Package 'ILS'

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Type Package

Title Interlaboratory Study

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Description It performs interlaboratory studies (ILS) to detect those laboratories that provide non-consistent results when comparing to others. It permits to work simultaneously with various testing materials, from standard univariate, and functional data analysis (FDA) perspectives. The univariate approach based on ASTM E691-08 consist of estimating the Mandel's h and k statistics to identify those laboratories that provide more significant different results, testing also the presence of outliers by Cochran and Grubbs tests, Analysis of variance (ANOVA) techniques are provided (F and Tuckey tests) to test differences in means corresponding to different laboratories per each material. Taking into account the functional nature of data retrieved in analytical chemistry, applied physics and engineering (spectra, thermograms, etc.). ILS package provides a FDA approach for finding the Mandel's k and h statistics distribution by smoothing bootstrap resampling.

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LazyData yes

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 $\boldsymbol{URL} \text{ https://github.com/mflores72000/ILS/}$

BugReports https://github.com/mflores72000/ILS/issues

Suggests knitr, rmarkdown

R topics documented:

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boot.sim.set

Bootstrap samples of a functional statistic

Description

data. bootstrap provides bootstrap samples for functional data.

Usage

```
boot.sim.set(x, smo = 0.05)
```

Arguments

x An object of classs fdata.

smo The smoothing parameter for the bootstrap samples.

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cochran.test

Function to compute the Cochran test statistic

Description

Function to estimate the Cochran test statistic.

Usage

```
cochran.test(x, ...)
## Default S3 method:
cochran.test(
    x,
    var.index = 1,
    replicate.index = 2,
    material.index = 3,
    laboratory.index = 4,
    data.name = NULL,
    alpha = 0.05,
    ...
)
## S3 method for class 'lab.qcdata'
cochran.test(x, alpha = 0.05, ...)
```

Arguments

x An object of class lab. qcdata (Univariate Quality Control Data).

. . . Other arguments passed to or from methods.

var.index A scalar with the column number corresponding to the observed variable (the

critical to quality variable). Alternativelly can be a string with the name of the

quality variable.

replicate.index

A scalar with the column number corresponding to the index each replicate.

material.index A scalar corresponding to the replicated number.

laboratory.index

A scalar that defines the index number of each laboratory.

data.name A string specifying the name of the variable which appears on the plots. If name

is not provided, it is taken from the object given as data.

alpha The significance level (0.05 by default)

DSC DSC

References

Wilrich Peter-T. (2013), Critical values of mandel's h and k, the grubbs and the Cochran test statistic. Asta-Advances in Statistical Analysis, 97(1):1-10.

ASTM E 691 (1999), Standard practice for conducting an interlaboratory study to determine the precision of a test method. American Society for Testing and Materials. West Conshohocken, PA, USA.

Examples

library(ILS)
data(Glucose)
Glucose.qcdata <- lab.qcdata(Glucose)
str(Glucose.qcdata)
cochran.test(Glucose.qcdata)</pre>

DSC

Differential Scanning Calorimetry curves

Description

90 samples of calcium oxalate were analyzed by differential scanning calorimetry technique (DSC), obtaining 90 DSC curves showing from an SDT device the difference of heat between a sample and an oxalate reference value depending on the temperature that the samples are heated at a constant temperature rate. The data set consists of 15 TG curves of 1000 observations from each of the 6 laboratories. Laboratory 2 to Laboratory 4 uses the same simultaneous SDT analyzer in similar conditions, Laboratory 6 uses a simultaneous SDT analyzer with an old calibration, and Laboratory 7 uses a simultaneous SDT analyzer with a calibration (2 degrees Celsius displaced from the zinc melting point).

Format

5 x 1000 x 6 dimension array, where each matrix consists of the 15 DSC curves obtained by testing 15 different oxalate samples, and evaluated at 1000 different temperature values. These 15 curves were obtained for each of the 6 laboratories that performed the experiments.

Xi Differential Scanning Calorimetry curves.

References

Naya, S., Tarrio-Saavedra. J., Lopez-Beceiro, J., Francisco Fernandez, M., Flores, M. and Artiaga, R. (2014), "Statistical functional approach for interlaboratory studies with thermal data". Journal of Thermal Analysis and Calorimetry, 118,1229-1243.

