

Package ‘fingerPro’

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Type Package

Title Sediment Source Fingerprinting

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Description Quantifies the provenance of the sediments in a catchment or study area. Based on a comprehensive characterization of the sediment sources and the end sediment mixtures a mixing model algorithm is applied to the sediment mixtures in order to estimate the relative contribution of each potential source. The package includes several statistical methods such as Kruskal-Wallis test, discriminant function analysis ('DFA'), principal component plot ('PCA') to select the optimal subset of tracer properties. The variability within each sediment source is also considered to estimate the statistical distribution of the sources contribution.

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URL <https://github.com/eead-csic-eesa>

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fingerPro-package *Sediment Source Fingerprinting*

Description

Soil erosion is one of the biggest challenges for food production and reservoirs siltation around the world. Information on sediment, nutrients and pollutant transport is required for effective control strategies. Source estimates are difficult to obtain using traditional monitoring techniques, but sediment source fingerprinting, has been proved to be a valuable tool. Sediment source fingerprinting offers the potential to assess sediment provenance as a basis to develop management plans and prevent erosion. The procedure focuses on developing methods that enable the apportionment of sediment sources to be identified from a composite sample of sediment mixture material. We developed an R-package as a tool to quantify the provenance of the sediments in a catchment. A mixing model algorithm is applied to the sediment mixture samples in order to estimate the relative contribution of each potential source. The package consists of a set of functions used to: i) characterise and pre-process the data, select the optimum subset of tracers; ii) unmix sediment samples and quantify the apportionment of each source; iii) assess the effect of the source variability; and iv) visualize and export the results.

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See Also

<https://github.com/eead-csic-eesa>

Examples

```

#Created on 22/08/2018

#If you want to use your own data
#setwd("the directory that contains your dataset")
#data <- read.table('your dataset', header = T, sep = '\t')
#install.packages("fingerPro")
#library(fingerPro)
#Example of the data included in the fingerPro package
#Load the dataset called "catchment"

# "Catchment": this dataset has been selected from a Mediterranean catchment for
#this purpose and contains high-quality radionuclides and geochemistry data.
#AG (cropland)
#PI and PI1 (Pine forest, at first looks different but when you display de LDA plot
#you will see that the wisser decision in join both pines as the same source)
#SS (subsoil)
data <- catchment
#boxPlot(data, columns = 1:6, ncol = 3)
#correlationPlot(data, columns = 1:5, mixtures = TRUE)
LDAPlot(data, P3D=FALSE)
#variables are collinear
#select the optimum set of tracers by implementing the statistical tests
data <- rangeTest(data)
data <- KWTest(data)
data <- DFATest(data)
#Check how the selected tracers discriminate between sources
LDAPlot(data, P3D=FALSE)
#change P3D=FALSE to P3D=TRUE to visualize the 3D LDAPlot
#2D and 3D LDAPlots suggest that two of the sources have to be combined
#reload the original dataset "catchment"
data <- catchment
# Combine sources PI1 and PI based on the previous LDAPlot
data$Land_Use[data$Land_Use == 'PI1'] <- 'PI'
#select the optimum set of tracers by implementing the statistical tests
data <- rangeTest(data)
data <- KWTest(data)
data <- DFATest(data)
LDAPlot(data, P3D=FALSE)
PCAPlot(data)
#Now the optimum tracer properties selected discriminate well, so proceed with the unmix function
result <- unmix(data, samples = 100L, iter =100L)
#Display the results
plotResults(result, y_high = 5, n = 1)
writeResults(result)

```

Description

The boxplot compactly shows the distribution of a continuous variable. It displays five summary statistics (the median, two hinges and two whiskers), and all "outlying" points individually.

Usage

```
boxPlot(data, columns = 1:ncol(data) - 2, ncol = 3)
```

Arguments

data	Data frame containing source and mixtures data
columns	Numeric vector containing the index of the columns in the chart (the first column refers to the first variable)
ncol	Number of charts per row

catchment

Land use and fingerprinting properties in a Mediterranean catchment

Description

A dataset containing the different tracer properties of the different land uses in a Mediterranean catchment and one mixture sample located at the output of the catchment. The variables are as follows:

Usage

```
catchment
```

Format

A data frame with 22 rows and 23 variables:

id reference number id of each sample analysed

Land_Use grouping variable, in this study refers to the different land uses in the catchment

Pbex, K40, Bi214, Ra226, Th232, U238, Nb, Sr, Rb, Pb, Zn, Fe, Mn, Cr, V, Ti, Ca, K, Al, Si, Mg
value of the tracer property for each sample

correlationPlot	<i>Correlation matrix chart</i>
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Description

The function displays a correlation matrix of each of the properties divided by the different sources to help the user in the decision.

Usage

```
correlationPlot(data, columns = c(1:ncol(data) - 1), mixtures = F)
```

Arguments

data	Data frame containing source and mixtures data
columns	Numeric vector containing the index of the columns in the chart (the first column refers to the grouping variable)
mixtures	Boolean to include or exclude the mixture samples in the chart

DFATest	<i>Discriminant function analysis test</i>
---------	--

Description

Performs a stepwise forward variable selection using the Wilk's Lambda criterion.

