# Package 'MorphoTools2'

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Type Package

Title Multivariate Morphometric Analysis

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Description Tools for multivariate analyses of morphological data, wrapped in one pack-

age, to make the workflow convenient and fast. Statistical and graphical tools provide a comprehensive framework for checking and manipulating input data, statistical analyses, and visualization of results. Several methods are provided for the analy-

sis of raw data, to make the dataset ready for downstream analyses. Integrated statistical methods include hierarchical classification, principal component analysis, principal coordinates analysis, non-metric multidimensional scaling, and multiple discriminant analyses: canonical, stepwise, and classificatory (linear, quadratic, and the non-parametric k nearest neighbours). The philosophy of the package will be described in Šlenker et al. (in prep).

URL https://github.com/MarekSlenker/MorphoTools2

BugReports https://github.com/MarekSlenker/MorphoTools2/issues

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License GPL-3

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boxMTest

Box's M-test for Homogeneity of Covariance Matrices

### **Description**

The boxMTest function performs Box's (1949) M-test for homogeneity of covariance matrices. The null hypothesis for this test is that the observed covariance matrices for the dependent variables are equal across groups.

### Usage

```
boxMTest(object)
```

### **Arguments**

object

an object of class morphodata.

#### Value

None. Used for its side effect.

### References

**Box G.E.P.** (1949). A general distribution theory for a class of likelihood criteria. *Biometrika* 36, 317-346.

```
data(centaurea)
# remove NAs and linearly dependent characters (characters with unique contributions
                  can be identified by stepwise discriminant analysis.)
centaurea = naMeanSubst(centaurea)
centaurea = removePopulation(centaurea, populationName = c("LIP", "PREL"))
centaurea = keepCharacter(centaurea, c("MLW", "ML", "IW", "LS", "IV", "MW", "MF",
                                    "AP", "IS", "LBA", "LW", "AL", "ILW", "LBS",
                                    "SFT", "CG", "IL", "LM", "ALW", "AW", "SF") )
# add a small constant to characters witch are invariant within taxa
centaurea$data[ centaurea$Taxon == "hybr", "LM" ][1] =
             centaurea$data[ centaurea$Taxon == "hybr", "LM" ][1] + 0.000001
centaurea$data[ centaurea$Taxon == "ph", "IV" ][1] =
             centaurea$data[ centaurea$Taxon == "ph", "IV" ][1] + 0.000001
centaurea$data[ centaurea$Taxon == "st", "LBS"][1] =
             centaurea$data[ centaurea$Taxon == "st", "LBS"][1] + 0.000001
boxMTest(centaurea)
```

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xplotCharacter Box Plots

### Description

These functions produce a box-and-whisker plot(s) of the given morphological character(s).

### Usage

### **Arguments**

object an object of class morphodata.

character a morphological character used to plot boxplot.

folderName folder to save produced boxplots.

outliers logical, if TRUE, the outliers are drawn.

lowerWhisker percentile to which the lower whisker is extended.

upperWhisker percentile to which the upper whisker is extended.

col background colour for the boxes. border colour of outliers and the lines.

frame logical, if TRUE, a 'frame' (box around the plot) is drawn.

main main title for the plot.

cex.main magnification to be used for the main title.

pch plotting symbol of the outliers. xlab, ylab title of the respective axes.

horizontal logical, indicating if the boxplot should be horizontal.

varwidth logical, if TRUE, the boxes are drawn with widths proportional to the square-roots

of the number of observations in the groups.

width the width of the figure. height the height of the figure.

units the units in which height and width are given. Can be "px" (pixels, the de-

fault), "in" (inches), "cm" or "mm".

... further arguments to be passed to boxplot or bxp.

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#### **Details**

These functions modify the classical boxplot function to allow whiskers to be extended to the desired percentiles. By default, the whiskers are extended to the 5th and 95th percentiles, because of the trimmed range (without the most extreme 10% of values) use to be used in taxa descriptions, determination keys, etc. Box defines 25th and 75th percentiles, bold horizontal line shows median (50th percentile). Missing values are ignored.

The boxplotAll function produces boxplots for each morphological character and saves them to a folder defined by the folderName argument. If it does not exist, a new folder is created.

#### Value

None. Used for its side effect of producing a plot(s).

### **Examples**

cda.calc

Canonical Discriminant Analysis

### **Description**

This function performs canonical discriminant analysis.

### Usage

```
cda.calc(object, passiveSamples = NULL)
```

### **Arguments**

```
object an object of class morphodata.

passiveSamples taxa or populations, which will be only predicted, see Details.
```

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#### **Details**

The cda.calc function performs canonical discriminant analysis using the candisc method from the candisc package. Canonical discriminant analysis finds linear combination of the quantitative variables that maximize the difference in the mean discriminant score between groups. This function allows exclude subset of samples (passiveSamples) from computing the discriminant function, and only passively predict them in multidimensional space. This approach is advantageous for testing the positions of "atypical" populations (e.g., putative hybrids) or for assessing positions of selected individuals (e.g., type herbarium specimens).

#### Value

```
an object of class cdadata with the following elements:
```

objects

ID IDs of each row of scores object.

Population population membership of each row of scores object.

Taxon taxon membership of each row of scores object. scores ordination scores of cases (objects, OTUs).

eigenValues eigenvalues, i.e., proportion of variation of the original dataset expressed by

individual axes.

eigenvaluesAsPercent

eigenvalues as percent, percentage of their total sum.

cumulativePercentageOfEigenvalues

cumulative percentage of eigenvalues.

groupMeans data. frame containing the means for the taxa.

rank number of non-zero eigenvalues.

coeffs.raw matrix containing the raw canonical coefficients.

coeffs.std matrix containing the standardized canonical coefficients.

totalCanonicalStructure

matrix containing the total canonical structure coefficients, i.e., total-sample cor-

relations between the original variables and the canonical variables.

canrsq squared canonical correlations.

```
data(centaurea)
centaurea = naMeanSubst(centaurea)
centaurea = removePopulation(centaurea, populationName = c("LIP", "PREL"))

cdaRes = cda.calc(centaurea)

summary(cdaRes)

plotPoints(cdaRes, col = c("red", "green", "blue", "red"),
    pch = c(20, 17, 8, 21), pt.bg = "orange", legend = TRUE)
```

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cdadata Class Cdadata

### **Description**

The cdadata class is designed for storing results of canonical discriminant analysis.

#### **Format**

Class cdadata.

objects ID IDs of each row of scores object.

Population population membership of each row of scores object.

**Taxon** taxon membership of each row of scores object.

scores ordination scores of cases (objects, OTUs).

**eigenValues** eigenvalues, i.e., proportion of variation of the original dataset expressed by individual axes.

eigenvalues As Percent eigenvalues as percent, percentage of their total sum.

cumulativePercentageOfEigenvalues cumulative percentage of eigenvalues.

groupMeans data. frame containing the means for the taxa.

rank number of non-zero eigenvalues.

coeffs.raw matrix containing the raw canonical coefficients.

**coeffs.std** matrix containing the standardized canonical coefficients.

**totalCanonicalStructure** matrix containing the total canonical structure coefficients, i.e., total-sample correlations between the original variables and the canonical variables.

canrsq squared canonical correlations.

centaurea 25 Morphological Characters of Three Species of the Centaurea phrygia Complex

### **Description**

The sample data include part of data sets from previously published studies by Koutecky (2007) and Koutecky et al. (2012): 25 morphological characters (see the cited studies for details) of the vegetative (stems and leaves) and reproductive structures (capitula and achenes) of three diploid species of the *Centaurea phrygia* complex: *C. phrygia* L. s.str. (abbreviated "ph"), *C. pseudophrygia* C.A.Mey. ("ps") and *C. stenolepis* A.Kern. ("st"). Moreover, a fourth group includes the putative hybrid of the *C. pseudophrygia* and *C. stenolepis* ("hybr"). The data represent 8, 12, 7 and 6 populations for each group, respectively, and 20 individuals per population, with one exception in which only 12 individuals were available. All morphological characters are either quantitative (sizes, counts, or ratios) or binary (two characters states or presence/absence). In four characters of achenes (AL, AW, ALW, AP), there are missing data because fruits were not available in all individuals. In two populations of *C. stenolepis* (LIP, PREL) fruits were completely missing. In total, the data set includes 652 individuals (453 complete) from 33 populations (31 complete).

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### Usage

```
data(centaurea)
```

#### **Format**

an object of class morphodata with the following elements:

ID IDs of each row of data object.

Population population membership of each row of data object.