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Examples

library(ILS)
data(DSC)
summary(DSC)

func.ils.formula

Descriptive measures for functional data.

Description

Central and dispersion measures for functional data.

Usage

```
func.ils.formula(formula, data = NULL, drop = FALSE, func = func.mean)
```

Arguments

formula	A formula, such as $y \sim \text{group}$, where y is a fdata object. to be split into groups according to the grouping variable group (usually a factor).
data	List that containing the variables in the formula. The item called "df" is a data frame with the grouping variable. The item called "y" is a fdata object.
drop	Logical indicating if levels that do not occur should be dropped (if f is a factor or a list).
func	Measures for functional data.
Glucose	Glucose in Serum

Description

Dataset corresponding to serum glucose (measurements of glucose concentration in blood used to control diabetes) testing. Eight laboratories conducted tests to five different blood samples tagged with different references, ranging them from low sugar content to very high. Three replicates were obtained for each sample. It is retrieved from ASTM E 691 standard.

Format

A data frame with 120 observations composed of the following 4 variables:

Glucose Glucose content in Serum.

Replicate Number of glucose measurement corresponding to each material.

Material Level of glucose, ranging from low content of sugar to very high level of glucose in blood.

Laboratory Laboratories conducted tests.

grubbs.test

References

ASTM E 691 (1999). Standard practice for conducting an interlaboratory study to determine the precision of a test method. American Society for Testing and Materials. West Conshohocken, PA, USA.

Examples

```
library(ILS)
data(Glucose)
summary(Glucose)
attach(Glucose)
str(Glucose)
table(Replicate, Material, Laboratory)
table(Laboratory, Material)
st <- with(Glucose, tapply(Glucose, list(Material, Laboratory), mean))
st</pre>
```

grubbs.test

Function to compute the Grubbs test statistic

Description

Function to estimate the Grubbs test statistic.

```
grubbs.test(x, ...)
## Default S3 method:
grubbs.test(
    x,
    var.index = 1,
    replicate.index = 2,
    material.index = 3,
    laboratory.index = 4,
    data.name = NULL,
    alpha = 0.05,
    ...
)
## S3 method for class 'lab.qcdata'
grubbs.test(x, alpha = 0.05, ...)
```

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Arguments

x An object of class lab. qcdata (Univariate Quality Control Data).

... Other arguments passed to or from methods.

var.index A scalar with the column number corresponding to the observed variable (the

critical to quality variable). Alternativelly can be a string with the name of the

quality variable.

replicate.index

A scalar with the column number corresponding to the index each replicate.

material.index A scalar corresponding to the replicated number.

laboratory.index

A scalar that defines the index number of each laboratory.

data.name A string specifying the name of the variable which appears on the plots. If name

is not provided, it is taken from the object given as data.

alpha The significance level (0.05 for default)

References

Wilrich Peter-T. (2013), Critical values of Mandel's h and k, the Grubbs and the Cochran test statistic. Asta-Advances in Statistical Analysis, 97(1):1-10.

ASTM E 691 (1999), Standard practice for conducting an interlaboratory study to determine the precision of a test method. American Society for Testing and Materials. West Conshohocken, PA, USA.

Examples

library(ILS)
data(Glucose)
Glucose.qcdata<- lab.qcdata(Glucose)
str(Glucose.qcdata)
grubbs.test(Glucose.qcdata)</pre>

h.qcs

Function to estimate the univariate Mandel's h statistic

Description

This function is used to compute the Mandel's h statistic.

h.qcs

Usage

```
h.qcs(x, ...)
## Default S3 method:
h.qcs(
    x,
    var.index = 1,
    replicate.index = 2,
    material.index = 3,
    laboratory.index = 4,
    data.name = NULL,
    alpha = 0.05,
    ...
)
## S3 method for class 'lab.qcdata'
h.qcs(x, alpha = 0.05, ...)
```

Arguments

x An object of class lab. qcdata (Univariate Quality Control Data).

