Package 'ILS'

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Type Package

Title Interlaboratory Study

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Depends R (>= 3.1.0), multcomp, depthTools, fda.usc, MASS

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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R topics documented:

`bootstrap.quantile` *Compute functional (FDA) Mandel's h and k statistics*

Description

This function is used to compute functional (FDA)Mandel's h and k, statistics, required to perform Interlaboratory studies, and to detect non-consistent laboratories where data show a functional form (curve). In addition, bootstrap resampling methodology is used to estimate functional distributions. This allow to perform bootstrap confidence bands for FDA h and k statistics.

Usage

```
bootstrap.quantile(x, ...)

## Default S3 method:
bootstrap.quantile(x, argvals = NULL, rangeval = NULL,
  statistic = c("h", "k"), method = c("Walter", "Depth"), alpha = 0.05,
  quantile = 0.9, ball = FALSE, nb = 200, smo = 0, draw = TRUE,
  draw.control = NULL, x.co = NULL, y.co = NULL, legend = TRUE,
  col = NULL, ...)

## S3 method for class 'lab.fqcd'
```

```
bootstrap.quantile(x, statistic = c("h", "k"),
  method = c("Walter", "Depth"), alpha = 0.05, quantile = 0.9,
  ball = FALSE, nb = 200, smo = 0, draw = TRUE, draw.control = NULL,
  x.co = NULL, y.co = NULL, legend = TRUE, col = NULL, ...)

## S3 method for class 'bootstrap.quantile'
print(x, ...)

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

Arguments

x	A bootstrap.quantile object for which a print is desired.
...	Arguments passed to or from methods.
argvals	Argvals, by default: 1:p.
rangeval	Range of discretization points, by default: range(argvals).
statistic	Sample statistic used for the interlaboratory analysis. By default, it uses sample h.
method	Quantile method used to estimate the critical quantile of the h and k statistics.
alpha	Significance level.
quantile	Probability with value in [0,1]
ball	Logical argument. If draw = TRUE and ball = TRUE, i bootstrap curves and quantiles functions are plotted. They correspond to (1-alpha/2)*100 [%] most central bootstrap resampling curves of q quantile. If draw = TRUE and ball = FALSE, the functional quantile q [%] is determined.
nb	Number of bootstrap resamples.
smo	Smoothing parameter for the bootstrap resamples, defined as a proportion of the sample variance matrix.
draw	Default TRUE, it plots the bootstrap samples and the h or k statistic. It depends on the ball parameter.
draw.control	List that specifies the col, lty and lwd plot arguments for the objects lab.fqcs, statistic, IN and OUT.
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
object	A bootstrap.quantile object 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.

Lopez-Pintado, S. and Romo, J. (2009), "On the concept of depth for functional data", Journal of the American Statistical Association, 104, 486-503.

Walter, S. (2011), Defining Quantiles for Functional Data: with an Application to the Reversal of Stock Price Decreases, Department of Math. and Stat. The Uni. of Melbourne.

Examples

```
## Not run:
library(ILS)
data(TG)
delta <- seq(from = 40 ,to = 850 ,length.out = 1000 )
curves.fqcd <- lab.fqcd(TG, argvals = delta,rangeval = c(40,80))
draw.control = list(col = c("blue","grey"),
                    lty = c(1, 1), lwd = c(2, 1))
#by Walter method
windows(20,10)
par(mfrow=c(1,2))
quantile95.w <- bootstrap.quantile(curves.fqcd, statistic = "h",
                                   method = "Walter", smo = 0,
                                   nb= 500, alpha = 0.05, quantile = 0.95,draw = TRUE,
                                  draw.control = draw.control,ylim=c(-3,3),x.co=50,y.co=3,
                                   main="Statistical h by the method's Walter")

## End(Not run)
```

`Cochram.test` *Function to compute the Grubbs test statistic.*

Description

Function to estimate the Cochram test statistic.

Usage

```
Cochram.test(x, ...)