Usage

```
DFATest(data, niveau = 0.1)
```

Arguments

data	Data frame containing source and mixtures
niveau	level for the approximate F-test decision

Value

Data frame only containing the variables that pass the DFA test

ggbiplot

*Biplot for Principal Components using ggplot2***Description**

Biplot for Principal Components using ggplot2

Usage

```
ggbiplot(pcoobj, choices = 1:2, scale = 1, pc.biplot = TRUE,
  obs.scale = 1 - scale, var.scale = scale, groups = NULL,
  ellipse = FALSE, ellipse.prob = 0.68, labels = NULL, labels.size = 3,
  alpha = 1, var.axes = TRUE, circle = FALSE, circle.prob = 0.69,
  varname.size = 3, varname.adjust = 1.5, varname.abbrev = FALSE)
```

Arguments

pcoobj	an object returned by pcomp() or princomp()
choices	which PCs to plot
scale	covariance biplot (scale = 1), form biplot (scale = 0). When scale = 1, the inner product between the variables approximates the covariance and the distance between the points approximates the Mahalanobis distance.
pc.biplot	for compatibility with biplot.princomp()
obs.scale	scale factor to apply to observations
var.scale	scale factor to apply to variables
groups	optional factor variable indicating the groups that the observations belong to. If provided the points will be colored according to groups
ellipse	draw a normal data ellipse for each group?
ellipse.prob	size of the ellipse in Normal probability
labels	optional vector of labels for the observations
labels.size	size of the text used for the labels
alpha	alpha transparency value for the points (0 = transparent, 1 = opaque)
var.axes	draw arrows for the variables?
circle	draw a correlation circle? (only applies when pcomp was called with scale = TRUE and when var.scale = 1)
varname.size	size of the text for variable names
varname.adjust	adjustment factor the placement of the variable names, >= 1 means farther from the arrow
varname.abbrev	whether or not to abbreviate the variable names
circle.prob	size of the ellipse in Normal probability

Value

a ggplot2 plot

inputSample	<i>Input sediment mixtures</i>
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Description

The function select and extract the sediment mixtures of the dataset.

Usage

```
inputSample(data)
```

Arguments

data	Data frame containing source and mixtures data
------	--

inputSource	<i>Input sediment sources</i>
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Description

The function select and extract the source samples of the dataset.

Usage

```
inputSource(data)
```

Arguments

data	Data frame containing source and mixtures data
------	--

KWTest	<i>Kruskal-Wallis rank sum test</i>
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Description

This function excludes from the original data frame the properties which do not show significant differences between sources.

Usage

```
KWTest(data, pvalue = 0.05)
```

Arguments

data	Data frame containing source and mixtures
pvalue	p-value threshold

Value

Data frame only containing the variables that pass the Kruskal-Wallis test

LDAPlot *Linear discriminat analysis chart*

Description

The function performs a linear discriminant analysis and displays the data in the relevant dimensions.

Usage

```
LDAPlot(data, P3D = FALSE)
```

Arguments

data	Data frame containing source and mixtures data
P3D	Boolean to switch between 2 to 3 dimensional chart

PCAPlot *Principal component analysis chart*

Description

The function performs a principal components analysis on the given data matrix and displays a biplot using `vqv.ggbiplot` package of the results for each different source to help the user in the decision.

Usage

```
PCAPlot(data, components = c(1:2))
```

Arguments

data	Data frame containing source and mixtures data
components	Numeric vector containing the index of the two principal components in the chart

plotResults	<i>Displays the results in the screen</i>
-------------	---

Description

The function performs a density chart of the relative contribution of the potential sediment sources for each sediment mixture in the dataset.

Usage

```
plotResults(data, y_high = 6.5, n = 1)
```

Arguments

data	Data frame containing the relative contribution of the potential sediment sources for each sediment mixture in the dataset
y_high	Number of the vertical height of the y-axis
n	Number of charts per row

rangeTest	<i>Range test</i>
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Description

Function that excludes the properties of the sediment mixture/s outside the minimum and maximum values in the sediment sources.

Usage

```
rangeTest(data)
```

Arguments

data	Data frame containing source and mixtures
------	---

Value

Data frame containing sediment sources and mixtures

unmix	<i>Unmix sediment mixtures</i>
-------	--------------------------------

Description

Asses the relative contribution of the potential sediment sources for each sediment mixture in the dataset.

Usage

```
unmix(data, samples = 100L, iter = 100L, seed = 123456L)
```

Arguments

data	Data frame containing sediment source and mixtures
samples	Number of samples in each hypercube dimension
iter	Iterations in the source variability analysis
seed	Seed for the random number generator

Value

Data frame containing the relative contribution of the sediment sources for each sediment mixture and iterations

unmix_c	<i>Mixing model</i>
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Description

Mixing model

Usage

```
unmix_c(sources, samples, trials = 100L, iter = 100L,
  seed = 69512L)
```

Arguments

sources	Data frame containing sediment sources data
samples	Data frame containing sediment mixtures data
trials	Number of samples in each hypercube dimension
iter	Iterations in the source variability analysis
seed	Seed for the random number generator

Value

Data frame containing the relative contribution of the sediment sources for each sediment mixture and iterations

writeResults *Save the results*

Description

The function saves the results in the workspace file for all the sediment mixture samples and for each sediment mixture sample separately

Usage

writeResults(data)

Arguments

data Data frame containing the relative contribution of the potential sediment sources for each sediment mixture in the dataset

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