a number of statistical methods. The procedure is independent of the distributional properties of samples and automatically selects features that best explain their differences, avoiding manual selection of specific points or summary statistics. It is appropriate for comparing samples of time series, images, spectrometric measures or similar multivariate observations. This package is described in Fachada et al. (2016) <doi:10.32614/RJ-2016-055>.

Depends R (>= 4.1.0)

Imports utils, graphics, methods, stats

Suggests biotools, MVN (>= 5.0), testthat (>= 0.8), knitr, roxygen2, devtools

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URL https://github.com/nunofachada/micompr

BugReports https://github.com/nunofachada/micompr/issues

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assumptions

Parametric tests assumptions

Description

Generic function to get the assumptions for parametric tests applied to the comparison of output observations.

Usage

```
assumptions(obj)
```

Arguments

obj

Object from which to get the assumptions.

Value

Assumptions for parametric tests applied to the comparison of outputs.

See Also

```
assumptions.cmpoutput, assumptions.micomp
```

```
assumptions.cmpoutput Get assumptions for parametric tests performed on output comparisons
```

Description

Get assumptions for parametric tests performed on output comparisons (i.e. from objects of class cmpoutput).

Usage

```
## S3 method for class 'cmpoutput'
assumptions(obj)
```

Arguments

obj

Object of class empoutput.

Value

Object of class assumptions_cmpoutput containing the assumptions for parametric tests performed on an output comparison. Basically a list containing the assumptions for the MANOVA (list of objects of class assumptions_manova, one per explained variance) and univariate parametric tests for each principal component (object of class assumptions_paruv).

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Examples

```
# Create a cmpoutput object from the provided datasets
cmp <- cmpoutput("All", 0.9, pphpc_ok$data[["All"]], pphpc_ok$obs_lvls)
# Get the assumptions for the parametric tests performed in cmp
acmp <- assumptions(cmp)</pre>
```

assumptions.micomp

Get assumptions for parametric tests performed on each comparisons

Description

Get assumptions for parametric tests performed on multiple comparisons (i.e. from objects of class micomp).

Usage

```
## S3 method for class 'micomp'
assumptions(obj)
```

Arguments

obj

Object of class micomp.

Value

Object of class assumptions_micomp containing the assumptions for parametric tests performed for the multiple comparisons held by the mcmp object. This object is a multi-dimensional list of assumptions_cmpoutput objects. Rows are associated with individual outputs, while columns are associated with separate comparisons.

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assumptions_manova

Determine the assumptions for the MANOVA test

Description

Determine two assumptions for the MANOVA test: a) multivariate normality of each group; b) homogeneity of covariance matrices.

Usage

```
assumptions_manova(data, factors)
```

Arguments

data Data used for the MANOVA test (rows correspond to observations, columns to

dependent variables).

factors Groups to which rows of data belong to (independent variables).

Value

An object of class assumptions_manova which is a list containing two elements:

mvntest List of results from the Royston multivariate normality test (mvn), one result per group. vartest Result of Box's M test for homogeneity of covariance matrices (boxM).

Note

This function requires the MVN and biotools packages.

```
# Determine the assumptions of applying MANOVA to the iris data
# (i.e. multivariate normality of each group and homogeneity of covariance
# matrices)
a <- assumptions_manova(iris[, 1:4], iris[, 5])</pre>
```

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assumptions_paruv	Determine the assumptions for the parametric comparison test

Description

Determine two assumptions for the parametric comparison tests (i.e. either t.test or aov) for each principal component, namely: a) univariate normality of each group; b) homogeneity of variances.

Usage

```
assumptions_paruv(data, factors)
```

Arguments

data Data used in the parametric test (rows correspond to observations, columns to

principal components).

factors Groups to which rows of data belong to.

Value

An object of class assumptions_paruv which is a list containing two elements:

uvntest List of results from the Shapiro-Wilk normality test (shapiro.test), one result per group per principal component.

vartest Result of Bartlett test for homogeneity of variances (bartlett.test).

Examples

```
# Determine the assumptions of applying ANOVA to each column (dependent
# variable) of the iris data (i.e. normality of each group and homogeneity of
# variances)
a <- assumptions_paruv(iris[, 1:4], iris[, 5])</pre>
```

centerscale

Center and scale vector

Description

Center and scale input vector using the specified method.

Usage

```
centerscale(v, type)
```

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Arguments

v Vector to center and scale.

type Type of scaling: "center", "auto", "range", "iqrange", "vast", "pareto", "level" or "none".

Value

Center and scaled vector using the specified method.