... Other arguments passed to or from methods.

var.index A scalar with the column number corresponding to the observed variable (the

critical to quality variable). Alternativelly can be a string with the name of the

quality variable.

replicate.index

A scalar with the column number corresponding to the index each replicate.

material.index A scalar corresponding to the replicated number.

laboratory.index

A scalar that defines the index number of each laboratory.

data.name A string specifying the name of the variable which appears on the plots. If name

is not provided, it is taken from the object given as data.

alpha The significance level (0.05 by default)

References

Wilrich Peter-T. (2013), Critical values of Mandel's h and k, the Grubbs and the Cochran test statistic. Asta-Advances in Statistical Analysis, 97(1):1-10.

ASTM E 691 (1999), Standard practice for conducting an interlaboratory study to determine the precision of a test method. American Society for Testing and Materials. West Conshohocken, PA, USA.

```
library(ILS)
data(Glucose)
```

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```
Glucose.qcdata <- lab.qcdata(Glucose)
str(Glucose.qcdata)
h<- h.qcs(Glucose.qcdata, alpha = 0.005)
summary(h)
plot(h)</pre>
```

IDT

Dataset composed of the initial decomposition temperature (IDT) of different samples of Calcium Oxalate, obtained by 7 different laboratories

Description

Initial decomposition temperature (IDT) is a parameter defined by temperature at which a material loss 5% of its weight when it is heated using a constant rate. One hundred and five calcium oxalate samples were tested by thermogravimetric analysis (TG), obtaining 105 TG curves from which the IDT is extracted. Summarizing, IDT dataset is composed of the IDT values of calcium oxalate obtained by 7 different laboratories that analyze 15 oxalate samples each one.: Laboratory 1 uses a simultaneous thermal analyzer (STA) with an old calibration program, Laboratory 2 to Laboratory 4 use a SDT simultaneous analyzer with an old calibration, and Laboratory 7 uses a SDT simultaneous analyzer with a biased calibration (2 degrees Celsius shifted from the zinc melting point).

Format

Dataframe of dimension 105 x 44. The first column corresponds to IDT variable, the second (Sample) is the replicate number, the third is the tested material (Material), and fourth is the laboratory.

IDT Initial decomposition temperature.

Sample The replicate number.

Run Tested material.

Laboratory Laboratories conducted tests.

References

Naya, S., Tarrio-Saavedra. J., Lopez-Beceiro, J., Francisco Fernandez, M., Flores, M. and Artiaga, R. (2014), "Statistical functional approach for interlaboratory studies with thermal data". Journal of Thermal Analysis and Calorimetry, 118,1229-1243.

```
library(ILS)
data(IDT)
summary(IDT)
attach(IDT)
str(IDT)
table(Sample,Run,Laboratory)
table(Laboratory,Run)
st <- with(IDT, tapply(IDT, list(Run,Laboratory), mean))
st</pre>
```

ils.fqcdata

ILS

Interlaboratoty Study

Description

Interlaboratory Study

Details

It performs interlaboratory studies (ILS) to detect those laboratories that provide non-consistent results when comparing to others. It permits to work simultaneously with various testing materials, from standard univariate, and functional data analysis (FDA) perspectives. The univariate approach based on ASTM E691-08 consist of estimating the Mandel's h and k statistics to identify those laboratories that provide more significant different results, testing also the presence of outliers by Cochran and Grubbs tests, Analysis of variance (ANOVA) techniques are provided (F and Tuckey tests) to test differences in the testing variable means corresponding to test differences in means corresponding to differente laboratories per each material. Taking into account the functional nature of data retrieved in analytical chemistry, applied physics and engineering (spectra, thermograms, etc.). ILS package provides a FDA approach for functional Mandel's k and h statistics by smoothing bootstrap resampling of distribution.

ils.fqcdata

Functional Quality Control Data

Description

It Creates an object of class 'ils.fqcd' to perform statistical quality control. This object is used to plot functional data.