Taxon taxon membership of each row of data object.

data data. frame of individuals (rows) and values of morphological characters (columns).

### References

**Koutecky P. (2007)**. Morphological and ploidy level variation of *Centaurea phrygia* agg. (Asteraceae) in the Czech Republic, Slovakia and Ukraine. *Folia Geobotanica* 42, 77-102.

**Koutecky P., Stepanek J., Badurova T. (2012)**. Differentiation between diploid and tetraploid *Centaurea phrygia*: mating barriers, morphology and geographic distribution. *Preslia* 84, 1-32.

characters

List Morphological Characters

# Description

Returns list morphological characters of object.

### Usage

```
characters(object)
```

### **Arguments**

object

an object of class morphodata, pcadata or cdadata.

### Value

A character vector containing names of morphological characters of object.

# Examples

```
data(centaurea)
```

characters(centaurea)

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classif.lda

Classificatory Discriminant Analysis

#### **Description**

These functions computes discriminant function for classifying observations. Linear discriminant function (classif.lda), quadratic discriminant function (classif.qda), or nonparametric k-nearest neighbours classification method (classif.knn) can be used.

# Usage

```
classif.lda(object, crossval = "indiv")
classif.qda(object, crossval = "indiv")
classif.knn(object, k, crossval = "indiv")
```

### **Arguments**

object an object of class morphodata.

crossval crossvalidation mode, sets individual ("indiv"; default, one-leave-out method)

or whole populations ("pop") as leave-out unit.

k number of neighbours considered for the k-nearest neighbours method.

### **Details**

The classif.lda and classif.qda performs classification using linear and quadratic discriminant functions with cross-validation using the lda and qda functions from the package MASS. The prior probabilities of group memberships are equal.

LDA and QDA analyses have some requirements: (1) no character can be a linear combination of any other character; (2) no pair of characters can be highly correlated; (3) no character can be invariant in any taxon; (4) for the number of taxa (g), characters (p) and total number of samples (n) should hold: 0 , and (5) there must be at least two groups (taxa), and in each group there must be at least two objects. Violation of some of these assumptions may result in warnings or error messages (rank deficiency).

Nonparametric classification method k-nearest neighbours is performed using the knn and knn.cv functions from the package class.

The mode of crossvalidation is set by the parameter crossval. The default "indiv" uses the standard one-leave-out method. However, as some hierarchical structure is usually present in the data (individuals from a population are not completely independent observations, as they are morphologically closer to each other than to individuals from other populations), the value "pop" sets whole populations as leave-out units. The latter method does not allow classification if there is only one population for a taxon and is more sensitive to "atypical" populations, which usually leads to a somewhat lower classification success rate.

The coefficients of the linear discriminant functions (above) can be directly applied to classify individuals of unknown group membership. The sums of constant and multiples of each character by

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the corresponding coefficient are compared among the groups. The unknown individual is classified into the group that shows the higher score. If the populations leave-out cross-validation mode is selected (crossval = "pop"): (1) each taxon must be represented by at least two populations; (2) coefficients of classification functions are computed as averages of coefficients retrieved after each run with one population removed.

#### Value

an object of class classifdata with the following elements:

ID IDs of each row.

Population population membership of each row.

Taxon taxon membership of each row.

classif.funs the classification functions computed for raw characters (descriptors). If crossval

= "pop", means of coefficients of classification functions are computed.

classif classification from discriminant analysis.

prob posterior probabilities of classification into each taxon (if calculated by classif.lda

or classif. qda), or proportion of the votes for the winning class (calculated by

classif.knn)

correct logical, correctness of classification.

#### See Also

```
classifSample.lda, classif.matrix, knn.select
```

```
data(centaurea)
# remove NAs and linearly dependent characters (characters with unique contributions
                   can be identified by stepwise discriminant analysis.)
centaurea = naMeanSubst(centaurea)
centaurea = removePopulation(centaurea, populationName = c("LIP", "PREL"))
centaurea = keepCharacter(centaurea, c("MLW", "ML", "IW", "LS", "IV", "MW", "MF",
                                    "AP", "IS", "LBA", "LW", "AL", "ILW", "LBS",
                                    "SFT", "CG", "IL", "LM", "ALW", "AW", "SF") )
# add a small constant to characters witch are invariant within taxa
centaurea$data[ centaurea$Taxon == "hybr", "LM" ][1] =
             centaurea$data[ centaurea$Taxon == "hybr", "LM" ][1] + 0.000001
centaurea$data[ centaurea$Taxon == "ph", "IV" ][1] =
             centaurea$data[ centaurea$Taxon == "ph", "IV" ][1] + 0.000001
centaurea$data[ centaurea$Taxon == "st", "LBS"][1] =
             centaurea$data[ centaurea$Taxon == "st", "LBS"][1] + 0.000001
# classification by linear discriminant function
classifRes.lda = classif.lda(centaurea, crossval = "indiv")
```

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```
# classification by quadratic discriminant function
classifRes.qda = classif.qda(centaurea, crossval = "indiv")

# classification by nonparametric k-nearest neighbour method
# use knn.select to find the optimal K.
knn.select(centaurea, crossval = "pop")
classifRes.knn = classif.knn(centaurea, k = 12, crossval = "pop")

# exporting results
classif.matrix(classifRes.lda, level = "taxon")
classif.matrix(classifRes.qda, level = "taxon")
classif.matrix(classifRes.knn, level = "taxon")
```

classif.matrix

Format the Classifdata to Summary Table

### **Description**

The classif.matrix method formats the results stored in classifidata class to a summary classification table of taxa, populations, or individuals.

#### Usage

```
classif.matrix(result, level = "taxon")
```

# **Arguments**

result an object of class classifdata.

level level of grouping of classification matrix, "taxon" (default), populations ("pop"),

or individuals ("indiv")

# Value

A data. frame, summary classification table.

```
data(centaurea)

centaurea = naMeanSubst(centaurea)
centaurea = removePopulation(centaurea, populationName = c("LIP", "PREL"))

# classification by linear discriminant function
classifRes.lda = classif.lda(centaurea, crossval = "indiv")

# exporting results
classif.matrix(classifRes.lda, level = "taxon")
classif.matrix(classifRes.lda, level = "pop")
```

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classifdata

Class classifdata

# **Description**

The classifidata class is designed for storing results of classificatory discriminant analysis.

### **Format**

Class classifdata.

ID IDs of each row.

Population population membership of each row.

Taxon taxon membership of each row.

**classif** classification from discriminant analysis.

**classif.funs** the classification functions computed for raw characters (descriptors). If crossval = "pop", means of coefficients of classification functions are computed.

**prob** posterior probabilities of classification into each taxon (if calculated by classif.lda or classif.qda), or proportion of the votes for the winning class (calculated by classif.knn) **correct** logical, correctness of classification.

classifSample.lda

Classificatory Discriminant Analysis

### **Description**

These functions compute discriminant function based on an independent training set and classify observations in sample set. Linear discriminant function (classifSample.lda), quadratic discriminant function (classifSample.qda), or nonparametric k-nearest neighbour classification method (classifSample.knn) can be used.

### Usage

```
classifSample.lda(sampleData, trainingData)
classifSample.qda(sampleData, trainingData)
classifSample.knn(sampleData, trainingData, k)
```

### **Arguments**

sampleData observations which should be classified. An object of class morphodata.

trainingData observations for computing discriminant function. An object of class morphodata.

k number of neighbours considered.

classifSample.lda 13

#### **Details**

The classifSample.lda and classifSample.qda performs classification using linear and quadratic discriminant function using the lda and qda functions from the package MASS. Nonparametric classification method classifSample.knn (k-nearest neighbours) is performed using the knn functions from the package class. The classifSample functions are designed to classify hybrid populations, type herbarium specimens, atypical samples, entirely new data, etc. Discriminant criterion is developed from the original (training) dataset and applied to the specific sample (set).

LDA and QDA analyses have some requirements: (1) no character can be a linear combination of any other character; (2) no pair of characters can be highly correlated; (3) no character can be invariant in any taxon (group); (4) for the number of taxa (g), characters (p) and total number of samples (n) should hold: 0 , and (5) there must be at least two groups (taxa), and in each group there must be at least two objects. Violation of some of these assumptions may result in warnings or error messages (rank deficiency).

### Value

an object of class classifdata with the following elements:

ID IDs of each row.

Population population membership of each row.

Taxon taxon membership of each row.

classif classification from discriminant analysis.

prob posterior probabilities of classification into each taxon (if calculated by classif.lda

or classif.qda), or proportion of the votes for the winning class (calculated by

classif.knn)

correct logical, correctness of classification.

#### See Also

```
classif.lda, classif.matrix, knn.select
```

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```
centaurea$data[ centaurea$Taxon == "st", "LBS"][1] + 0.000001
```

```
trainingSet = removePopulation(centaurea, populationName = "LES")
LES = keepPopulation(centaurea, populationName = "LES")

# classification by linear discriminant function
classifSample.lda(LES, trainingSet)

# classification by quadratic discriminant function
classifSample.qda(LES, trainingSet)

# classification by nonparametric k-nearest neighbour method
# use knn.select to find the optimal K.
knn.select(trainingSet)
classifSample.knn(LES, trainingSet, k = 12)
```

clust

Hierarchical Clustering

### **Description**

Hierarchical cluster analysis of objects.