References

Berg, R., Hoefsloot, H., Westerhuis, J., Smilde, A., and Werf, M. (2006). Centering, scaling, and transformations: improving the biological information content of metabolomics data. *BMC Genomics* **7**, 142. DOI: 10.1186/1471-2164-7-142

```
v \leftarrow c(-100, 3, 4, 500, 10, 25, -8, -33, 321, 0, 2)
centerscale(v, "center")
# [1] -165.81818 -62.81818 -61.81818 434.18182 -55.81818 -40.81818
# [7] -73.81818 -98.81818 255.18182 -65.81818 -63.81818
centerscale(v, "auto")
# [1] -0.9308937 -0.3526577 -0.3470437 2.4374717 -0.3133601 -0.2291509
# [7] -0.4144110 -0.5547596 1.4325760 -0.3694995 -0.3582716
centerscale(v, "range")
# [1] -0.2763636 -0.1046970 -0.1030303 0.7236364 -0.0930303 -0.0680303
# [7] -0.1230303 -0.1646970 0.4253030 -0.1096970 -0.1063636
centerscale(v, "iqrange")
# [1] -6.085071 -2.305254 -2.268557 15.933278 -2.048374 -1.497915 -2.708924
# [8] -3.626355 9.364470 -2.415346 -2.341952
centerscale(v, "vast")
# [1] -0.34396474 -0.13030682 -0.12823247   0.90064453 -0.11578638 -0.08467115
# [7] -0.15312466 -0.20498338   0.52933609 -0.13652987 -0.13238117
centerscale(v, "pareto")
# [1] -12.424134 -4.706731 -4.631804 32.531614 -4.182247 -3.058353
# [7] -5.530919 -7.404075 19.119816 -4.931509 -4.781657
centerscale(v, "level")
# [1] -2.5193370 -0.9544199 -0.9392265 6.5966851 -0.8480663 -0.6201657
# [7] -1.1215470 -1.5013812 3.8770718 -1.0000000 -0.9696133
centerscale(v, "none")
# [1] -100
            3 4 500
                          10 25 -8 -33 321
                                                     0
                                                          2
```

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cmpoutput Compares output observations from two or more groups
--

Description

Compares output observations from two or more groups.

Usage

```
cmpoutput(name, ve_npcs, data, obs_lvls, lim_npcs = TRUE, mnv_test = "Pillai")
```

Arguments

name	Comparison name (useful when calling this function to perform multiple comparisons).
ve_npcs	Percentage ($0 < ve_npcs < 1$) of variance explained by the q principal components (i.e. number of dimensions) used in MANOVA, or the number of principal components ($ve_npcs > 1$, must be integer). Can be a vector, in which case the MANOVA test will be applied multiple times, one per specified variance to explain / number of principal components.
data	A $n \times m$ matrix, where n is the total number of output observations (runs) and m is the number of variables (i.e. output length).
obs_lvls	Levels or groups associated with each observation.
lim_npcs	Limit number of principal components used for MANOVA to minimum number of observations per group?
mnv_test	The name of the test statistic to be used in MANOVA, as described in summary.manova.

Value

Object of class empoutput containing the following data:

scores *n* x *n* matrix containing projections of output data in the principal components space. Rows correspond to observations, columns to principal components.

obs_lvls Levels or groups associated with each observation.

varexp Percentage of variance explained by each principal component.

npcs Number of principal components specified in ve_npcs OR which explain the variance percentages given in ve_npcs.

ve Percentage (between 0 and 1) of variance explained by the q principal components (i.e. number of dimensions) used in MANOVA.

name Comparison name (useful when calling this function to perform multiple comparisons).

p.values *P*-values for the performed statistical tests, namely:

manova List of *p*-values for the MANOVA test for each number of principal component in npcs.

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parametric Vector of *p*-values for the parametric test applied to groups along each principal component (*t*-test for 2 groups, ANOVA for more than 2 groups).

nonparametric Vector of *p*-values for the non-parametric test applied to groups along each principal component (Mann-Whitney U test for 2 groups, Kruskal-Wallis test for more than 2 groups).

parametric_adjusted Same as field parametric, but *p*-values are adjusted using weighted Bonferroni procedure. Percentages of explained variance are used as weights.

nonparametric_adjusted Same as field nonparametric, but *p*-values are adjusted using weighted Bonferroni procedure. Percentages of explained variance are used as weights.

tests manova Objects returned by the manova function for each value specified in ve_npcs.

parametric List of objects returned by applying t.test (two groups) or aov (more than two groups) to each principal component.

nonparametric List of objects returned by applying wilcox. test (two groups) or kruskal. test (more than two groups) to each principal component.

Examples

```
# Comparing the first output ("Pop.Sheep") of one the provided datasets.
cmp <-
cmpoutput("SheepPop", 0.8, pphpc_ok$data[["Pop.Sheep"]], pphpc_ok$obs_lvls)

# Compare bogus outputs created from 2 random sources, 5 observations per
# source, 20 variables each, yielding a 10 x 20 data matrix.
data <- matrix(c(rnorm(100), rnorm(100, mean = 1)), nrow = 10, byrow = TRUE)
olvls <- factor(c(rep("A", 5), rep("B", 5)))
cmp <- cmpoutput("Bogus", 0.7, data, olvls)</pre>
```

concat_outputs

Concatenate multiple outputs with multiple observations

Description

Concatenate multiple outputs with multiple observations.

Usage

```
concat_outputs(outputlist, centscal = "none")
```

Arguments

outputlist List of outputs. Each output is a $n \times m$ matrix, where n is the number of obser-

vations and *m* is the number of variables (i.e. output length).

centscal Centering and scaling method: "center", "auto", "range", "iqrange", "vast", "pareto",

"level" or "none". This task is delegated to the centerscale function.

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Value

An $n \times p$ matrix, representing the n observations of the concatenated output, each observation of length p, which is the sum of individual output lengths.