```
ils.fqcdata(
    x,
    p = NULL,
    index.laboratory = NULL,
    argvals = NULL,
    rangeval = NULL,
    names = NULL
```

ils.fqcs

Arguments

x A (n x m) matrix or data-frame. The m is the number of points observed in each

curve, and n is the number of curves for each laboratory.

p The number of laboratories.

index.laboratory

The laboratory index. The index laboratory length should be equal a p.

argvals Argvals, by default: 1:m.

rangeval The range of discretization points, by default: range(argvals).

names Optional. A list with tree components: main an overall title, xlab title for x axis

and ylab title for y axis.

References

Febrero-Bande, M. and Oviedo, M. (2012), "Statistical computing in functional data analysis: the R package fda.usc". Journal of Statistical Software 51 (4), 1-28.

Naya, S., Tarrio-Saavedra. J., Lopez-Beceiro, J., Francisco Fernandez, M., Flores, M. and Artiaga, R. (2014), Statistical functional approach for interlaboratory studies with thermal data". Journal of Thermal Analysis and Calorimetry, 118,1229-1243.

Examples

```
library(ILS)
data(TG)
delta <- seq(from = 40 ,to = 850 ,length.out = 1000 )
fqcdata <- ils.fqcdata(TG, p = 7, argvals = delta)
xlab <- "Temperature (C)"
ylab <- "Mass (%)"
main <- "TG curves obtained from calcium oxalate"
plot(x = fqcdata, main = main, xlab=xlab, ylab=xlab,col = 1:7,legend = TRUE)</pre>
```

ils.fqcs

It developes an object of class 'ils.fqcs'

Description

Create an object of class 'ils.fqcs' to perform statistical quality control. This function is used to compute requested FDA.

```
ils.fqcs(x, ...)
## Default S3 method:
ils.fqcs(x, argvals = NULL, rangeval = NULL, ...)
## S3 method for class 'ils.fqcdata'
```

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```
ils.fqcs(x, ...)
## S3 method for class 'ils.fqcs'
print(x, ...)
## S3 method for class 'ils.fqcs'
summary(object, ...)
```

Arguments

x An object of class ils.fqcs for which a print is desired.

... Other arguments passed to or from methods.

argvals Argvals, by default: 1:m.

rangeval The range of discretization points, by default: range(argvals).

object An object of class ils.fqcs for which a summary is desired.

References

Febrero-Bande, M. and Oviedo, M. (2012), "Statistical computing in functional data analysis: the R package fda.usc". Journal of Statistical Software 51 (4), 1-28

Cuevas A., Febrero-Bande, M. and Fraiman, R. (2006), "On the use of the bootstrap for estimating functions with functional data". Computational Statistics & Data Analysis 51, 2, 1063-1074.

Naya, S., Tarrio-Saavedra. J., Lopez-Beceiro, J., Francisco Fernandez, M., Flores, M. and Artiaga, R. (2014), "Statistical functional approach for interlaboratory studies with thermal data". Journal of Thermal Analysis and Calorimetry, 118,1229-1243.

Examples

```
library(ILS)
data(TG)
delta <- seq(from = 40 ,to = 850 ,length.out = 1000 )
fqcdata <- ils.fqcdata(TG, p = 7, argvals = delta)
xlab <- "Temperature/ C"
ylab <- "Mass/ %"
fqcstat <- ils.fqcs(fqcdata)
plot(fqcstat, xlab = xlab, ylab = ylab,legend = TRUE)</pre>
```

k.qcs

Function to calcute the Mandel's k statistic

Description

This function is used to compute the statistic k of Mandel.

k.qcs

Usage

```
k.qcs(x, ...)
## Default S3 method:
k.qcs(
    x,
    var.index = 1,
    replicate.index = 2,
    material.index = 3,
    laboratory.index = 4,
    data.name = NULL,
    alpha = 0.05,
    ...
)
## S3 method for class 'lab.qcdata'
k.qcs(x, alpha = 0.05, ...)
```

Arguments

x An object of class lab. qcdata (Univariate Quality Control Data).

... Other arguments passed to or from methods.

var.index A scalar with the column number corresponding to the observed variable (the

critical to quality variable). Alternativelly can be a string with the name of the

quality variable.

replicate.index

A scalar with the column number corresponding to the index each replicate.

material.index A scalar corresponding to the replicated number.

laboratory.index

A scalar that defines the index number of each laboratory.

data.name A string specifying the name of the variable which appears on the plots. If name

is not provided, it is taken from the object given as data.

alpha The significance level (0.05 by default)

References

Wilrich Peter-T. (2013), Critical values of Mandel's h and k, the Grubbs and the Cochran test statistic. Asta-Advances in Statistical Analysis, 97(1):1-10.