### Usage

### **Arguments**

object an object of class morphodata.

distMethod the distance measure to be used. This must be one of: "Euclidean" (default),

"Manhattan", "Minkowski", "Jaccard", "simpleMatching", or "Gower". See

details.

clustMethod the agglomeration method to be used: "average" (= "UPGMA"; default), "complete",

"ward.D" (= "Ward"), "ward.D2", "single", "Mcquitty" (= "WPGMA"), "median"

(= "WPGMC") or "centroid" (= "UPGMC"). See hclust for details.

binaryChs, nominalChs, ordinalChs

names of categorical ordinal, categorical nominal (multistate), and binary char-

acters. Needed for Gower's dissimilarity coefficient only, see details.

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#### **Details**

This function performs agglomerative hierarchical clustering. Typically, populations are used as OTUs (operational taxonomic units). Characters are standardised to a zero mean and a unit standard deviation.

Various measures of distance between the observations (rows) are applicable: (1) coefficients of distance for quantitative and binary characters: "Euclidean", "Manhattan", "Minkowski"; (2) similarity coefficients for binary characters: "Jaccard" and simple matching ("simpleMatching"); (3) coefficient for mixed data: "Gower". Note that the other than default methods for clustering and distance measurement are rarely used in morphometric analyses.

The Gower's dissimilarity coefficient can handle different types of variables. Characters have to be divided into four categories: (1) quantitative characters, (2) categorical ordinal characters, (3) categorical nominal (multistate) characters, and (4) binary characters. All characters are considered to be quantitative characters unless otherwise specified. Other types of characters have to be explicitly specified. To mark characters as ordinal, nominal, or binary, enumerate them by names using ordinalChs, nominalChs, and binaryChs arguments, respectively.

#### Value

An object of class 'hclust'. It encodes a stepwise dendrogram.

```
data(centaurea)
clustering.UPGMA = clust(centaurea)
plot(clustering.UPGMA, cex = 0.6, frame.plot = TRUE, hang = -1,
       main = "", sub = "", xlab = "", ylab = "distance")
# using Gower's method
data = list(
    ID = as.factor(c("id1","id2","id3","id4","id5","id6")),
   Population = as.factor(c("Pop1", "Pop1", "Pop2", "Pop2", "Pop3", "Pop3")),
   Taxon = as.factor(c("TaxA", "TaxA", "TaxA", "TaxB", "TaxB")),
    data = data.frame(
     stemBranching = c(1, 1, 1, 0, 0, 0), # binaryChs
    petalColour = c(1, 1, 2, 3, 3, 3), # nominalChs; 1=white, 2=red, 3=blue
   leaves = c(1,1,1,2,2,3), # nominalChs; 1=simple, 2=palmately compound, 3=pinnately compound
     taste = c(2, 2, 2, 3, 1, 1), # ordinal; 1=hot, 2=hotter, 3=hottest
     stemHeight = c(10, 11, 14, 22, 23, 21),
                                                  # quantitative
     leafLength = c(8, 7.1, 9.4, 1.2, 2.3, 2.1) # quantitative
)
attr(data, "class") = "morphodata"
clustering.GOWER = clust(data, distMethod = "Gower", clustMethod = "UPGMA",
                              binaryChs = c("stemBranching"),
                               nominalChs = c("petalColour", "leaves"),
                              ordinalChs = c("taste"))
```

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cormat

Correlations of Characters

### **Description**

The cormat function calculates the matrix of the correlation coefficients of the characters.

### Usage

```
cormat(object, method = "Pearson")
cormatSignifTest(object, method = "Pearson", alternative = "two.sided")
```

### **Arguments**

object an object of class morphodata.

method a character string indicating which correlation coefficient is to be used for the

test. One of "Pearson" (default), or "Ppearman" can be applied.

alternative indicates the alternative hypothesis and must be one of "two.sided" (default),

"greater" (positive association) or "less" (negative association).

#### **Details**

This function returns table with pairwise correlation coefficients for each pair of morphological characters. The result is formatted as a data.frame to allow export with the exportRes function.

Significance tests are usually unnecessary for morphometric analysis. Anyway, if tests are needed, they can be computed using the cormatSignifTest function.

### Value

A data. frame, storing correlation coefficients for each pair of morphological characters.

```
data(centaurea)

correlations.p = cormat(centaurea, method = "Pearson")
correlations.s = cormat(centaurea, method = "Spearman")

## Not run: exportRes(correlations.p, file = "correlations.pearson.txt")
## Not run: exportRes(correlations.s, file = "correlations.spearman.txt")

correlations.p = cormatSignifTest(centaurea, method = "Pearson")
```

descrTaxon 17

### Description

These functions calculate the descriptive statistics of each character in the whole dataset, each taxon and each population.

# Usage

```
descrTaxon(object, format = NULL, decimalPlaces = 3)
descrPopulation(object, format = NULL, decimalPlaces = 3)
descrAll(object, format = NULL, decimalPlaces = 3)
```

# **Arguments**

object an object of class morphodata.

format form to which will be formatted descriptive characters. See Details.

decimalPlaces the number of a digit to the right of a decimal point.

### **Details**

The following statistics are computed: number of observations, mean, standard deviation, and the percentiles: 0% (minimum), 5%, 25% (lower quartile), 50% (median), 75% (upper quartile), 95% and 100% (maximum).

The format argument brings a handy way how to receive only what is wanted and in format what is desired. Otherways, if format remains NULL, output table contains all calculated descriptors. The format argument is a single string, where keywords will be replaced by particular values.

Keywords: "\$MEAN" = mean; "\$\$D" = standard deviation; "\$MIN" = minimum; "\$5%" = 5th percentile; "\$25%" = 25th percentile (lower quartile); "\$MEDIAN" = median (50th percentile); "\$75%" = 75th percentile (upper quartile); "\$95%" = 95th percentile; "\$MAX" = maximum.

#### Value

A data. frame with calculated statistical descriptors.

```
data(centaurea, decimalPlaces = 3)

descrTaxon(centaurea)

descrTaxon(centaurea, format = "($MEAN ± $SD)")

descrPopulation(centaurea, format = "$MEAN ($MIN - $MAX)")
```

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```
descrAll(centaurea, format = "$MEAN \pm $SD ($5% - $95%)")
```

exportRes	Export Data	
-----------	-------------	--

# Description

This function is designed for exporting results, stored in objects of MorphoTools2 package.

# Usage

# Arguments

object	an object to be exported.
file	either a character string naming a file or a connection opened for writing (e.g., "clipboard"). "" indicates output to the console.
dec	the character used for decimal points.
sep	the column separator character.
row.names	logical, if TRUE, row names of the object are to be written.
col.names	logical, if TRUE, column names of the object are to be written.

## Value

None. Used for its side effect.

```
data(centaurea)

descr = descrTaxon(centaurea, format = "($MEAN ± $SD)")
## Not run: exportRes(descr, file = "centaurea_descrTax.txt")
```

head.morphodata 19

head.morphodata

Return the First or Last Parts of an Object

# **Description**

Returns the first or last parts of a object.

# Usage

```
## S3 method for class 'classifdata'
head(x, n = 6, ...)

## S3 method for class 'classifdata'
tail(x, n = 6, ...)

## S3 method for class 'morphodata'
head(x, n = 6, ...)

## S3 method for class 'morphodata'
tail(x, n = 6, ...)
```

# Arguments

```
an object of class morphodata or classifdata.
n number of rows to print.
arguments to be passed to or from other methods.
```

### **Details**

Object passed as parameter is formated to data.frame. A head() (tail()) returns the first (last) n rows when  $n \ge 0$  or all but the last (first) n rows when n < 0.

### Value

A data. frame, containing the first or last n individuals of the passed object.