Examples

```
# Collect 20 observations of 3 outputs with different scales and lengths
# Output 1, length 100
out1 <- matrix(rnorm(2000, mean = 0, sd = 1), nrow = 20)
# Output 2, length 200
out2 <- matrix(rnorm(4000, mean = 100, sd = 200), nrow = 20)
# Output 1, length 50
out3 <- matrix(rnorm(1000, mean = -1000, sd = 10), nrow = 20)
# Concatenate and range scale outputs, resulting matrix dimensions will be
# 20 x 350
outconcat <- concat_outputs(list(out1, out2, out3), "range")</pre>
```

grpoutputs

Load and group outputs from files

Description

Load and group outputs from files containing multiple observations of the groups to be compared.

Usage

```
grpoutputs(
  outputs,
  folders,
  files,
  lvls = NULL,
  concat = F,
  centscal = "range",
  ...
)
```

Arguments

outputs

A vector with the labels of each output, or an integer with the number of outputs (in which case output labels will be assigned automatically). In either case, the number of outputs should account for an additional concatenated output, as specified in the concat parameter.

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folders	Vector of folder names where to read files from. These are recycled if length(folders) < length(files).
files	Vector of filenames or file sets to load in each folder. File sets can be given as regular expressions, or as wildcards by wrapping them with glob2rx.
lvls	Vector of factor levels (groups). Must be the same length as files, i.e. each file set will be associated with a different level or group. If not given, default group names will be used.
concat	If TRUE add an additional output which corresponds to the concatenation of all outputs, properly centered and scaled.
centscal	Method for centering and scaling outputs if concat is TRUE. It can be one of "center", "auto", "range" (default), "iqrange", "vast", "pareto" or "level". Centering and scaling is performed by the centerscale function.
•••	Options passed to read.table, which is used to read the files specified in the files parameter.

Details

Each file corresponds to an observation, and should have a tabular format where columns correspond to outputs and rows to variables or dimensions. Observations (files) are grouped by factor levels which correspond to the file groups given in the files parameter. Factor levels differentiate observations from distinct groups.

Value

Object of class grpoutputs containing the following data:

data List of all outputs, each one grouped into a *n* x *m* matrix, where *n* is the total number of output observations and *m* is the number of variables or dimensions (i.e. output length).

groupsize Vector containing number of observations for each level or group.

obs_lvls Factor vector of levels or groups associated with each observation.

lvls Vector of factor levels in the order they occur (as given in parameter with the same name).

concat Boolean indicating if this object was created with an additional concatenated output.

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micomp

Multiple independent comparisons of observations

Description

Performs multiple independent comparisons of output observations.

Usage

```
micomp(
  outputs,
  ve_npcs,
  comps,
  concat = F,
  centscal = "range",
  lim_npcs = TRUE,
  mnv_test = "Pillai",
  ...
)
```

Arguments

outputs

A vector with the labels of each output, or an integer with the number of outputs (in which case output labels will be assigned automatically).

ve_npcs

Percentage ($\emptyset < \text{ve_npcs} < 1$) of variance explained by the q principal components (i.e. number of dimensions) used in MANOVA, or the number of principal components ($\text{ve_npcs} > 1$, must be integer). Can be a vector, in which case the MANOVA test will be applied multiple times, one per specified variance to explain / number of principal components.

comps

A list of lists, where each list contains information regarding an individual comparison. Each list can have one of two configurations:

1. Lists with the first configuration are used to load data from files, and require the following fields:

name A string specifying the comparison name.

folders Vector of folder names where to read files from. These are recycled if length(folders) < length(files).

files Vector of filenames (with wildcards) to load in each folder.

- **Ivls** Vector of level or group names, must be the same length as files, i.e. each file set will be associated with a different group. If not given, default group names will be set.
- 2. Lists with the second configuration are used to load data from environment variables, and require the following fields:

name A string specifying the comparison name.

grpout Either an object of class grpoutputs or a list with the following two fields:

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data List of all outputs, where tags correspond to output names and values correspond to the output data. Output data is a *n* x *m* matrix, where *n* is the total number of output observations and *m* is the number of variables (i.e. output length).

obs_lvls Levels or groups associated with each observation.

concat	Create an additional, concatenated output? Ignored for sublists passed in the comps which follow the second configuration.
centscal	Method for centering and scaling outputs if concat is TRUE. It can be one of "center", "auto", "range" (default), "iqrange", "vast", "pareto" or "level". Centering and scaling is performed by the centerscale function.
lim_npcs	Limit number of principal components used for MANOVA to minimum number of observations per group?
mnv_test	The name of the test statistic to be used in MANOVA, as described in summary.manova.
	Options passed to read.table, which is used to read the files specified in lists using the first configuration in the comp parameter.