ASTM E 691 (1999), Standard practice for conducting an interlaboratory study to determine the precision of a test method. American Society for Testing and Materials. West Conshohocken, PA, USA.

```
library(ILS)
data(Glucose)
```

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```
Glucose.qcdata <- lab.qcdata(Glucose)
str(Glucose.qcdata)
k<- k.qcs(Glucose.qcdata, alpha = 0.005)
summary(k)
plot(k)</pre>
```

lab.aov

Function to compute the AOV

Description

Function to compute the analysis of variance of ILS data, taking into account the laboratories and material factors.

Usage

```
lab.aov(x, ...)

## Default S3 method:
lab.aov(
    x,
    var.index = 1,
    replicate.index = 2,
    material.index = 3,
    laboratory.index = 4,
    data.name = NULL,
    level = 0.95,
    plot = FALSE,
    pages = 0,
    ...
)

## S3 method for class 'lab.qcdata'
lab.aov(x, level = 0.95, plot = FALSE, pages = 0, ...)
```

Arguments

x An object of class lab.qcdata (Univariate Quality Control Data).

... Other arguments passed to or from methods.

var.index A scalar with the column number corresponding to the observed variable (the critical to quality variable). Alternatively can be a string with the name of the

quality variable.

replicate.index

A scalar with the column number corresponding to the index each replicate.

 $\label{lem:material.index} \begin{tabular}{ll} A scalar corresponding to the replicated number. \\ laboratory.index \end{tabular}$

A scalar that defines the index number of each laboratory.

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data.name A string specifying the name of the variable which appears on the plots. If name

is not provided, it is taken from the object given as data.

level Requested confidence level (0.95 by default).

plot If TRUE, confidence intervals are plot.

pages By default 0, it indicates the number of pages over which to spread the output.

For example, if pages=1, all terms will be plotted on one page with the layout performed automatically. If pages=0, one plot will be displayed by each tested

material.

References

WHothorn T., Bretz, F., and Westfall, P. (2008), Simultaneous inference in general parametric models. Biometrical Journal, 50(3):346-363.

Heyden, Y., Smeyers-Verbeke, J. (2007), Set-up and evaluation of interlaboratory studies. J. Chromatogr. A, 1158:158-167.

Examples

```
## Not run:
library(ILS)
data(Glucose)
Glucose.qcdata <- lab.qcdata(Glucose)
str(Glucose.qcdata)
lab.aov(Glucose.qcdata,level = 0.95, plot = TRUE, pages = 1)
## End(Not run)</pre>
```

lab.qcdata

Quality Control Data

Description

It creates a 'lab.qcdata' class object to perform the interlaboratory study. This object is used to plot ILS data and more.

```
lab.qcdata(
  data,
  var.index = 1,
  replicate.index = 2,
  material.index = 3,
  laboratory.index = 4,
  data.name = NULL
)
```

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Arguments

data A matrix or data-frame that contains the data, replicate index, type of material,

and the laboratory.

var.index A scalar with the column number corresponding to the observed variable (the

critical to quality variable). Alternativelly can be a string with the name of the

quality variable.

replicate.index

A scalar with the column number corresponding to the index each replicate.

material.index A scalar corresponding to the replicated number.

laboratory.index

A scalar that defines the index number of each laboratory.

data.name A string specifying the name of the variable which appears on the plots. If name

is not provided, it is taken from the object given as data.

Examples

```
library(ILS)
data(Glucose)
Glucose.qcdata <- lab.qcdata(Glucose)
str(Glucose.qcdata)
summary(Glucose.qcdata)</pre>
```

lab.qcs

Create an object of class 'lab.qcs' to perform statistical quality control. This function is used to compute statistics required for plotting Statitics

Description

It develops an object of lab.qcs-codelinkclass to perform statistical quality control. This function is used to compute the requested statistics to be summarized and ploted.

Usage

```
lab.qcs(x, ...)
## S3 method for class 'lab.qcs'
print(x, ...)
## S3 method for class 'lab.qcs'
summary(object, ...)
```

Arguments

x An object of class lab. qcs for which a print is desired.

... Other arguments passed to or from methods.

object An object of class lab. qcs for which a summary is desired.

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Examples

```
library(ILS)
data(Glucose)
Glucose.qcdata <- lab.qcdata(Glucose)
str(Glucose.qcdata)
Glucose.qcs <- lab.qcs(Glucose.qcdata)
str(Glucose.qcs)
summary(Glucose.qcs)</pre>
```

mandel.fqcs

This function is used to compute the FDA Mandel's h and k statistic

Description

It develops an object of 'mandel.fqcs' class to perform statistical quality control analysis. This function is used to compute the functional approach of Mandel's h and k statistic. It is specifically designed to deal with experimental data results defined by curves such as thermograms and spectra.