```
data(centaurea)
head(centaurea)
tail(centaurea)
```

20 histCharacter

	histCharacter	Histograms of Characters	
--	---------------	--------------------------	--

### **Description**

Histograms are produced for the level of taxa/groups, to displays a within-group distribution of each taxon for a particular character, and its deviation from the normal distribution (red line).

### Usage

### **Arguments**

object an object of class morphodata.

character a morphological character used to plot histogram.

folderName folder to save produced histograms.
col colour to be used to fill the bars.

taxon taxa which should be plotted, default is to plot all of the taxa.

main a main title for the plot.

histogram logical, if TRUE, the histograms will be drawn.

densityLine logical, if TRUE, the density line smoothing out the histogram will be drawn.

normDistLine logical, if TRUE, the normal distribution curve will be drawn.

width the width of the figure. height the height of the figure.

units the units in which height and width are given. Can be "px" (pixels, the de-

fault), "in" (inches), "cm" or "mm".

... further arguments to be passed to hist or graphical parameters par.

### Value

None. Used for its side effect of producing a plot(s).

```
data(centaurea)
histCharacter(centaurea, character = "IW", breaks = seq(0.5, 2.5, 0.1))
## Not run: histAll(centaurea, folderName = "../histograms")
```

keepTaxon 21

keepTaxon	Keep Items (Taxa, Populations, Samples, Morphological Characters)
	in an Morphodata Object (and Remove Others)

# Description

These functions keep only selected taxa, populations, samples or morphological characters in morphodata object. The samples can be kept by names using sampleName argument, or by the threshold. Each sample holding less or equal portion of missing data than the desired threshold (missingPercentage) will be kept. Only one parameter can be specified in one run.

# Usage

```
keepTaxon(object, taxonName)
keepPopulation(object, populationName)
keepSample(object, sampleName = NULL, missingPercentage = NA)
keepCharacter(object, characterName)
```

### **Arguments**

object an object of class morphodata.

taxonName vector of taxa to be kept.

populationName vector of populations to be kept.

sampleName vector of samples to be kept.

 ${\tt missingPercentage}$ 

a numeric, samples holding less or equal portion of missing data than specified

by  ${\tt missingPercentage}$  will be kept.

characterName vector of characters to be kept.

### Value

an object of class morphodata with the following elements:

IDs of each row of data object.

Population population membership of each row of data object.

Taxon taxon membership of each row of data object.

data data. frame of individuals (rows) and values of measured morphological char-

acters (columns).

22 knn.select

### **Examples**

```
data(centaurea)
centaurea.hybr = keepTaxon(centaurea, "hybr")
centaurea.PhHybr = keepTaxon(centaurea, c("ph", "hybr"))
centaurea.PREL = keepPopulation(centaurea, "PREL")
centaurea.NA_0.1 = keepSample(centaurea, missingPercentage = 0.1)
centaurea.stem = keepCharacter(centaurea, c("SN", "SF", "ST"))
```

knn.select

Search for the Optimal K-nearest Neighbours

### Description

This function search for the optimal number of neighbours for the given data set for k-nearest neighbour cross-validatory classification.

### Usage

```
knn.select(object, crossval = "indiv")
```

# **Arguments**

object an object of class morphodata.

crossval crossvalidation mode, sets individual ("indiv"; default, one-leave-out method)

or whole populations ("pop") as leave-out unit.

### **Details**

The knn. select function compute number of correctly classified individuals for k values ranging from 1 to 30 and highlight the value with the highest success rate. Ties (i.e., when there are the same numbers of votes for two or more groups) are broken at random, and thus several iterations may yield different results. Therefore, the functions compute 10 iterations, and the average success rates for each k are used; the minimum and maximum success rates for each k are also displayed as error bars. Note that several k values may have nearly the same success rates; if this is the case, the similarity of iterations may also be considered.

The mode of crossvalidation is set by the parameter crossval. The default "indiv" uses the standard one-leave-out method. However, as some hierarchical structure is usually present in the data (individuals from a population are not completely independent observations, as they are morphologically closer to each other than to individuals from other populations), the value "pop" sets whole populations as leave-out units. The latter method does not allow classification if there is only one population for a taxon and is more sensitive to "atypical" populations, which usually leads to a somewhat lower classification success rate.

missingCharactersTable

### Value

Optimal number of neighbours is written to the console, and plot displaying all Ks is produced.

#### See Also

```
classif.lda, classifSample.lda, classif.qda, classifSample.qda, classifSample.knn
```

### **Examples**

```
data(centaurea)
centaurea = naMeanSubst(centaurea)
centaurea = removePopulation(centaurea, populationName = c("LIP", "PREL"))
# classification by nonparametric k-nearest neighbour method
knn.select(centaurea, crossval = "indiv")
classifRes.knn = classif.knn(centaurea, k = 12, crossval = "indiv")
```

missingCharactersTable

Summarize Missing Data

### **Description**

Summarize percentage and number of missing values on the desired grouping level.

### Usage

```
missingCharactersTable(object, level)
```

### **Arguments**

object an object of class morphodata.

level of grouping, one of the following: "taxon", populations ("pop"), or indi-

viduals ("indiv")

# Value

A data. frame summarizing a number of missing values.

```
data(centaurea)
missingCharactersTable(centaurea, level = "pop")
```

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missingSamplesTable Summarize Missing Data

### **Description**

Summarize number of missing values for each character on the desired grouping level.

# Usage

```
missingSamplesTable(object, level)
```

# Arguments

object an object of class morphodata.

level of grouping, one of the following: "taxon", populations ("pop"), or indi-

viduals ("indiv".)

#### Value

A data. frame summarizing a number of missing values.

### **Examples**

```
data(centaurea)
missingSamplesTable(centaurea, level = "pop")
```

morphodata

Class morphodata

# Description

The morphodata class is designed for storing morphological data of individuals, their IDs and it's appertaining to population and taxon.

### **Format**

Class morphodata.

ID IDs of each row of data object.

Population population membership of each row of data object.

Taxon taxon membership of each row of data object.

data data. frame of individuals (rows) and values of measured morphological characters (columns).

naMeanSubst 25

naMeanSubst	Replace Missing Data by Population Average

# Description

This function substitutes missing data using the average value of the respective character in the respective population.

### Usage

```
naMeanSubst(object)
```

### **Arguments**

object an object of class morphodata.

### **Details**

Generally, most of the multivariate analyses require a full data matrix. The preferred approach is to reduce the data set to complete observations only (i.e., perform the casewise deletion of missing data) or to remove characters for which there are missing values. The use of mean substitution, which introduces values that are not present in the original data, is justified only if (1) there are relatively few missing values, (2) these missing values are scattered throughout many characters (each character includes only a few missing values) and (3) removing all individuals or all characters with missing data would unacceptably reduce the data set.

#### Value

an object of class morphodata with the following elements:

IDs of each row of data object.

Population population membership of each row of data object.

Taxon taxon membership of each row of data object.

data data. frame of individuals (rows) and values of measured morphological char-

acters (columns).

```
data(centaurea)
centaurea = naMeanSubst(centaurea)
```

26 nmds.calc

nmds.calc

Non-metric Multidimensional Scaling (NMDS)

### **Description**

This function performs Non-metric multidimensional scaling.

### Usage

### **Arguments**

object an object of class morphodata.

distMethod the distance measure to be used. This must be one of: "Euclidean", "Manhattan",

"Minkowski", "Jaccard", "simpleMatching", or "Gower". See details.

k number of dimensions. binaryChs, nominalChs, ordinalChs

names of categorical ordinal, categorical nominal (multistate), and binary char-

acters. Needed for Gower's dissimilarity coefficient only, see details.

#### **Details**

The nmds.calc function performs non-metric multidimensional scaling using the monoMDS function from package vegan. The main threat of NMDS is, that this method doesn't preserve distances among objects in the original character space and approximates only the order of the dissimilarities among objects, based on any coefficient of similarity or distance.

Further, multiple runs of the NMDS analysis are needed to ensure that the stable ordination has been reached, as anyone run may get "trapped" in local optima which are not representative of true similarities.

The stress value reflects how well the ordination summarizes the observed relationship among the samples. A rule of thumb, 0.1-0.2 is considered fairly good, but there is no general rule since the stress is greatly influenced by the number of points. Since stress decreases as dimensionality increases, the optimal solution is when the decrease in stress is small after decreasing the number of dimensions.

Various measures of distance between the observations (rows) are applicable: (1) coefficients of distance for quantitative and binary characters: "Euclidean", "Manhattan", "Minkowski"; (2) similarity coefficients for binary characters: "Jaccard" and simple matching ("simpleMatching"); (3) coefficient for mixed data: ("Gower").

The Gower's dissimilarity coefficient can handle different types of variables. Characters have to be divided into four categories: (1) quantitative characters, (2) categorical ordinal characters, (3) categorical nominal (multistate) characters, and (4) binary characters. All characters are considered to be quantitative characters unless otherwise specified. Other types of characters have to be explicitly specified. To mark characters as ordinal, nominal, or binary, enumerate them by names using ordinalChs, nominalChs, and binaryChs arguments, respectively.

nmds.calc 27

#### Value

```
an object of class \ensuremath{\mathsf{nmdsdata}} with the following elements:
```

objects

ID IDs of each row of scores object.

Population population membership of each row of scores object.

Taxon taxon membership of each row of scores object.

scores ordination scores of cases (objects, OTUs).

stress value, e.i., goodness of fit.

groupMeans data. frame containing the means for the taxa.

distMethod used distance measure.

rank number of possitive eigenvalues.