Value

An object of class micomp, which is a two-dimensional list of cmpoutput objects. Rows are associated with individual outputs, while columns are associated with separate comparisons.

```
# Create a micomp object from existing files and folders
dir nl ok <-
  system.file("extdata", "nl_ok", package = "micompr")
dir_jex_ok <-
  system.file("extdata", "j_ex_ok", package = "micompr")
dir_jex_noshuff <-</pre>
  system.file("extdata", "j_ex_noshuff", package = "micompr")
dir_jex_diff <-
  system.file("extdata", "j_ex_diff", package = "micompr")
files <- glob2rx("stats400v1*.tsv")</pre>
mic \leftarrow micomp(7, 0.8,
              list(list(name = "NLOKvsJEXOK",
                         folders = c(dir_nl_ok, dir_jex_ok),
                         files = c(files, files),
                        lvls = c("NLOK", "JEXOK")),
                   list(name = "NLOKvsJEXNOSHUFF",
                         folders = c(dir_nl_ok, dir_jex_noshuff),
                         files = c(files, files),
                         lvls = c("NLOK", "JEXNOSHUFF")),
                   list(name = "NLOKvsJEXDIFF",
                         folders = c(dir_nl_ok, dir_jex_diff),
                         files = c(files, files),
                         lvls = c("NLOK", "JEXDIFF"))),
              concat = TRUE)
```

```
# Create a micomp object from package datasets (i.e. grpoutputs objects)
# directly
mic <- micomp(c("o1", "o2", "o3", "o4"), 0.9,
              list(list(name = "NLOKvsJEXOK", grpout = pphpc_ok),
                   list(name = "NLOKvsJEXNOSHUFF", grpout = pphpc_noshuff),
                   list(name = "NLOKvsJEXDIFF", grpout = pphpc_diff)))
# Create a micomp object using manually inserted data
mic <- micomp(6, 0.5, list(
 list(name = "NLOKvsJEXOK",
      grpout = list(data = pphpc_ok$data,
                     obs_lvls = pphpc_ok$obs_lvls)),
 list(name = "NLOKvsJEXNOSHUFF",
      grpout = list(data = pphpc_noshuff$data,
                     obs_lvls = pphpc_noshuff$obs_lvls)),
 list(name = "NLOKvsJEXDIFF",
      grpout = list(data = pphpc_diff$data,
                     obs_lvls = pphpc_diff$obs_lvls))))
```

plot.assumptions_cmpoutput

Plot p-values for testing the assumptions of the parametric tests used in output comparison

Description

Plot method for objects of class assumptions_cmpoutput containing *p*-values produced by testing the assumptions of the parametric tests used for comparing an output.

Usage

```
## S3 method for class 'assumptions_cmpoutput' plot(x, ...)
```

Arguments

- x Objects of class assumptions_cmpoutput.
- ... Extra options passed to plot.default.

Details

Several bar plots are presented, showing the *p*-values yielded by the Shapiro-Wilk (shapiro.test) and Royston tests (mvn) for univariate and multivariate normality, respectively, and for the Bartlett (bartlett.test) and Box's M (boxM) for testing homogeneity of variances and of covariance matrices, respectively. The following bar plots are shown:

- One bar plot for the *p*-values of the Bartlett test, one bar (*p*-value) per individual principal component.
- *s* bar plots for *p*-values of the Shapiro-Wilk test, where *s* is the number of groups being compared. Individual bars in each plot are associated with a principal component.
- *t* bar plot for the *p*-values of the Royston test with *s* bars each, where *t* is the number of unique MANOVA tests performed (one per requested explained variances) and *s* is the number of groups being compared. These plots will not show if there is only one principal component being considered.
- One plot for the *p*-values of the Box's M test, one bar (*p*-value) per unique MANOVA tests performed (one per requested explained variances).

Value

None.

Examples

```
# Create a cmpoutput object from the provided datasets
cmp <- cmpoutput("All", 0.9, pphpc_ok$data[["All"]], pphpc_ok$obs_lvls)
# Display a bar plot with the p-values of the assumptions for the parametric
# tests performed in cmp
plot(assumptions(cmp))</pre>
```

plot.assumptions_manova

Plot p-values for testing the multivariate normality assumptions of the MANOVA test

Description

Plot method for objects of class assumptions_manova which presents a bar plot containing the *p*-values produced by the Royston multivariate normality test (mvn) for each group being compared.

Usage

```
## S3 method for class 'assumptions_manova' plot(x, ...)
```

Arguments

x Objects of class assumptions_manova.

Extra options passed to barplot. The col parameter defines colors for p-values below 1, 0.05 and 0.01, respectively.

Value

None.

Examples

```
# Plot the Royston test p-value for multivariate normality of each group
# (species) of the iris data
plot(assumptions_manova(iris[, 1:4], iris[, 5]))
# Plot the same data with logarithmic scale for p-values
plot(assumptions_manova(iris[, 1:4], iris[, 5]), log = "y")
```

```
plot.assumptions_micomp
```

Plot p-values for testing the assumptions of the parametric tests used in multiple output comparison

Description

Plot method for objects of class assumptions_cmpoutput containing p-values produced by testing the assumptions of the parametric tests used for multiple output comparisons.

Usage

```
## S3 method for class 'assumptions_micomp' plot(x, ...)
```

Arguments

- x Object of class assumptions_micomp.
- ... Extra options passed to barplot.

Details

Several bar plots are presented, one for each comparison and output combination, showing the several statistical tests employed to verify the assumptions of the parametric tests.

Value

None.

plot.assumptions_paruv

Examples

plot.assumptions_paruv

Plot p-values for testing the assumptions of the parametric tests used in output comparison

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Description

Plot method for objects of class assumptions_paruv containing *p*-values produced by testing the assumptions of the parametric tests used for comparing outputs.

Usage

```
## S3 method for class 'assumptions_paruv'
plot(x, ...)
```

Arguments

x Objects of class assumptions_paruv.

Extra options passed to barplot. The col parameter defines colors for p-values below 1, 0.05 and 0.01, respectively.

Details

One bar plot is presented for the Bartlett test (bartlett.test), showing the respective *p*-values along principal component. *s* bar plots are presented for the Shapiro-Wilk (shapiro.test), where *s* is the number of groups being compared; individual bars in each plot represent the *p*-values associated with each principal component.