```
mandel.fqcs(x, ...)
## Default S3 method:
mandel.fqcs(
  Х,
  p = NULL,
  index.laboratory = NULL,
  argvals = NULL,
  rangeval = NULL,
  names = NULL,
)
## S3 method for class 'ils.fqcdata'
mandel.fqcs(
  Х,
  fdep = depth.mode,
  outlier = TRUE,
  trim = 0.01,
  alpha = 0.01,
  nb = 200,
  smo = 0.05,
)
```

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Arguments

A (n x m) matrix or data-frame. The m is the number of points observed in each

curve, and n is the number of curves for each laboratory.

... Other arguments passed to or from other methods.

p The number of laboratories.

index.laboratory

The laboratory index. The index laboratory length should be equal a p.

argvals Argvals, by default: 1:m.

rangeval The range of discretization points, by default: range(argvals).

names Optional. A list with tree components: main an overall title, xlab title for x axis

and ylab title for y axis.

fdep Type of depth measure, by default depth.mode.

outlier = TRUE

trim The alpha of the trimming.

alpha Significance level, by defaul 1%.

nb The number of bootstrap samples.

smo The smoothing parameter for the bootstrap samples.

References

Febrero-Bande, M. and Oviedo, M. (2012), "Statistical computing in functional data analysis: the R package fda.usc". Journal of Statistical Software 51 (4), 1-28.

Cuevas A., Febrero-Bande, M. and Fraiman, R. (2006), "On the use of the bootstrap for estimating functions with functional data". Computational Statistics & Data Analysis 51, 2, 1063-1074.

Naya, S., Tarrio-Saavedra. J., Lopez-Beceiro, J., Francisco Fernandez, M., Flores, M. and Artiaga, R. (2014), "Statistical functional approach for interlaboratory studies with thermal data". Journal of Thermal Analysis and Calorimetry, 118,1229-1243.

```
## Not run:
library(ILS)
data(TG)
delta <- seq(from = 40 ,to = 850 ,length.out = 1000 )
fqcdata <- ils.fqcdata(TG, p = 7, argvals = delta)
mandel.tg <- mandel.fqcs(fqcdata.tg,nb = 200)
plot(mandel.tg,legend = F,col=c(rep(3,5),1,1))
## End(Not run)</pre>
```

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outliers.ils

Detecting outliers for functional dataset

Description

Procedure for detecting functional outliers.

Usage

```
outliers.ils(x, fdep = depth.FM, trim = 0.01)
```

Arguments

x An object of classs fdata.

fdep Type of depth measure, by default depth.mode.

trim The percentage of the trimming, by default is 1%.

plot.ils.fqcdata

Plotting method for 'ils.fqcdata' objects

Description

Generic function to plot objects of 'ils.fqcdata' class