```
data(centaurea)
nmdsRes = nmds.calc(centaurea, distMethod = "Euclidean", k = 3)
summary(nmdsRes)
plotPoints(nmdsRes, axes = c(1,2), col = c("red", "green", "blue", "black"),
 pch = c(20,17,8,21), pt.bg = "orange", legend = TRUE, legend.pos = "bottomright")
# using Gower's method
data = list(
    ID = as.factor(c("id1","id2","id3","id4","id5","id6")),
   Population = as.factor(c("Pop1", "Pop1", "Pop2", "Pop2", "Pop3", "Pop3")),
   Taxon = as.factor(c("TaxA", "TaxA", "TaxA", "TaxB", "TaxB")),
   data = data.frame(
    stemBranching = c(1, 1, 1, 0, 0, 0), # binaryChs
     petalColour = c(1, 1, 2, 3, 3), \# nominalChs; 1=white, 2=red, 3=blue
   leaves = c(1,1,1,2,2,3), \ \# \ nominal Chs; \ 1=simple, \ 2=palmately \ compound, \ 3=pinnately \ compound
     taste = c(2, 2, 2, 3, 1, 1), # ordinal; 1=hot, 2=hotter, 3=hottest
     stemHeight = c(10, 11, 14, 22, 23, 21),
                                                     # quantitative
     leafLength = c(8, 7.1, 9.4, 1.2, 2.3, 2.1) # quantitative
)
attr(data, "class") = "morphodata"
nmdsGower = nmds.calc(data, distMethod = "Gower", k = 2, binaryChs = c("stemBranching"),
                      nominalChs = c("petalColour", "leaves"), ordinalChs = c("taste"))
plotPoints(nmdsGower, axes = c(1,2), col = c("red", "green"),
           pch = c(20,17), pt.bg = "orange", legend = TRUE, legend.pos = "bottomright")
```

28 pca.calc

nmdsdata

Class nmdsdata

### Description

The nmdsdata class is designed for storing results of non-metric multidimensional scaling (NMDS).

#### **Format**

Class nmdsdata.

objects ID IDs of each row of scores object.

**Population** population membership of each row of scores object.

**Taxon** taxon membership of each row of scores object.

scores ordination scores of cases (objects, OTUs).

stress stress value, e.i., goodness of fit.

**groupMeans** data. frame containing the means for the taxa.

distMethod used distance measure.

rank number of possitive eigenvalues.

pca.calc

Principal Component Analysis

### **Description**

This function performs principal component analysis.

### Usage

```
pca.calc(object)
```

### Arguments

object

an object of class morphodata.

### **Details**

The pca.calc function performs an R type principal component analysis using the R base princomp function. Principal component analysis is a variable reduction procedure. It reduces original variables into a smaller number of principal components (artificial variables) that will account for most of the variance in the observed variables.

### Value

```
an object of class pcadata with the following elements:
```

objects

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ID IDs of each row of scores object.

Population population membership of each row of scores object.

Taxon taxon membership of each row of scores object.

scores ordination scores of cases (objects, OTUs).

eigenVectors matrix of eigenvectors (i.e., a matrix of characters loadings).

eigenValues eigenvalues of principal components, i.e., proportion of variation of the original

dataset expressed by individual axes.

eigenvaluesAsPercent

eigenvalues as percent, percentage of their total sum.

 $\verb|cumulativePercentageOfEigenvalues|\\$ 

cumulative percentage of eigenvalues.

groupMeans data. frame containing the means for the taxa.

rank number of principal components.

center, scale the centring and scaling of the input data.

### **Examples**

```
data(centaurea)
centaurea = naMeanSubst(centaurea)
centaurea = removePopulation(centaurea, populationName = c("LIP", "PREL"))
pcaRes = pca.calc(centaurea)
summary(pcaRes)
plotPoints(pcaRes, axes = c(1,2), col = c("red", "green", "blue", "black"),
    pch = c(20,17,8,21), pt.bg = "orange", legend = TRUE, legend.pos = "bottomright")
```

pcadata

Class pcadata

### Description

The pcadata class is designed for storing results of principal component analysis (PCA).

### **Format**

Class pcadata.

objects ID IDs of each row of scores object.

**Population** population membership of each row of scores object.

**Taxon** taxon membership of each row of scores object.

**scores** ordination scores of cases (objects, OTUs).

eigenVectors matrix of eigenvectors (i.e., a matrix of characters loadings).

30 pcoa.calc

**eigenValues** eigenvalues of principal components, i.e., proportion of variation of the original dataset expressed by individual axes.

eigenvaluesAsPercent eigenvalues as percent, percentage of their total sum.

cumulativePercentageOfEigenvalues cumulative percentage of eigenvalues.

groupMeans data. frame containing the means for the taxa.

rank number of principal components.

center, scale the centring and scaling of the input data.

pcoa.calc

Principal Coordinates Analysis (PCoA)

## Description

This function performs principal coordinates analysis.

### Usage

### **Arguments**

object an object of class morphodata.

distMethod the distance measure to be used. This must be one of: "Euclidean", "Manhattan",

"Minkowski", "Jaccard", "simpleMatching", or "Gower". See details.

binaryChs, nominalChs, ordinalChs

names of categorical ordinal, categorical nominal (multistate), and binary char-

acters. Needed for Gower's dissimilarity coefficient only, see details.

### **Details**

The pcoa.calc function performs principal coordinates analysis using the cmdscale function from package stats. Principal coordinates analysis estimates coordinates for a set of objects in a space. Distances among objects is approximationy of the dissimilarities, based on any similarity or distance coefficient.

Various measures of distance between the observations (rows) are applicable: (1) coefficients of distance for quantitative and binary characters: "Euclidean", "Manhattan", "Minkowski"; (2) similarity coefficients for binary characters: "Jaccard" and simple matching ("simpleMatching"); (3) coefficient for mixed data: ("Gower").

The Gower's dissimilarity coefficient can handle different types of variables. Characters have to be divided into four categories: (1) quantitative characters, (2) categorical ordinal characters, (3) categorical nominal (multistate) characters, and (4) binary characters. All characters are considered to be quantitative characters unless otherwise specified. Other types of characters have to be explicitly specified. To mark characters as ordinal, nominal, or binary, enumerate them by names using ordinalChs, nominalChs, and binaryChs arguments, respectively.

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#### Value

```
an object of class pcoadata with the following elements:
objects
                      ID IDs of each row of scores object.
             Population population membership of each row of scores object.
                  Taxon taxon membership of each row of scores object.
                 scores ordination scores of cases (objects, OTUs).
eigenValues
                 eigenvalues of principal coordinates.
eigenvaluesAsPercent
                  eigenvalues as percent, percentage of their total sum.
cumulativePercentageOfEigenvalues
                 cumulative percentage of eigenvalues.
                  data. frame containing the means for the taxa.
groupMeans
distMethod
                 used distance measure.
```

number of possitive eigenvalues.

### **Examples**

rank