Value

None.

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Examples

```
# Plot the Shapiro-Wilk and Bartlett test p-values for each dependent
# variable of the iris data
plot(assumptions_paruv(iris[, 1:4], iris[, 5]))
# Plot the same data with logarithmic scale for p-values
plot(assumptions_paruv(iris[, 1:4], iris[, 5]), log = "y")
```

plot.cmpoutput

Plot comparison of an output

Description

Plot objects of class empoutput.

Usage

```
## S3 method for class 'cmpoutput'
plot(x, ...)
```

Arguments

x Object of class empoutput.

Extra options passed to plot. default. The col option determines the colors to use on observations of different groups (scatter plot only).

Details

This method produces four sub-plots, namely:

- Scatter plot containing the projection of output observations on the first two dimensions of the principal components space.
- Bar plot of the percentage of variance explain per principal component.
- Bar plot of *p*-values for the parametric test for each principal component.
- Bar plot of *p*-values for the non-parametric test for each principal component.

Value

None.

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Examples

```
# Comparing the concatenated output of the pphpc_ok dataset, which
# contains simulation output data from two similar implementations of the
# PPHPC model.

plot(cmpoutput("All", 0.95, pphpc_ok$data[["All"]], pphpc_ok$obs_lvls))
```

plot.grpoutputs

Plot grouped outputs

Description

Plot objects of class grpoutputs.

Usage

```
## S3 method for class 'grpoutputs' plot(x, ...)
```

Arguments

x Object of class grpoutputs.

... Extra options passed to plot.default.

Details

Each output is plotted individually, and observations are plotted on top of each other. Observations from different groups are plotted with different colors (which can be controlled through the col parameter given in ...).

This function can be very slow for a large number of observations.

Value

None.

Examples

```
# Determine paths for the data folder containing outputs of different
# lengths
dir_na <- system.file("extdata", "testdata", "NA", package = "micompr")
# Sets of files A and B have 3 files each
filesA <- glob2rx("stats400v1*n20A.tsv")
filesB <- glob2rx("stats400v1*n20B.tsv")</pre>
```

Instantiate grpoutputs object

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```
go <-
  grpoutputs(7, dir_na, c(filesA, filesB), lvls = c("A", "B"), concat = TRUE)
# Plot grpoutputs object
plot(go)</pre>
```

plot.micomp

Plot projection of output observations on the first two dimensions of the principal components space

Description

For each comparison and output combination, draw a scatter plot containing the projection of output observations on the first two dimensions of the principal components space.

Usage

```
## S3 method for class 'micomp'
plot(x, ...)
```

Arguments

x An object of class micomp.

Extra options passed to plot.default. The col option determines the colors to use on observations of different groups.

Value

None.

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pphpc_diff	Data from two implementations of the PPHPC model, one of which setup with a different parameter

Description

A dataset containing simulation output data from two implementations of the PPHPC model, one of which setup with a different parameter.

Usage

pphpc_diff

Format

A grpoutputs object containing simulation output data from 20 runs of the PPHPC model, 10 runs from each implementation. The model has six outputs, but the object contains a seventh output corresponding to the concatenation of the six outputs

Source

Runs are obtained from the NetLogo and Java (EX with 8 threads) implementations of the PPHPC model available at https://github.com/nunofachada/pphpc. The config400v1.txt configuration was used in both cases, with the exception of restart parameter, c_r , in the Java implementation, which was set to 9 instead of 10.

pphpc_noshuff	Data from two implementations of the PPHPC model, one of which has agent list shuffling deactivated

Description

A dataset containing simulation output data from two implementations of the PPHPC model, one of which has agent list shuffling deactivated.

Usage

pphpc_noshuff

Format

A grpoutputs object containing simulation output data from 20 runs of the PPHPC model, 10 runs from each implementation. The model has six outputs, but the object contains a seventh output corresponding to the concatenation of the six outputs

Source

Runs are obtained from the NetLogo and Java (EX with 8 threads) implementations of the PPHPC model available at https://github.com/nunofachada/pphpc. The config400v1.txt configuration was used in both cases. Runs with the Java implementation were performed with the '-u' option, i.e. with agent list shuffling turned off.

pphpc_ok

Data from two similar implementations of the PPHPC model

Description

A dataset containing simulation output data from two implementations of the PPHPC model.

Usage

pphpc_ok

Format

A grpoutputs object containing simulation output data from 20 runs of the PPHPC model, 10 runs from each implementation. The model has six outputs, but the object contains a seventh output corresponding to the concatenation of the six outputs

Source

Runs are obtained from the NetLogo and Java (EX with 8 threads) implementations of the PPHPC model available at https://github.com/nunofachada/pphpc. The configuration was used in both cases.

```
print.assumptions_cmpoutput
```

Print method for the assumptions of parametric tests used in a comparison of an output

Description

Print method for objects of class assumptions_cmpoutput, which contain the assumptions for the parametric tests used in a comparison of an output.

Usage

```
## S3 method for class 'assumptions_cmpoutput'
print(x, ...)
```

Arguments

x Object of class assumptions_cmpoutput.

... Currently ignored.

Value

None.

Examples

print.assumptions_manova

Print information about the assumptions of the MANOVA test

Description

Print information about objects of class assumptions_manova, which represent the assumptions of the MANOVA test performed on a comparison of outputs.

Usage

```
## S3 method for class 'assumptions_manova' print(x, ...)
```

Arguments

- x Object of class assumptions_manova.
- ... Currently ignored.

Value

The argument x, invisibly, as for all print methods.