```
## S3 method for class 'ils.fqcdata'
plot(
    x,
    type = "1",
    main = NULL,
    xlab = NULL,
    ylab = NULL,
    ylim = NULL,
    y.co = NULL,
    y.co = NULL,
    legend = TRUE,
    col = NULL,
    ...
)
```

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Arguments

x An object class of ils. fqcdata (Functional Quality Control Data)

type 1-character string giving the type of plot desired. The following values are pos-

sible for fdata class object: "I" for lines (by default), "p" for points, , "o" for overplotted points and lines, "b", "c" for (empty if "c") points joined by lines, "s" and "S" for stair steps and "h" for histogram-like vertical lines. Finally, "n" does not produce any points or lines. The following values are possible for fdata2d class object: "image.contour" (by default) to display three-dimensional data and add the contour lines, "image" to display three-dimensional data, "contour" to display a contour plot, "persp" to display a perspective plots of a surface over the x-y plane and "filled.contour" to display a contour plot with the areas

between the contours filled in solid color.

main Main title for the plot.

xlab Title for the x axis.

ylab Title for the y axis.

ylim The y limits of the plot.

x.co It specifies the x co-ordinates to be used to place a legend.

y.co It specifies the y co-ordinates to be used to place a legend.

legend Logical argument. Default is TRUE then The legend default is used.

col Color specifications

... Other arguments passed to matplot function (for fdata class).

References

Febrero-Bande, M. and Oviedo, M. (2012), "Statistical computing in functional data analysis: the R package fda.usc". Journal of Statistical Software 51 (4), 1-28. Naya, S., Tarrio-Saavedra. J., Lopez-Beceiro, J., Francisco Fernandez, M., Flores, M. and Artiaga, R. (2014), "Statistical functional approach for interlaboratory studies with thermal data". Journal of Thermal Analysis and Calorimetry, 118,1229-1243.

```
## Not run:
library(ILS)
data(TG)
delta <- seq(from = 40 ,to = 850 ,length.out = 1000 )
fqcdata <- ils.fqcdata(TG, p = 7, argvals = delta)
windows()
xlab <- "Temperature (C)"
ylab <- "Mass (%)"
main <- "TG curves obtained from calcium oxalate"
plot(x = fqcdata, main = main, xlab=xlab, ylab=ylab,legend = TRUE)
## End(Not run)</pre>
```

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plot.ils.fqcs

Plotting method for 'ils.fqcs' objects

Description

Generic function to plot objects of 'ils.fqcs' class. Results of functional ILS studies are graphically shown.

Usage

```
## S3 method for class 'ils.fqcs'
plot(x, type = "1", xlab = NULL, ylab = NULL, legend = TRUE, col = NULL, ...)
```

Arguments

x An object of class ils.fqcs (Functional Quality Control Statistics).

type 1-character string giving the type of plot desired. The following values are pos-

sible for fdata class object: "I" for lines (by default), "p" for points, , "o" for overplotted points and lines, "b", "c" for (empty if "c") points joined by lines, "s" and "S" for stair steps and "h" for histogram-like vertical lines. Finally, "n" does not produce any points or lines. The following values are possible for fdata2d class object: "image.contour" (by default) to display three-dimensional data and add the contour lines, "image" to display three-dimensional data, "contour" to display a contour plot, "persp" to display a perspective plots of a surface over the x-y plane and "filled.contour" to display a contour plot with the areas

between the contours filled in solid color.

xlab Title for the x axis. ylab Title for the y axis.

legend Logical argument. Default is TRUE then The legend default is used.

col Color specifications.

... Other arguments to be passed to or from methods.

References

Febrero-Bande, M. and Oviedo, M. (2012), "Statistical computing in functional data analysis: the R package fda.usc". Journal of Statistical Software 51 (4), 1-28.

Naya, S., Tarrio-Saavedra. J., Lopez-Beceiro, J., Francisco Fernandez, M., Flores, M. and Artiaga, R. (2014), "Statistical functional approach for interlaboratory studies with thermal data". Journal of Thermal Analysis and Calorimetry, 118,1229-1243.

```
library(ILS)
data(TG)
delta <- seq(from = 40 ,to = 850 ,length.out = 1000 )</pre>
```

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```
fqcdata <- ils.fqcdata(TG, p = 7, argvals = delta)
xlab <- "Temperature/ C"
ylab <- "Mass/ %"
fqcstat <- ils.fqcs(fqcdata)
plot(fqcstat, xlab = xlab, ylab = ylab,legend = TRUE)</pre>
```

plot.lab.qcdata

Plot method for 'lab.qcdata' objects

Description

Generic function for plotting objects of 'lab.qcdata' class. Results of univariate ILS studies are graphically shown.

Usage

```
## S3 method for class 'lab.qcdata'
plot(x, xlab = NULL, ylab = NULL, col = "blue", ...)
```

Arguments

```
x An object of class lab. qcdata (Univariate Quality Control Data).
xlab Title for the x axis.
ylab Title for the y axis.
col Color of type material, when there only one.
... Other arguments to be passed to or from methods.
```

Examples

```
library(ILS)
data(Glucose)
Glucose.qcdata <- lab.qcdata(Glucose)
str(Glucose.qcdata)
plot(Glucose.qcdata)</pre>
```

plot.lab.qcs

Plot method for 'lab.qcs' objects

Description

Generic function for plotting objects of 'lab.qcs' class. Results of univariate ILS studies are graphically shown.

