

Package ‘AQuality’

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Description The functions proposed in this package allows to evaluate the process of measurement of the chemical components of water numerically or graphically. TSSS(), ICHS and datacheck() functions are useful to control the quality of measurements of chemical components of a sample of water. If one or more measurements include an error, the generated graph will indicate it with a position of the point that represents the sample outside the confidence interval. The function CI() allows to evaluate the possibility of contamination of a water sample after being obtained. Validation() is a function that allows to calculate the quality parameters of a technique for the measurement of a chemical component.

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AQuality-package	<i>Water and Measurements Quality</i>
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Description

The package allows you to evaluate graphically the quality of measurements of water components

Details

The package includes five functions: TSSS(), ICHS(), datacheck(), validation() and CI(). The TSSS() function allows evaluating the quality of a set of measurement of water components, which correlate with total soluble solids. On the other hand, the ICHS() function allows evaluating the quality of a set of measurement of water components, which correlate with conductivity. The function CI() allows to evaluate the possibility of contamination of a water sample after being obtained. The function datacheck indicates the registers of a database that do not match simultaneously correlation of mass summation of chemical components with total soluble solids and correlation of charge summation of chemical components with conductivity. The function validation() allows to calculate the quality parameters of a technique for the measurement of a chemical component.

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CI	<i>Contamination Index</i>
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Description

Calculate an index that allows to estimate the possibility of microbiological contamination of a water sample after being obtained.

Usage

```
CI(sample,data)
```

Arguments

sample	Code of the sample whose quality you want to know.
data	Data.frame containing code of the database samples, and the concentration of the following chemical components: phosphate, nitrate, nitrite, tkm, ammonium, chemical demand of oxygen (dco), biological demand of oxygen (dbo) and organic matter.

Details

The CI() function performs the calculation of a score whose value allows to estimate the possibility of microbiological contamination of a water sample after being obtained.

Value

The CI() function returns a number (score). If $\text{score} \geq 0$ and $\text{score} \leq 2$, the sample is not contaminable. If $\text{score} > 2$ and $\text{score} \leq 4$, the sample is hardly contaminable. If $\text{score} > 4$ and $\text{score} \leq 6$, the sample is possibly contaminable. If $\text{score} > 6$ and $\text{score} \leq 8$, the sample is easily contaminable.

Author(s)

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datacheck

Two Criteria Database Check

Description

Generate a list of records that probably have errors in chemical components concentrations, based in two criteria: correlation between chemical components concentrations with total soluble solids, and correlation between chemical ionic components concentrations with conductivity

Usage

```
datacheck(dataICHs, dataTSSS, conflevel = 0.95, pchdata = 19, coldata = "green",
  cexdata = 0.5, pchsample = 19, colsample = "red", cexsample = 3, xaxis = xaxis,
  yaxis = yaxis, title = title, linetyprediction = 2, linewidthprediction = 1,
  linecolorprediction = 5)
```

Arguments

dataICHs	Registers of a database with concentrations of chemical components of water, including concentration of ionic chemical components and conductivity.
dataTSSS	Registers of a database with concentrations of chemical components of water, including concentration of chemical components and total soluble solids.
conflevel	Significance level used in the predict function.
pchdata	Symbol used to graph all the data in the data.frame.
coldata	Color of the symbols of all the data in the data.frame.
cexdata	Symbol size of all data in the data frame.
pchsample	Symbol chosen to represent the point whose measurement quality is to be represented.
colsample	Color chosen to represent the point whose measurement quality is to be represented.

cexsample	Size of the symbol chosen to represent the point whose measurement quality is to be represented.
xaxis	X axis label.
yaxis	Y axis label.
title	Title of the graph including the code of the chosen sample.
linetypprediction	Linear model prediction line type.
linewidthprediction	Linear model prediction line thickness.
linecolorprediction	Linear model prediction line color.

Details

The `datacheck()` function performs two linear regressions using the functions `TSSS()` and `ICHS()` of this package. `TSSS()` function performs a linear model using column 2 (total soluble solids) as the dependent variable and the other components of water as independent variables (columns 3 onwards). Based on the linear model, a data prediction interval is obtained with a certain confidence level and displays as a red point the samples that are outside the prediction interval. The `ICHS()` function performs a linear model using column 2 (conductivity) as the independent variable and the other components of water as dependent variables (columns 3 onwards). Based on the linear model, a data prediction interval is obtained with a certain confidence level and `ICHS` graphs in red points those samples that are outside the prediction interval. The `datacheck()` function selects the samples of the database, that are outside of both prediction intervals. If a sample is outside both prediction intervals, probably has an important error and must be revised.

Value

The `datacheck()` function returns a graph with two plots. The first plot displays the linear regression of charge summation as a function of conductivity, and the second one, the linear regression of mass summation as a function of total soluble solids. In both plots are presented the prediction interval and the samples that are outside of it, which probably has a problem of accuracy or precision, are displayed as red dots. The identification code of the samples that are outside both prediction intervals are displayed as a list.