## Default S3 method:
Cochram.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.qcd'
Cochram.test(x, alpha = 0.05, ...)
```

Arguments

x	R object (used to select the method). See details.
...	Arguments passed to or from methods.
var.index	Scalar with the column number corresponding to the observed variable (the critical to quality variable). Alternatively, a string with the name of a quality variable can be provided.
replicate.index	Scalar with the column number corresponding to the index each replicate.
material.index	Scalar corresponding to the replicated number.
laboratory.index	Scalar that defines the index number of each laboratory.
data.name	String specifying the name of the variable which appears on the plots. If name is not provided, it is retrieved from the object.
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 cochram 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.qcd <- lab.qcd(Glucose)
str(Glucose.qcd)
Cochram.test(Glucose.qcd)
```

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

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
```

Grubbs.test *Function to compute the Grubbs test statistic.*

Description

Function to estimate the Grubbs test statistic.

Usage

```
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.qcd'
Grubbs.test(x, alpha = 0.05, ...)
```

Arguments

x	an R object (used to select the method). See details.
...	arguments passed to or from methods.
var.index	Scalar with the column number corresponding to the observed variable (the critical to quality variable). Alternatively, a string with the name of a quality variable can be provided.
replicate.index	Scalar with the column number corresponding to the index each replicate.
material.index	Scalar corresponding to the replicated number.
laboratory.index	Scalar that defines the index number of each laboratory.
data.name	String specifying the name of the variable which appears on the plots. If name is not provided, it is retrieved from the object.
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 Cochram 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.qcd <- lab.qcd(Glucose)
str(Glucose.qcd)
Grubbs.test(Glucose.qcd)
```

---

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

Description

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

Usage

```
h.fqcs(x, ...)

## Default S3 method:
h.fqcs(x, argvals = NULL, rangeval = NULL, ...)

## S3 method for class 'lab.fqcd'
h.fqcs(x, ...)
```

Arguments

x	A (m x p) matrix or data-frame. Alternatively an (m x p x n) array. The m parameter is the number of curves, p defines the number of points observed in each curve, and n is the number of replicates.
...	Arguments passed to or from methods.
argvals	Argvals, by default: 1:p.
rangeval	Range of discretization points, by default: range(argvals).

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 )
curves.fqcd <- lab.fqcd(TG, argvals = delta)
fh <- h.fqcs(curves.fqcd)
xlab <- "Temperature(Grade Celsius)"
ylab <- "Mass (%)"
main <- "Functional hi  Estimation"
p <- fh$p
plot(fh,main = main, xlab = xlab, ylab = ylab,col=1:p,ylim=c(-3,3))
legend(10,3,paste("Lab",1:p),
      col=1:p,lty=1,lwd=2,cex=0.7)
```

h.qcs *Function to estimate the univariate Mandel's h statistic*

Description

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

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.qcd'
h.qcs(x, alpha = 0.05, ...)
```

Arguments

x	R object (used to select the method). See details.
...	Arguments passed to or from methods.
var.index	Scalar with the column number corresponding to the observed variable (the critical to quality variable). Alternatively, a string with the name of a quality variable can be provided.
replicate.index	Scalar with the column number corresponding to the index each replicate.
material.index	Scalar corresponding to the replicated number.
laboratory.index	Scalar that defines the index number of each laboratory.
data.name	String specifying the name of the variable which appears on the plots. If name is not provided, it is retrieved from the object.
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 Cochram 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.qcd <- lab.qcd(Glucose)
str(Glucose.qcd)
h<- h.qcs(Glucose.qcd, alpha = 0.005)
summary(h)
plot(h)
```

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, 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

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.

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(IDT)
summary(IDT)
attach(IDT)
str(IDT)
table(Sample,Run,Laboratory)
table(Laboratory,Run)
st <- with(IDT, tapply(IDT, list(Run,Laboratory), mean))
st
```

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.

k.fqcs *This function is used to compute the FDA Mandel's k statistic*

Description

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

Usage

```
k.fqcs(x, ...)

## Default S3 method:
k.fqcs(x, argvals = NULL, rangeval = NULL, ...)

## S3 method for class 'lab.fqcd'
k.fqcs(x, ...)
```

Arguments

x	A (m x p) matrix or data-frame. Alternatively an (m x p x n) array. The m parameter is the number of curves, p defines the number of points observed in each curve, and n is the number of replicates.
...	Arguments passed to or from methods.
argvals	Argvals, by default: 1:p.
rangeval	Range of discretization points, by default: range(argvals).