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Usage

```
## S3 method for class 'lab.qcs'
plot(x, title = NULL, xlab = NULL, ylab = NULL, col = NULL, ylim = NULL, ...)
```

Arguments

Χ	An object of class lab.qcs (Univariate Quality Control Statistics).
title	Main title for the plot.
xlab	Title for the x axis.
ylab	Title for the y axis.
col	Color specifications.
ylim	A Numeric vectors of length 2 (coordinates ranges).
	Other arguments to be passed to or from methods.

Examples

```
library(ILS)
data(Glucose)
Glucose.qcdata <- lab.qcdata(Glucose)
Glucose.qcs <- lab.qcs(Glucose.qcdata)
plot(Glucose.qcs)</pre>
```

plot.mandel.fqcs

Plotting method for 'mandel.fqcs' objects

Description

Generic function to plot objects of 'mandel.fqcs' class. Results of functional ILS studies are graphically shown.

```
## S3 method for class 'mandel.fqcs'
plot(
    x,
    xlab = NULL,
    ylab = NULL,
    x.co = NULL,
    y.co = NULL,
    legend = TRUE,
    col = NULL,
    ...
)
```

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Arguments

Χ	An object of class mandel.fqcs.
xlab	Title for the x axis.
ylab	Title for the y axis.
x.co	It speficies the x co-ordinates to be used to place a legend.
y.co	It specifies the y co-ordinates to be used to place a legend.
legend	Logical argument. Default is TRUE then The legend default is used.
col	Color specifications.
	Other arguments to be passed to or from methods.

References

Febrero-Bande, M. and Oviedo, M. (2012), "Statistical computing in functional data analysis: the R package fda.usc". Journal of Statistical Software 51 (4), 1-28.

Naya, S., Tarrio-Saavedra. J., Lopez-Beceiro, J., Francisco Fernandez, M., Flores, M. and Artiaga, R. (2014), "Statistical functional approach for interlaboratory studies with thermal data". Journal of Thermal Analysis and Calorimetry, 118,1229-1243.

Examples

```
## Not run:
library(ILS)
data(TG)
delta <- seq(from = 40 ,to = 850 ,length.out = 1000 )
fqcdata <- ils.fqcdata(TG, p = 7, argvals = delta)
mandel.tg <- mandel.fqcs(fqcdata.tg,nb = 200)
plot(mandel.tg,legend = F,col=c(rep(3,5),1,1))
## End(Not run)
# $H(t)$ y $K(t)$</pre>
```

TG

Thermogravimetry curves

Description

One hundred and five Calcium oxalate samples were tested by thermogravimetric (TG) analysis, obtaining 105 TG curves that shows the mass loss of oxalate depending on time when samples are heated at a constant temperature rate. Dataset is composed by fifteen TG curves of 1000 observations each of overall 7 different laboratories. Laboratory 1 uses a simultaneous thermal analyzer (STA) with an old calibration program, Laboratory 2 to Laboratory 4 use a SDT simultaneous analyzer, Laboratory 6 utilizes a SDT simultaneous analyzer with an old calibration, and Laboratory 7 uses a SDT simultaneous analyzer with a biased calibration (2 degrees Celsius shifted from the zinc melting point).

Format

A 15 x 1000 x 7 dimension array , where each matrix consists of the 15 TG curves obtained testing 15 different oxalate samples, and evaluated in 1000 different values of temperature. These 15 curves were obtained for each of the overall 7 laboratories that have performed the esperiments.

Vi Thermogravimetric.

References

Naya, S., Tarrio-Saavedra. J., Lopez-Beceiro, J., Francisco Fernandez, M., Flores, M. and Artiaga, R. (2014), "Statistical functional approach for interlaboratory studies with thermal data". Journal of Thermal Analysis and Calorimetry, 118,1229-1243.

Examples

library(ILS)
data(TG)
summary(TG)

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