Author(s)

Maela Lupo, Andrea Porpatto, Alfredo Rigalli

dataCI

Data Sets~~

Description

Data.frame with data for testing the `CI()` (Contamination Index) function. Column 1: sample identification code. Column 2: onwards: measurement of chemical components of water used to calculate CI, expressed in ppm.

Usage

```
data("dataCI")
```

Format

A data frame with 6 observations on the following 9 variables.

code a character vector
phosphate a numeric vector
nitrate a numeric vector
nitrite a numeric vector
ammonium a numeric vector
dco a numeric vector
tkn a numeric vector
organicmatter a character vector
dbo a numeric vector

Examples

```
# Including data.frame: dataCI in workspace.  
data("dataCI")  
# Column names of data.frame: dataCI  
names(dataCI)  
# Data set type of columns of data.frame: dataCI.  
str(dataCI)  
# Calculation of CI for the sample A1  
#The following code should calculate the CI for the sample A1 included in dataCI, which  
# is not acceptable as drinking water and is possibly contaminable.  
CI("A1",dataCI)  
#The following code should calculate the CI for the sample A2 included in dataCI, which  
#is acceptable as drinking water and is hardly contaminable.  
CI("A3",dataCI)
```

dataICHS

Data Sets

Description

Data.frame with data for testing the ICHS() (Ionic Charge Summation) function. Column 1: sample identification code. Column 2: measurement of water conductivity. Column3 onwards: measurement of ionic chemical components of water expressed in milliequivalent per litre.

Usage

```
data("dataICHS")
```

Format

A data frame with 411 observations on the following 14 variables.

```
codigo a character vector
conductividad a numeric vector
cargacloruro a numeric vector
cargacarbonato a numeric vector
cargabicarbonato a numeric vector
cargafosfato a numeric vector
carganitrato a numeric vector
carganitrito a numeric vector
cargafloruro a numeric vector
cargaarcenico a numeric vector
cargaamonio a numeric vector
cargasulfato a numeric vector
cargasodio a numeric vector
cargacalcio a numeric vector
```

Examples

```
# Including data.frame: data in workspace.
data("dataICHS")
# Column names of data.frame: data
names(dataICHS)
# Data set type of columns of data.frame: data.
str(dataICHS)
# Visualization of sample A45
#The following code should display a graphic with all samples in green dots and sample
# A45 as red big dot
ICHS("A45",dataICHS)
```

dataTSSS

Data Sets~~

Description

Data.frame with data for testing the TSSS() (total soluble solids summation) function. Column 1: sample identification code. Column 2: measurement of total soluble solids. Column3 onwards: measurement of chemical components of water expressed in the same units as column 2.

Usage

```
data("dataTSSS")
```

Format

A data frame with 411 observations on the following 16 variables.

codigo a character vector
solidostotales a numeric vector
cloruro a numeric vector
carbonato a numeric vector
bicarbonato a numeric vector
fosfato a numeric vector
nitrato a numeric vector
nitrito a numeric vector
fluoruro a numeric vector
arsenico a numeric vector
amonio a numeric vector
sulfato a numeric vector
sodio a numeric vector
tkn a numeric vector
calcio a numeric vector
magnesio a numeric vector

Examples

```
# Including data.frame: data in workspace.  
data("dataTSSS")  
# Column names of data.frame: data  
names(dataTSSS)  
# Data set type of columns of data.frame: data.  
str(dataTSSS)  
# Visualization of sample A45  
#The following code should display a graphic with all samples in green dots and sample  
# A45 as red big dot  
TSSS("A45",dataTSSS)
```

datavalidation*Data Sets~~*

Description

Data.frame with data for calculating the quality parameters of a technique for the measurement of a chemical component of water with the validation() function. The data.frame includes concentration and absorbance measurement of standards of the calibration curve and a solution of known concentration, called quality control (qc). The data.frame includes measurements of the absorbance of the tube at three different days. Column 1: name of the tube. The tubes b, s1, s2,s3 and s4 represent different concentrations of a calibration curve. Column 2: concentration: the concentration of each tube, expressed in micrograms. Column 3: abs: absorbance of each tube which were measured spectrophotometrically. Column 4: day: the day when the measurement was done.

Usage

```
data("datavalidation")
```

Format

A data frame with 46 measurement of the following variables.

tube a character vector

concentration a numeric vector

abs a numeric vector

day a numeric vector

Examples

```
# Including data.frame: datavalidation in workspace.
data("datavalidation")
# Column names of data.frame: datavalidation
names(datavalidation)
# Data set type of columns of data.frame: datavalidation.
str(datavalidation)
# Calculation of quality parameters of the Total Kjeldhal Nitrogen (tkn) measurement technique
validation(datavalidation,numest=4,measurementunit='ug',techniquename='tkn',graph=TRUE)
```

ICHS

Ionic Charge Summation

Description

Plots ionic charge summation as a function of conductivity.