```
data(centaurea)
pcoRes = pcoa.calc(centaurea, distMethod = "Manhattan")
summary(pcoRes)
plotPoints(pcoRes, axes = c(1,2), col = c("red", "green", "blue", "black"),
  pch = c(20,17,8,21), pt.bg = "orange", legend = TRUE, legend.pos = "bottomright")
# using Gower's method
data = list(
    ID = as.factor(c("id1","id2","id3","id4","id5","id6")),
    Population = as.factor(c("Pop1", "Pop1", "Pop2", "Pop2", "Pop3", "Pop3")),
    Taxon = as.factor(c("TaxA", "TaxA", "TaxA", "TaxB", "TaxB")),
    data = data.frame(
     stemBranching = c(1, 1, 1, 0, 0, 0), # binaryChs
    petalColour = c(1,\ 1,\ 2,\ 3,\ 3),\quad \#\ nominalChs;\ 1=white,\ 2=red,\ 3=blue
   leaves = c(1,1,1,2,2,3), # nominalChs; 1=simple, 2=palmately compound, 3=pinnately compound
     taste = c(2, 2, 2, 3, 1, 1), # ordinal; 1=hot, 2=hotter, 3=hottest
     stemHeight = c(10, 11, 14, 22, 23, 21),
                                                     # quantitative
     leafLength = c(8, 7.1, 9.4, 1.2, 2.3, 2.1) # quantitative
attr(data, "class") = "morphodata"
pcoaGower = pcoa.calc(data, distMethod = "Gower", binaryChs = c("stemBranching"),
                      nominalChs = c("petalColour", "leaves"), ordinalChs = c("taste"))
```

32 plot3Dpoints

pcoadata

Class pcoadata

### **Description**

The pcoadata class is designed for storing results of principal coordinates analysis (PCoA).

### **Format**

Class pcoadata.

**objects ID** IDs of each row of scores object.

Population population membership of each row of scores object.

Taxon taxon membership of each row of scores object.

scores ordination scores of cases (objects, OTUs).

eigenValues eigenvalues of principal coordinates.

eigenvalues As Percent eigenvalues as percent, percentage of their total sum.

cumulativePercentageOfEigenvalues cumulative percentage of eigenvalues.

groupMeans data. frame containing the means for the taxa.

distMethod used distance measure.

rank number of possitive eigenvalues.

plot3Dpoints

The Default Scatterplot 3D Function

### **Description**

A generic function for plotting ordination scores stored in pcadata, pcoadata, nmdsdata, and cdadata objects.

# Usage

```
plot3Dpoints(result, axes = c(1,2,3), xlab = NULL, ylab = NULL, zlab = NULL,
    pch = 16, col = "black", pt.bg = "white", phi = 10, theta = 2,
    ticktype = "detailed", bty = "u", type = "p", labels = FALSE,
    legend = FALSE, legend.pos = "topright", ncol = 1, ...)
```

plot3Dpoints 33

# Arguments

result	an object of class pcadata, pcoadata, nmdsdata, or cdadata.
axes	x, y, z axes of plot.
xlab, ylab, zlab	
	a title of the respective axes.
pch	a vector of plotting characters or symbols, see points.
col	the colours for points. Multiple colours can be specified so that each taxon can be given its own colour. If there are fewer colours than taxa, they are recycled in the standard fashion.
pt.bg	the background colours for points. Multiple colours can be specified, as above.
theta, phi	the angles defining the viewing direction. Theta gives the azimuthal direction and phi the colatitude, see persp.
ticktype	character: "simple" draws just an arrow parallel to the axis to indicate direction of increase; "detailed" draws normal ticks as per 2D plots.
bty	the type of the box. One of "g", "b2", "b1", "f", "u" can be specified.
type	the type of plot points, "p" for points, or "h" for vertical spikes.
labels	logical, if TRUE, point's labels are displayed.
legend	logical, if TRUE, legend is displayed. Only restricted number of legend parameters are supported. For more precise legend plotting, use plotAddLegend directly.
legend.pos	a single keyword from the list "bottomright", "bottom", "bottomleft", "left", "topleft", "top", "topright", "right", and "center", to be used to position the legend.
ncol	the number of columns in which to set the legend items.
• • •	further arguments to be passed to plot3D, persp, par.

### Value

None. Used for its side effect of producing a plot.

34 plotAddEllipses

plotAddEllipses	Add Prediction Ellipses to a Plot

## **Description**

This function draws prediction ellipses around taxa.

## Usage

```
plotAddEllipses(result, axes = c(1,2), probability = 0.95, col = "black", type = "l", lty = 1, lwd = 1, ...)
```

# **Arguments**

result	result of pca.calc, pcoa.calc, nmds.calc, or cda.calc, has to by plotted at first.
axes	x, y axes of plot.
probability	probability, that a new independent observation from the same population will fall in that ellipse.
col	the colours for labels.
type	character indicating the type of plotting, for details, see plot: "p" for points, "1" for lines, "b" for both points and lines, "c" for empty points joined by lines, "o" for overplotted points and lines, "s" and "S" for stair steps and "h" for histogram-like vertical lines.
lty	the line type. Line types can either be specified as one of following types: 0=blank, 1=solid (default), 2=dashed, 3=dotted, 4=dotdash, 5=longdash, 6=twodash.
lwd	the line width.
	further arguments to be passed to lines or other graphical parameters in par.

### **Details**

Prediction ellipses with given probability define the regions where will fall any new independent observation from the respective taxa. The prediction ellipses are quantified using covariance matrices of taxa scores and chi-squared distribution with two degrees of freedom (Friendly et al. 2013).

### Value

None. Used for its side effect of adding elements to a plot.

### References

**Friendly M., Monette G., Fox J. (2013)**. Elliptical insights: understanding statistical methods through elliptical geometry. *Statistical Science* 28, 1-39.

plotAddLabels.characters

### **Examples**

plotAddLabels.characters

Add Labels to a Plot

### Description

This is a generic function for drawing labels to the character arrows of pcadata and cdadata objects.

# Usage

```
plotAddLabels.characters(result, labels = characters(result), include = TRUE, axes = c(1,2), pos = NULL, offset = 0.5, cex = 0.7, col = NULL, ...)
```

### **Arguments**

result	an object of class pcadata or cdadata.
labels	a vector of label names, which should be included / excluded from plotting, see include.
include	logical, specify if labels in labels argument should be plotted or excluded from plotting.
axes	x, y axes of plot.
pos	a position specifier for the text. Values of 1, 2, 3 and 4, respectively indicate positions below, to the left of, above and to the right of the point.
offset	when pos is specified, this value controls the distance (offset) of the text label from the point in fractions of a character width.
cex	character expansion factor for text.
col	the colours for labels.
	further arguments to be passed to text or other graphical parameters in par.

### Value

None. Used for its side effect of adding elements to a plot.

### **Examples**

```
data(centaurea)
centaurea = naMeanSubst(centaurea)
centaurea = removePopulation(centaurea, populationName = c("LIP", "PREL"))

pcaRes = pca.calc(centaurea)

plotCharacters(pcaRes, labels = FALSE)
plotAddLabels.characters(pcaRes, labels = c("MW", "IW", "SFT", "SF", "LW"), pos = 2, cex = 1)
plotAddLabels.characters(pcaRes, labels = c("LLW", "ILW", "LBA"), pos = 4, cex = 1)
plotAddLabels.characters(pcaRes, labels = c("ML", "IV", "MLW"), pos = 1, cex = 1)
```

plotAddLabels.points Add Labels to a Plot

### **Description**

This is a generic function for drawing labels to the data points of pcadata, pcoadata, nmdsdata, and cdadata objects.

### Usage

### **Arguments**

result	result of pca.calc, pcoa.calc, nmds.calc, or cda.calc, has to by plotted at first.
labels	a vector of label names, which should be included $\!\!\!/$ excluded from plotting, see include.
include	logical, specify if labels in labels argument should be plotted or excluded from plotting.
axes	x, y axes of plot.
pos	a position specifier for the text. Values of 1, 2, 3 and 4, respectively indicate positions below, to the left of, above and to the right of the point.
offset	when pos is specified, this value controls the distance (offset) of the text label from the point in fractions of a character width.
cex	character expansion factor for text.
col	the colours for labels.
	further arguments to be passed to text or other graphical parameters in par.

plotAddLegend 37

## Value

None. Used for its side effect of adding elements to a plot.

## **Examples**

plotAddLegend

Add Legend to a Plot

# **Description**

This function can be used to add legend to plot.

# Usage