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 )
curves.fqcd <- lab.fqcd(TG, argvals = delta)
fk <- k.fqcs(curves.fqcd)
p <- fk$p
xlab <- "Temperature (Grade Celsius)"
ylab <- "Mass (%)"
main <- "Functional ki  Estimation"
plot(fk,main = main, xlab = xlab, ylab = ylab, ylim=c(0,3),col=1:p)
legend(10,3,paste("Lab",1:p),
      col=1:p,lty=1,lwd=2,cex=0.7)
```

---

k.qcs *Function to calcute the Mandel's k statistic*

Description

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

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.qcd'
k.qcs(x, alpha = 0.05, ...)
```

Arguments

x	an R object (used to select the method). See details.
...	arguments passed to or from methods.
var.index	Scalar with the column number corresponding to the observed variable (the critical to quality variable). Alternatively, a string with the name of a quality variable can be provided.
replicate.index	Scalar with the column number corresponding to the index each replicate.
material.index	Scalar corresponding to the replicated number.
laboratory.index	Scalar that defines the index number of each laboratory.
data.name	String specifying the name of the variable which appears on the plots. If name is not provided, it is retrieved from the object.
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 Cochram 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.qcd <- lab.qcd(Glucose)
str(Glucose.qcd)
k<- k.qcs(Glucose.qcd, alpha = 0.005)
summary(k)
plot(k)
```

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.qcd'
lab.aov(x, level = 0.95, plot = FALSE, pages = 0, ...)
```

Arguments

x	Object lab.qcd.
...	Arguments passed to or from methods.
var.index	Scalar with the column number corresponding to the observed variable (the critical to quality variable). Alternatively, a string with the name of a quality variable can be provided.
replicate.index	Scalar with the column number corresponding to the index each replicate.
material.index	Scalar corresponding to the replicated number.
laboratory.index	Scalar that defines the index number of each laboratory.
data.name	String specifying the name of the variable which appears on the plots. If name is not provided, it is retrieved from the object.
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.qcd <- lab.qcd(Glucose)
str(Glucose.qcd)
lab.aov(Glucose.qcd,level = 0.95, plot = TRUE, pages = 1)

## End(Not run)
```

---

lab.fqcd *Functional Quality Control Data*

Description

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

Usage

```
lab.fqcd(x, argvals = NULL, rangeval = NULL)
```

Arguments

x	A (m x p) matrix or data-frame. Alternatively an (m x p x n) array. The m parameter is the number of curves, p defines the number of points observed in each curve, and n is the number of replicates.
argvals	Argvals, by default: 1:p.
rangeval	Range of discretization points, by default: range(argvals).

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 )
curves.fqcd <- lab.fqcd(TG, argvals = delta)
windows()
xlab <- "Temperature (0C)"
ylab <- "Mass (%)"
main <- "TG curves obtained from calcium oxalate"
p <- curves.fqcd$p
col <- terrain.colors(p)
plot(x = curves.fqcd, main, xlab, ylab,legend = FALSE,col = col)
legend(45,70,c(paste("Lab",c(1:7))),
      col = col,lty = 1, lwd = c(rep(1,7),2), cex = 0.7)

## End(Not run)
```

`lab.fqcs` *It developes an object of class 'lab.fqcs'*

Description

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

Usage

```
lab.fqcs(x, ...)

## Default S3 method:
lab.fqcs(x, argvals = NULL, rangeval = NULL, ...)

## S3 method for class 'lab.fqcd'
lab.fqcs(x, ...)

## S3 method for class 'lab.fqcs'
print(x, ...)

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

Arguments

`x`	A `lab.fqcs` object for which a print is desired.
`...`	Arguments passed to or from methods.
`argvals`	Argvals, by default: 1:p.

rangeval	Range of discretization points, by default: range(argvals).
object	A lab.fqcs object 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

```
## Not run:
library(ILS)
data(TG)
delta <- seq(from = 40 ,to = 850 ,length.out = 1000 )
curves.fqcd <- lab.fqcd(TG, argvals = delta)
p <- curves.fqcd$p
curves.fqcs <- lab.fqcs(curves.fqcd)
summary(curves.fqcs)
names(curves.fqcs)

##### Statistical Functional
windows(20,10)
xlab <- "Temperature (C)"
ylab <- "Mass (%)"
main <- "Statistical Functional"
col <- 1:p