```
# Print information concerning the assumptions of applying MANOVA to the iris
# data (i.e. multivariate normality of each group and homogeneity of
# covariance matrices)
assumptions_manova(iris[, 1:4], iris[, 5])
```

```
print.assumptions_micomp
```

Print information about the assumptions concerning the parametric tests performed on multiple comparisons of outputs

Description

Print information about objects of class assumptions_micomp, which represent the assumptions concerning the parametric tests performed on multiple comparisons of outputs.

Usage

```
## S3 method for class 'assumptions_micomp' print(x, ...)
```

Arguments

- x Object of class assumptions_micomp.
- ... Currently ignored.

Value

The argument x, invisibly, as for all print methods.

Examples

```
print.assumptions_paruv
```

Print information about the assumptions of the parametric test

Description

Print information about objects of class assumptions_paruv, which represent the assumptions of the parametric test (i.e. either t.test or aov) performed on a comparison of outputs.

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Usage

```
## S3 method for class 'assumptions_paruv'
print(x, ...)
```

Arguments

- x Object of class assumptions_paruv.
- ... Currently ignored.

Value

The argument x, invisibly, as for all print methods.

Examples

```
# Print information about the assumptions of applying ANOVA to each column
# (dependent variable) of the iris data (i.e. normality of each group and
# homogeneity of variances)
assumptions_paruv(iris[, 1:4], iris[, 5])
```

print.cmpoutput

Print information about comparison of an output

Description

Print information about objects of class empoutput.

Usage

```
## S3 method for class 'cmpoutput'
print(x, ...)
```

Arguments

- x Object of class empoutput.
- ... Currently ignored.

Value

The argument x, invisibly, as for all print methods.

26 print.grpoutputs

Examples

```
# Comparing the fifth output of the pphpc_diff dataset, which contains
# simulation output data from two implementations of the PPHPC model executed
# with a different parameter.
cmpoutput("WolfPop", 0.7, pphpc_diff$data[[5]], pphpc_diff$obs_lvls)
```

print.grpoutputs

Print information about grouped outputs

Description

Print information about objects of class grpoutputs.

Usage

```
## S3 method for class 'grpoutputs'
print(x, ...)
```

Arguments

x Object of class grpoutputs.

... Currently ignored.

Value

The argument x, invisibly, as for all print methods.

```
# Determine paths for data folders, each containing outputs for 10 runs of
# the PPHPC model
dir_nl_ok <- system.file("extdata", "nl_ok", package = "micompr")
dir_jex_diff <- system.file("extdata", "j_ex_diff", package = "micompr")
files <- glob2rx("stats400v1*.tsv")

# Create a grpoutputs object
go <- grpoutputs(6, c(dir_nl_ok, dir_jex_diff), c(files, files))
# Print information about object (could just type "go" instead)
print(go)</pre>
```

print.micomp 27

print.micomp

Print information about multiple comparisons of outputs

Description

Print information about objects of class micomp.

Usage

```
## S3 method for class 'micomp'
print(x, ...)
```

Arguments

x Object of class micomp.... Currently ignored.

Value

The argument x, invisibly, as for all print. methods.

Examples

pvalf

Format p-values

Description

Generic function to format *p*-values.

Usage

```
pvalf(pval, params)
```

Arguments

pval Numeric *p*-value to format (between 0 and 1).

params A list of method-dependent options.

28 pvalf.default

Value

A string representing the formatted *p*-value.

See Also

```
pvalf.default
```

pvalf.default

Default p-value formatting method

Description

Format a *p*-value for printing in a LaTeX table. Requires the *ulem* LaTeX package for underlining the *p*-values.

Usage

```
## Default S3 method:
pvalf(pval, params = list())
```

Arguments

pval Numeric value between 0 and 1.

params A list of options. This function accepts the following options:

 $m{minval}$ If p-value is below this value, return this value preceded by a "<" sign

instead instead.

lim1val If p-value is below this value, it will be double-underlined.

lim2val If *p*-value is below this value, it will be underlined. **na_str** String to use for NAs. By default NAs are returned as is.

Value

A string representing the formatted pval.

```
summary.assumptions_cmpoutput
```

Summary method for the assumptions of parametric tests used in a comparison of an output

Description

Summary method for objects of class assumptions_cmpoutput, which contain the assumptions for the parametric tests used in a comparison of an output.

Usage

```
## S3 method for class 'assumptions_cmpoutput'
summary(object, ...)
```

Arguments

```
object Object of class assumptions_cmpoutput.
... Currently ignored.
```

Value

A list with the following items:

manova A matrix of *p*-values for the MANOVA assumptions. All rows, expect the last one, correspond to the Royston test for multivariate normality for each group; the last row corresponds to Box's M test for homogeneity of covariance matrices. Columns correspond to number of principal components required to explain the percentage of user-specified variance.

ttest A matrix of *p*-values for the *t*-test assumptions. All rows, expect the last one, correspond to the Shapiro-Wilk normality test for each group; the last row corresponds to Bartlett's for equality of variances. Columns correspond to the principal components on which the *t*-test was applied.