```
plotAddLegend(result, x = "topright", y = NULL, pch = 16, col = "black",
    pt.bg = "white", pt.cex = cex, pt.lwd = 1, x.intersp = 1,
    y.intersp = 1, box.type = "o", box.lty = "solid", box.lwd = 1,
    box.col = "black", box.bg = "white", cex = 1, ncol = 1, horiz = FALSE, ...)
```

# **Arguments**

result	result of pca.calc, pcoa.calc, nmds.calc, or cda.calc, has to by plotted at first.
x, y	the x and y coordinates or a single keyword from the list "bottomright", "bottom", "bottomleft", "left", "topleft", "top", "topright", "right", and "center", to be used to position the legend.
pch	the plotting symbols of points appearing in the legend.
col	the colours of points appearing in the legend.
pt.bg	the background colour for the points, corresponding to its argument bg.
pt.cex	character expansion factor for the points.

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pt.lwd the line width for the points. x.intersp, y.intersp character interspacing factor for horizontal (x) and vertical (y) line distances. the type of box to be drawn around the legend. The applicable values are "o" box.type (the default) and "n". box.lty, box.lwd, box.col, box.bg the line type, width colour and background colour for the legend box (if box. type character expansion factor for text. cex the number of columns in which to set the legend item. ncol logical; if TRUE, set the legend horizontally rather than vertically (specifying horiz horiz overrides the ncol specification). further arguments to be passed to legend or other graphical parameters in par. . . .

#### Value

None. Used for its side effect of adding elements to a plot.

# **Examples**

plotAddSpiders

Add Spiders to a Plot

## **Description**

This function connects taxa's points with its centroids, thus forms a "spider" diagram.

#### Usage

```
plotAddSpiders(result, axes = c(1,2), col = "black", lty = 1, lwd = 1, ...)
```

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# **Arguments**

result	result of pca.calc, pcoa.calc, nmds.calc, or cda.calc, has to by plotted at first.
axes	x, y axes of plot.
col	the colours for labels.
lty	the line type. Line types can either be specified as one of following types: 0=blank, 1=solid (default), 2=dashed, 3=dotted, 4=dotdash, 5=longdash, 6=twodash.
lwd	the line width.
• • •	further arguments to be passed to lines or other graphical parameters in par.

## Value

None. Used for its side effect of adding elements to a plot.

# **Examples**

```
data(centaurea)
centaurea = naMeanSubst(centaurea)
centaurea = removePopulation(centaurea, populationName = c("LIP", "PREL"))
pcaRes = pca.calc(centaurea)
plotPoints(pcaRes, col = c(rgb(255, 0, 0, max = 255, alpha = 150), # red
                           rgb(0, 255, 0, max = 255, alpha = 150), # green
                           rgb(0, 0, 255, max = 255, alpha = 150), # blue
                           rgb(0, 0, 0, max = 255, alpha = 150)), # black
            legend = FALSE, x \lim = c(-5, 7.5), y \lim = c(-5, 5.5)
plotAddLegend(pcaRes, col = c("red", "green", "blue", "black"), ncol = 2)
plotAddSpiders(pcaRes, col = c("red", "green", "blue", "black"))
plotPoints(pcaRes, col = c("red", "green", "blue", "black"), legend = TRUE, cex = 0.4)
plotAddSpiders(pcaRes, col = c(rgb(255, 0, 0, max = 255, alpha = 150), # red
                               rgb(0, 255, 0, max = 255, alpha = 150), # green
                               rgb(0, 0, 255, max = 255, alpha = 150), # blue
                               rgb(0, 0, 0, max = 255, alpha = 150))) # black
```

plotCharacters

Draws Character's Contribution as Arrows

# **Description**

The character's contribution to ordination axes are visualised as arrows.

40 plotCharacters

### Usage

```
plotCharacters(result, axes = c(1, 2), xlab = NULL, ylab = NULL, main = NULL, xlim = NULL, ylim = NULL, col = "red", length = 0.1, angle = 15, labels = TRUE, cex = 0.7, ...)
```

#### **Arguments**

result an object of class pcadata or cdadata. x, y axes of plot. axes a title of the respective axes. xlab, ylab xlim, ylim numeric vectors of length 2, giving the x and y coordinates ranges. main a main title for the plot. col the colour for arrows. length length of the edges of the arrow head (in inches). angle angle from the shaft of the arrow to the edge of the arrow head. labels logical, if TRUE, labels are displayed. Only restricted number of parameters are supported. For more precise labels plotting, use plotAddLabels.characters directly. character expansion factor for labels. cex

## Details

The distribution of samples in ordination space is driven by morphological characters. Each character has its own contribution to ordination axes. These contributions are visualised as arrows. The direction and length of the arrows characterize the impact of the morphological characters on the separation of objects along a given axis. This information is stored in eigenvectors or total canonical structure coefficients for principal component analysis of canonical discriminant analysis, respectively.

further arguments to be passed to arrows or other graphical parameters in par.

The plotCharacters method is not applicable to results of the principal coordinates analysis (pcoa.calc) and non-metric multidimensional scaling (nmds.calc) analyses, as the influence of original characters on new axes can not be directly derived, and variation explained by individual axes is unknown.

## Value

None. Used for its side effect of producing a plot.

## **Examples**

```
data(centaurea)
centaurea = naMeanSubst(centaurea)
centaurea = removePopulation(centaurea, populationName = c("LIP", "PREL"))
pcaRes = pca.calc(centaurea)
plotCharacters(pcaRes)
```

plotPoints 41

plotPoints	The Default Scatterplot Function	

# Description

A generic function for plotting ordination scores stored in pcadata, pcoadata, nmdsdata, and cdadata objects.

# Usage

# Arguments

result	an object of class pcadata, pcoadata, nmdsdata, or cdadata.
axes	x, y axes of plot.
xlab, ylab	a title of the respective axes.
pch	a vector of plotting characters or symbols: see points.
col	the colours for points. Multiple colours can be specified so that each taxon can be given its own colour. If there are fewer colours than taxa, they are recycled in the standard fashion.
pt.bg	the background colours for points. Multiple colours can be specified, as above.
breaks	a numeric, giving the width of one histogram bar.
xlim, ylim	the range of x and y axes.
labels	logical, if TRUE, labels are displayed. Only restricted number of parameters are supported. For more precise labels plotting, use plotAddLabels.points directly.
legend	logical, if TRUE, legend is displayed. Only restricted number of legend parameters are supported. For more precise legend plotting, use plotAddLegend directly.
legend.pos	a single keyword from the list "bottomright", "bottom", "bottomleft", "left", "topleft", "top", "topright", "right", and "center", to be used to position the legend.
ncol	the number of columns in which to set the legend items.
• • •	further arguments to be passed to plot.default or other graphical parameters in par.

## **Details**

This generic method holds separate implementations of plotting points for pcadata, pcoadata, nmdsdata, and cdadata objects. If only one axis exists, sample scores are displayed as a histogram.

42 populOTU

## Value

None. Used for its side effect of producing a plot.

## **Examples**

```
data(centaurea)
centaurea = naMeanSubst(centaurea)
centaurea = removePopulation(centaurea, populationName = c("LIP", "PREL"))

pcaRes = pca.calc(centaurea)

plotPoints(pcaRes, axes = c(1,2), col = c("red", "green", "blue", "red"),
    pch = c(20, 17, 8, 21), pt.bg = "orange", legend = TRUE, legend.pos = "bottomright")

plotPoints(pcaRes, main = "My PCA plot", frame.plot = FALSE, cex = 0.8)

cdaRes = cda.calc(centaurea)

plotPoints(cdaRes, col = c("red", "green", "blue", "red"),
    pch = c(20, 17, 8, 21), pt.bg = "orange", legend = TRUE)
```

popul0TU

Population Means

## **Description**

This function calculates the average value for each character in each population, with the pairwise deletion of missing data.

## Usage

```
populOTU(object)
```

# Arguments

object

an object of class morphodata.

## **Details**

This function returns morphodata object, where each population is used as the operational taxonomic unit (OTUs), thus is represented by single "individual" (row) with average values for each character. Note that when using populations as OTUs, they are handled with the same weight in all analyses (disregarding population size, within-population variation, etc.)

qqnormCharacter 43

## Value

an object of class morphodata with the following elements:

IDs of each row of data object.

Population population membership of each row of data object.

Taxon taxon membership of each row of data object.

data data.frame of individuals (rows) and values of measured morphological char-

acters (columns).

## **Examples**

```
data(centaurea)
pops = populOTU(centaurea)
```

qqnormCharacter

Quantile-Quantile Plots

## Description

Q-Q plots are produced for the level of taxa/groups, to displays a deviation of morphological characters of each taxon from the normal distribution (line).

# Usage

## **Arguments**

object an object of class morphodata.

character a morphological character used to plot Q-Q plot.

folderName folder to save produced Q-Q plots.

taxa which should be plotted, default is to plot all of the taxa.

main main title for the plot.

width the width of the figure.

height the height of the figure.

units the units in which height and width are given. Can be "px" (pixels, the de-

fault), "in" (inches), "cm" or "mm".

... further arguments to be passed to qqnorm or graphical parameters par.

44 read.morphodata

## Value

None. Used for its side effect of producing a plot(s).

# **Examples**