Usage

```
ICHS(sample, data, conflevel = 0.95, pchdata = 19, coldata = "green", cexdata = 0.5,
      pchsample = 19, colsample = "red", cexsample = 3, xaxis = "CONDUCTIVITY",
      yaxis = "IONIC CHARGE SUMMATION", title = paste("Sample ", as.character(sample)),
      linetyprediction = 2, linewidthprediction = 1, linecolorprediction = 5)
```

Arguments

sample	Code of the sample whose quality you want to know.
data	Data.frame containing code of the database samples, conductivity, measurements of ionic water components.
conflevel	Significance level used in the predict function.
pchdata	Symbol used to graph all the data in the data.frame.
coldata	Color of the symbols of all the data in the data.frame.
cexdata	Symbol size of all data in the data frame.

pchsample	Symbol chosen to represent the point whose measurement quality is to be represented.
colsample	Color chosen to represent the point whose measurement quality is to be represented.
cexsample	Size of the symbol chosen to represent the point whose measurement quality is to be represented.
xaxis	X axis label.
yaxis	Y axis label.
title	Title of the graph including the code of the chosen sample.
linetypprediction	Linear model prediction line type.
linewidthprediction	Linear model prediction line thickness.
linecolorprediction	Linear model prediction line color.

Details

The ICHS() function performs a linear model using column 2 (conductivity) as the independent variable and the other components of water as dependent variables (columns 3 onwards). Based on the linear model, a data prediction interval is obtained with a certain confidence level (conflevel). Then, ICHS() graphs the values of the entire database and finally graphs as a point with different color, the sample whose measurement quality you want to observe.

Value

The ICHS() function returns a graph of the sum of ionic chemical components as a function of the measurement of conductivity for each sample. It contains the confidence interval indicated in a dotted line, and the sample under observation. If the point that represents the sample is within the region delimited by the lines of the confidence interval, it is presumed that there were no serious measurement errors of the components analyzed.

Author(s)

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TSSS

Total Soluble Solids Summation

Description

Plot total soluble solids summation as a function of total soluble solids measurement.

Usage

```
TSSS(sample, data, conflevel = 0.95, pchdata = 19, coldata = "green", cexdata = 0.5,
pchsample = 19, colsample = "red", cexsample = 3, xaxis = "TOTAL SOLUBLE SOLIDS",
yaxis = "MASS SUMMATION", title = paste("Sample ", as.character(sample)),
linetyprediction = 2, linewidthprediction = 1, linecolorprediction = 5)
```

Arguments

sample	Code of the sample whose quality you want to know.
data	Data.frame containing code of the database samples, total soluble solids, measurements of other water components.
conflevel	Significance level used in the predict function.
pchdata	Symbol used to graph all the data in the data.frame.
coldata	Color of the symbols of all the data in the data.frame.
cexdata	Symbol size of all data in the data frame.
pchsample	Symbol chosen to represent the point whose measurement quality is to be represented.
colsample	Color chosen to represent the point whose measurement quality is to be represented.
cexsample	Size of the symbol chosen to represent the point whose measurement quality is to be represented.
xaxis	X axis label.
yaxis	Y axis label.
title	Title of the graph including the code of the chosen sample.
linetyprediction	Linear model prediction line type.
linewidthprediction	Linear model prediction line thickness.
linecolorprediction	Linear model prediction line color.

Details

The TSSS() function performs a linear model using column 2 (total soluble solids) as the dependent variable and the other components of water as independent variables (columns 3 onwards). Based on the linear model, a data prediction interval is obtained with a certain confidence level (conflevel). Then, TSSS() graphs the values of the entire database and finally graphs as a point with different color, the sample whose measurement quality you want to observe.

Value

The TSSS() function returns a graph of the sum of soluble solids as a function of the measurement of total soluble solids for each sample. It contains the confidence interval and the sample under observation indicated in a dotted line. If the point that represents the sample is within the region delimited by the lines of the confidence interval, it is presumed that there were no serious measurement errors of the components analyzed.

Author(s)

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validation

Quality parameters of a measurement technique

Description

Calculate the quality parameters of a technique for the measurement of a chemical component.

Usage

```
validation(datavalidation, numest = NULL, measurementunit = NULL,  
techniquename = NULL, date = Sys.Date(), graph = FALSE)
```

Arguments

datavalidation	Data.frame with data for points of a calibration curve of five points, including a reagent blank and four standards. The data.frame also includes a solution of known concentration called quality control (qc). The columns include name of the tube, concentration, absorbance and day of measurement.
numest	The number of standards solution used for the calibration curve. This number do not include the reagent blank.
measurementunit	The unit of measurement of the concentration.
techniquename	The name of the technique whose quality parameters are calculated.
date	The date when the procedure is performed.
graph	Graph argument allows to plot the calibration curve.

Details

The validation() function calculates a set of quality parameters of a technique for the measurement of a chemical component. The function needs the values of a property (absorbance in the example) of standard solutions with different known concentration of one chemical component of water, measured in three different days. The function also needs the values of the property of a solution with a known concentration of the component, different from the standards of the calibration curve, which is called quality control solution (qc).

Value

The datavalidation() function returns a graph of the calibration curve if the argument graph takes the value TRUE. The function calculates and returns a list with the values of the slope of the calibration curve, the detection limit (LOD), the quantification limit (LOQ), correlation coefficient, sensitivity, accuracy, intraassay repetitivity, interassayrepetitivity, linear range and uncertainty.

Author(s)

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