```
summary.assumptions_micomp
```

Summary method for the assumptions of parametric tests used in multiple comparisons of outputs

Description

Summary method for objects of class assumptions_micomp, which contain the assumptions for the parametric tests used in multiple comparisons of outputs.

Usage

```
## S3 method for class 'assumptions_micomp'
summary(object, ...)
```

Arguments

```
objectObject of class assumptions_micomp....Currently ignored.
```

Value

A list in which each component is associated with a distinct comparison. Each component contains a matrix, in which columns represent individual outputs and rows correspond to the statistical tests evaluating the assumptions of the parametric tests used in each output. More specifically, each matrix has rows with the following information:

Royston (*group*, *ve=%/npcs=*) One row per group per variance to explain / number of PCs, with the *p*-value yielded by the Royston test (mvn) for the respective group and variance/npcs combination.

Box's M (ve=%/npcs=) One row per variance to explain with the p-value yielded by Box's M test (boxM).

Shapiro-Wilk (*group*) One row per group, with the *p*-value yielded by the Shapiro-Wilk test (shapiro.test) for the respective group.

Bartlett One row with the *p*-value yielded by Bartlett's test (bartlett.test).

summary.cmpoutput 31

summary.cmpoutput

Summary method for comparison of an output

Description

Summary method for objects of class empoutput.

Usage

```
## S3 method for class 'cmpoutput'
summary(object, ...)
```

Arguments

object Object of class cmpoutput.

... Currently ignored.

Value

A list with the following components:

output.name Output name.

num.pcs Number of principal components which explain var. exp percentage of variance.

var.exp Minimum percentage of variance which must be explained by the number of principal components used for the MANOVA test.

manova.pvals P-value of the MANOVA test.

parametric.test Name of the used parametric test.

parametric.pvals Vector of \$p\$-values returned by applying the parametric test to each principal component.

parametric.pvals.adjusted Vector of \$p\$-values returned by applying the parametric test to each principal component, adjusted with the weighted Bonferroni procedure, percentage of explained variance used as weight.

nonparametric.test Name of the used non-parametric test.

nonparametric.pvals Vector of \$p\$-values returned by applying the non-parametric test to each principal component.

nonparametric.pvals.adjusted Vector of \$p\$-values returned by applying the non-parametric test to each principal component, adjusted with the weighted Bonferroni procedure, percentage of explained variance used as weight.

32 summary.grpoutputs

Examples

```
# Comparing the concatenated output of the pphpc_noshuff dataset, which
# contains simulation output data from two implementations of the PPHPC model
# executed with a minor implementation difference.
summary(
  cmpoutput("All", 0.6, pphpc_noshuff$data[["All"]], pphpc_noshuff$obs_lvls)
)
```

summary.grpoutputs

Summary method for grouped outputs

Description

Summary method for objects of class grpoutputs.

Usage

```
## S3 method for class 'grpoutputs'
summary(object, ...)
```

Arguments

```
object Object of class grpoutputs.
... Currently ignored.
```

Value

A list with the following components:

output.dims Dimensions for each output, i.e. number of observations and number of variables (i.e. output length).

group.sizes Number of output observations in each group.

```
# Determine paths for data folders, each containing outputs for 10 runs of
# the PPHPC model
dir_nl_ok <- system.file("extdata", "nl_ok", package = "micompr")
dir_jex_noshuff <-
    system.file("extdata", "j_ex_noshuff", package = "micompr")
files <- glob2rx("stats400v1*.tsv")

# Create a groutputs object
go <-
groutputs(c("o1", "o2"), c(dir_nl_ok, dir_jex_noshuff), c(files, files))</pre>
```

summary.micomp 33

summary.micomp

Summary method for multiple comparisons of outputs

Description

Summary method for objects of class micomp.

Usage

```
## S3 method for class 'micomp'
summary(object, ...)
```

Arguments

```
object Object of class micomp.
... Currently ignored.
```

Value

A list in which each component is associated with a distinct comparison. Each component contains a matrix, in which columns represent individual outputs and rows have information about the outputs. More specifically, each matrix has the following rows:

#PCs (ve=%) Number of principal components required to explain the specified percentage of variance. There is one row of this kind for each percentage of variance specified when creating the micomp object.

MANOVA (ve=%) *P*-value for the MANOVA test applied to the #PCs required to explain the specified percentage of variance. There is one row of this kind for each percentage of variance specified when creating the micomp object.

par.test *P*-value for the parametric test (first principal component).

nonpar.test *P*-value for the non-parametric test (first principal component).

par.test.adjust *P*-value for the parametric test (first principal component), adjusted with the weighted Bonferroni procedure, percentage of explained variance used as weight.

nonpar.test.adjust *P*-value for the non-parametric test (first principal component), adjusted with the weighted Bonferroni procedure, percentage of explained variance used as weight.

34 tikzscat

tikzscat	Simple TikZ scatter plot	

Description

Create a simple 2D TikZ scatter plot, useful for plotting PCA data.

Usage