```
data(centaurea)
qqnormCharacter(centaurea, character = "SF")
## Not run: qqnormAll(centaurea, folderName = "../qqnormPlots")
```

read.morphodata

Data Input and Description

# Description

This function imports data and produces a morphodata object from it.

# Usage

```
read.morphodata(file, dec = ".", sep = "\t", ...)
## S3 method for class 'morphodata'
samples(object)
populations(object)
taxa(object)
```

# **Arguments**

file	the file which the data are to be read from or a connection for reading (e.g., "clipboard").
dec	the character used for decimal points.
sep	the column separator character.
object	an object of class morphodata.
	further arguments to be passed to read.table function.

## **Details**

The function expects the following data structure:

- (1) the first row contains variable names;
- (2) the following rows contains individuals, single individual per row;
- (3) the first three columns include unique identifiers for individuals, populations and taxa/groups, respectively. Columns have to be named as "ID", "Population" and "Taxon";

removeTaxon 45

(4) starting from the fourth column, any number of quantitative or binary morphological characters may be recorded. Any variable names can be used (avoiding spaces and special characters);

If there are missing values in the data, they must be represented as empty cells or by the text NA, not zero, space or any other character. Example dataset in txt and xlsx formats are stored in the "extdata" directory of the MorphoTools2 package installation directory. To find the path to the package location run system.file("extdata", package = "MorphoTools2").

#### Value

an object of class morphodata with the following elements:

ID IDs of each row of data object.

Population population membership of each row of data object.

Taxon taxon membership of each row of data object.

data data. frame of individuals (rows) and values of measured morphological char-

acters (columns).

#### See Also

characters

# **Examples**

removeTaxon

Remove Items (Taxa, Populations, Morphological Characters) from Morphodata Object

# **Description**

These functions remove particular taxa, populations, samples or morphological characters from morphodata object. The samples can be deleted by names using sampleName argument, or each sample above the desired threshold missingPercentage will be deleted. Only one parameter can be specified in one run.

46 removeTaxon

# Usage

```
removeTaxon(object, taxonName)
removePopulation(object, populationName)
removeSample(object, sampleName = NULL, missingPercentage = NA)
removeCharacter(object, characterName)
```

## **Arguments**

object of class morphodata.
taxonName vector of taxa to be removed.

populationName vector of populations to be removed.
sampleName vector of samples to be removed.

missingPercentage

a numeric, samples holding more missing data than specified by missingPercentage

will be removed.

characterName vector of characters to be removed.

# Value

an object of class morphodata with the following elements:

ID IDs of each row of data object.

Population population membership of each row of data object.

Taxon taxon membership of each row of data object.

data data.frame of individuals (rows) and values of measured morphological char-

acters (columns).

## **Examples**

```
data(centaurea)
centaurea.3tax = removeTaxon(centaurea, "hybr")
centaurea.PsSt = removeTaxon(centaurea, c("ph", "hybr"))
centaurea.short = removePopulation(centaurea, c("LIP", "PREL"))
centaurea.NA_0.1 = removeSample(centaurea, missingPercentage = 0.1)
centaurea.short = removeCharacter(centaurea, "LL")
```

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shapiroWilkTest

Shapiro-Wilk Normality Test

# Description

Calculates the Shapiro-Wilk normality test of characters for taxa.

# Usage

```
shapiroWilkTest(object, p.value = 0.05)
```

# **Arguments**

object an object of class morphodata.

p.value a number or NA are acceptable. In the case of number, the output will be format-

ted as "normally distributed" or "NOT normally distributed". In the case

of NA, exact p-values will be returned.

#### Value

A data. frame, storing results of Shapiro-Wilk normality test.

# **Examples**

```
data(centaurea)
sW = shapiroWilkTest(centaurea)
## Not run: exportRes(sW, file = "sW_test.txt")
sW = shapiroWilkTest(centaurea, p.value = NA)
## Not run: exportRes(sW, file = "sW_test.txt")
```

stepdisc.calc

Stepwise Discriminant Analysis

# Description

This function perform stepwise discriminant analysis.

# Usage

```
stepdisc.calc(object, FToEnter = 0.15, FToStay = 0.15)
```

48 summary

# **Arguments**

object an object of class morphodata.

FToEnter significance levels for a variable to enter the subset.

FToStay significance levels for a variable to stay in the subset.

#### **Details**

The stepdisc.calc function performs a stepwise discriminant analysis to select the "best" subset of the quantitative variables for use in discriminating among the groups (taxa).

## Value

None. Used for its side effect.

# Examples

```
data(centaurea)
centaurea = naMeanSubst(centaurea)
centaurea = removePopulation(centaurea, populationName = c("LIP", "PREL"))
stepdisc.calc(centaurea)
```

summary

Object Summaries

# Description

 $summary\ methods\ for\ classes\ morphodata,\ pcadata,\ pcadata,\ nmdsdata,\ cdadata,\ and\ classifdata.$ 

## Usage

```
## S3 method for class 'morphodata'
summary(object, ...)
## S3 method for class 'pcadata'
summary(object, ...)
## S3 method for class 'pcoadata'
summary(object, ...)
## S3 method for class 'nmdsdata'
summary(object, ...)
## S3 method for class 'cdadata'
summary(object, ...)
## S3 method for class 'cdadata'
summary(object, ...)
```

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# **Arguments**

object an object of class morphodata, pcadata, pcoadata, nmdsdata, cdadata, or

classifdata.

... additional arguments affecting the summary produced.

## Value

None. Used for its side effect.

transformCharacter Transformation of Character

# **Description**

This function transforms morphological characters by applying another function passed in the argument.

# Usage

transformCharacter(object, character, FUN, newName = NULL)

#### **Arguments**

object an object of class morphodata.

character a morphological character that should be transformed. FUN the transforming function to be applied to character.

newName a name to rename the original character. If NULL, the name of the transformed

character remains the same.

#### Details

Transformation is applied to characters to improve their distribution (to become normally distributed or at least to achieve lesser deviation from normality). The FUN argument takes any function, able to accept as input any value of the character specified by character argument.

Note that, when using a log transformation, a constant should be added to all values to make them all positive before transformation (if there are zero values in the data), because the argument of the logarithm can be only positive numbers. The arcsine transformation is applicable for proportions and percentages (for values ranging from 0 to 1).

#### Value

an object of class morphodata with the following elements:

IDs of each row of data object.

Population population membership of each row of data object.

Taxon taxon membership of each row of data object.

data data. frame of individuals (rows) and values of measured morphological char-

acters (columns).

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## **Examples**

```
data(centaurea)
# For a right-skewed (positive) distribution can be used:
# Logarithmic transformation
cTransf = transformCharacter(centaurea, character = "SF", FUN = function(x) log(x+1))
cTransf = transformCharacter(centaurea, character = "SF", FUN = function(x) log10(x+1))
# Square root transformation
cTransf = transformCharacter(centaurea, character = "SF", FUN = function(x) sqrt(x))
# Cube root transformation
cTransf = transformCharacter(centaurea, character = "SF", FUN = function(x) x^{(1/3)})
# Arcsine transformation
cTransf = transformCharacter(centaurea, character = "SF", FUN = function(x) asin(sqrt(x)))
# For a left-skewed (negative) distribution can be used:
# Logarithmic transformation
cTransf = transformCharacter(centaurea, character="SF", FUN=function(x) log((max(x)+1)-x))
cTransf = transformCharacter(centaurea, character="SF", FUN=function(x) log10((max(x)+1)-x))
# Square root transformation
 {\sf cTransf = transformCharacter(centaurea, character="SF", FUN=function(x) \ sqrt((max(x)+1)-x)) } 
# Cube root transformation
cTransf = transformCharacter(centaurea, character="SF", FUN=function(x) ((max(x)+1)-x)^(1/3))
# Arcsine transformation
cTransf = transformCharacter(centaurea, character="SF", FUN=function(x) asin(sqrt((max(x))-x)))
```

viewMorphodata

Invoke a Data Viewer

# **Description**

Invoke a spreadsheet-style data viewer on a data stored in morphodata class.

# Usage

```
viewMorphodata(object)
```

# **Arguments**

object an object of class morphodata.

#### Value

None. Used for its side effect.

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# Examples

```
data(centaurea)
## Not run: viewMorphodata(centaurea)
```

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