```
tikzscat(data, obs_lvls, marks, tscale, axes_color = "gray")
```

Arguments

data	Data to plot, $m \times 2$ numeric matrix, where m is the number of observations or points to plot.
obs_lvls	Levels or groups associated with each observation.
marks	Character vector determining how to draw the points in TikZ, for example: c("mark=square*,mark options={color=red},mark size=0.8pt", "mark=diamond*,mark options={color=black},mark size=1pt", "mark=triangle*,mark options={color=green},mark size=1pt").

tscale The scale property of the TikZ figure.

axes_color Axes color (must be a LaTeX/TikZ color).

Details

This function creates a simple TikZ 2D scatter plot within a tikzpicture environment. The points are plotted on a normalized figure with x and y axes bounded between [-1, 1]. To render adequately, the final LaTeX document should load the plotmarks TikZ library.

Value

A string containing the TikZ figure code for plotting the specified data.

toLatex.cmpoutput 35

toLatex.cmpoutput

Convert cmpoutput object to LaTeX table

Description

This method converts cmpoutput objects to character vectors representing LaTeX tables.

Usage

```
## S3 method for class 'cmpoutput'
toLatex(object, cmp_name = "Comp. 1", ...)
```

Arguments

object A cmpoutput object.

cmp_name Comparison name (to appear in table).

... Any options accepted by the toLatex.micomp function.

Details

This method simply wraps the cmpoutput object into a micomp object, and invokes toLatex.micomp on the wrapped object.

Value

A character vector where each element holds one line of the corresponding LaTeX table.

```
# Create a cmpoutput object by comparing the first output ("Pop.Sheep") of
# one the provided datasets.
cmp <-
    cmpoutput("SheepPop", 0.9, pphpc_ok$data[["Pop.Sheep"]], pphpc_ok$obs_lvls)
# Print latex table source to screen
toLatex(cmp)</pre>
```

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toLatex.micomp

Convert micomp object to LaTeX table

Description

This method converts micomp objects to character vectors representing LaTeX tables.

Usage

```
## S3 method for class 'micomp'
toLatex(
  object,
  orientation = T,
  data_show = c("npcs-1", "mnvp-1", "parp-1", "nparp-1", "scoreplot"),
  data_labels = NULL,
  labels\_cmp\_show = T,
  labels_col_show = T,
  label_row_show = T,
  tag_comp = "Comp.",
  tag_data = "Data",
  tag_outputs = "Outputs",
  table_placement = "ht",
  latex_envs = c("center"),
  booktabs = F,
  booktabs_cmalign = "1",
  caption = NULL,
  caption_cmd = "\\caption",
  label = NULL,
  col_width = F,
  pvalf_f = pvalf.default,
  pvalf_params = list(),
  scoreplot_marks = c("mark=square*,mark options={color=red},mark size=0.8pt",
    "mark=diamond*,mark options={color=black},mark size=1pt",
    "mark=triangle*,mark options={color=green},mark size=1pt"),
  scoreplot_scale = 6,
  scoreplot_before = "\raisebox{-.5}\height}{\resizebox {1.2cm} {1.2cm} {",}
  scoreplot_after = "}}"
)
```

Arguments

orientation

object A micomp object.
... Currently ignored.

If TRUE, outputs are placed along columns, while data is placed along rows. If FALSE, outputs are placed along rows, while data is placed along columns.

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data_show

Vector of strings specifying what data to show. Available options are:

npcs-i Number of principal components required to explain i-th user-specified percentage of variance.

mnvp-i MANOVA *p*-values for the i-th user-specified percentage of variance to explain.

parp-j Parametric test *p*-values for the j-th principal component.

nparp-j Non-parametric test *p*-values for the j-th principal component.

aparp-j Parametric test *p*-values adjusted with weighted Bonferroni procedure for the j-th principal component.

anparp-j Non-parametric test *p*-values adjusted with weighted Bonferroni procedure for the j-th principal component.

varexp-j Explained variance for the j-th principal component.

scoreplot Output projection on the first two principal components.

sep Place a separator (e.g. midrule) between data.

data_labels

Vector of strings specifying the labels of the data to show. If NULL, default labels are used for all elements. If individual elements are set to NA, default labels will be used for those elements.

labels_cmp_show

Show the column containing the comparison labels?

labels_col_show

Show the column containing the data labels (orientation == T) or the output labels (orientation == F)?

label_row_show

tag_comp

Show the tag_outputs tag? If TRUE, the row identifier part will have two levels, the tag_outputs label and output names (orientation == T), or the tag_data and data labels (orientation == F). If FALSE only the output names or data labels are shown.

Tag identifying comparison labels.

tag_data Tag identifying data labels.
tag_outputs Tag identifying outputs.

table_placement

LaTeX table placement.

latex_envs Wrap table in the specified LaTeX environments.

booktabs Use booktabs table beautifier package?

booktabs_cmalign

How to align cmidule when using the booktabs package.

caption Table caption.

caption_cmd Command used for table caption.

label Table label for cross-referencing.

col_width Resize table to page column width?

pvalf_f P-value formatter function, which receives a numeric value between 0 and 1

and returns a string containing the formatted value. Default is pvalf.default

(requires ulem LaTeX package).

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```
pvalf_params Parameters for pvalf_f function. Default is empty list.

scoreplot_marks

Vector of strings specifying how TikZ should draw points belonging to each group in the score plot.

scoreplot_scale

TikZ scale for each score plot figure.

scoreplot_before

LaTeX code to paste before each TikZ score plot figure.

scoreplot_after

LaTeX code to paste after each TikZ score plot figure.
```

Details

This method is inspired by the functionality provided by the xtable and print.xtable functions (from the xtable package), but follows the standard behavior of the toLatex generic.

Value

A character vector where each element holds one line of the corresponding LaTeX table.

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