## End(Not run)
```

---

lab.qcd *Quality Control Data*

Description

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

Usage

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

Arguments

data	Matrix or data-frame that contains the data, replicate index, type of material, and the laboratory.
var.index	Scalar with the column number corresponding to the observed variable (the critical to quality variable). Alternatively, a string with the name of a quality variable can be provided.
replicate.index	Scalar with the column number corresponding to the index each replicate.
material.index	Scalar corresponding to the replicated number.
laboratory.index	Scalar that defines the index number of each laboratory.
data.name	String specifying the name of the variable which appears on the plots. If name is not provided, it is retrieved from the object.

Examples

```
library(ILS)
data(Glucose)
Glucose.qcd <- lab.qcd(Glucose)
str(Glucose.qcd)
summary(Glucose.qcd)
```

---

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	Object lab.qcd (Functional Quality Control Data)
...	Arguments passed to or from methods.
object	A lab.qcs object for which a summary is desired.

Examples

```
library(ILS)
data(Glucose)
Glucose.qcd <- lab.qcd(Glucose)
str(Glucose.qcd)
Glucose.qcs <- lab.qcd(Glucose.qcd)
str(Glucose.qcs)
summary(Glucose.qcs)
```

`plot.lab.fqcd` *Plotting method for 'lab.fqcd' objects*

Description

Generic function to plot objects of 'lab.fqcd' class

Usage

```
## S3 method for class 'lab.fqcd'
plot(x, main = NULL, xlab = NULL, ylab = NULL,
  ylim = NULL, x.co = NULL, y.co = NULL, legend = TRUE, col = NULL,
  ...)
```

Arguments

`x`	Object lab.fqcd (Functional Quality Control Data)
`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 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
`...`	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

```
library(ILS)
data(TG)
delta <- seq(from = 40 ,to = 850 ,length.out = 1000 )
curves.fqcd <- lab.fqcd(TG, argvals = delta)
xlab <- "Temperature/ C"
ylab <- "Mass/ %"
main <- "TG curves obtained from calcium oxalate"
p <- dim(curves.fqcd$curves)[3]
col <- 1:p
plot(x = curves.fqcd, main, xlab, ylab, col= col,legend = FALSE)
legend(45,70,paste("Lab",col),
      col = col, lty = 1, lwd = 2, cex =0.8)
```

---

plot.lab.fqcs *Plotting method for 'lab.fqcs' objects*

Description

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

Usage

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

Arguments

x	Object functional data or a list with objects of functional data type
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 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
...	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

```
library(ILS)
data(TG)
delta <- seq(from = 40 ,to = 850 ,length.out = 1000 )
curves.fqcd <- lab.fqcd(TG, argvals = delta)
curves.fqcs <- lab.fqcs(curves.fqcd)
summary(curves.fqcs)
names(curves.fqcs)
class(curves.fqcs$mean.i)
xlab <- "Temperature/ C"
ylab <- "Mass/ %"
main <- "Functional Mean Estimation by Laboratory"
p <- dim(curves.fqcd$curves)[3]
col <- 1:p
plot(curves.fqcs$mean.i,main = main, xlab = xlab, ylab = ylab, col = col,legend = FALSE)
legend(45,70,paste("Lab",1:p),
      col = col,lty = 1,lwd = 2,cex = 0.7)
```

`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.

Usage

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

Arguments

`x`	Functional data object or a list with functional objects
`title`	Main title for the plot
`xlab`	Title for the x axis
`ylab`	Title for the y axis
`col`	Color specifications

ylim	Numeric vectors of length 2 (coordinates ranges)
...	arguments to be passed to or from methods.

`QuantileDepth` *Creates a 'lab.fqcs' object to estimate functional quantiles using data depth procedures.*

Description

It defines a `lab.fqcs` object to estimate functional quantiles using data depth procedures (Lopez-Pintado and Romo, 2009). The required functional quantiles are obtained from data depths values of each curve. If quantile argument is 0.9, 0.95 and 0.05 functional quantiles are obtained.

Usage

```
QuantileDepth(x, quantile = 0.95)
```

Arguments

x	Object of type fdata
quantile	Probability defined in the interval [0,1]

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.

Lopez-Pintado, S. and Romo, J. (2009), "On the concept of depth for functional data", Journal of the American Statistical Association, 104, 486-503.

Examples

```
## Not run:
library(ILS)
data(TG)
delta <- seq(from = 40 ,to = 850 ,length.out = 1000 )
curves.fqcd <- lab.fqcd(TG, argvals = delta)
n <- curves.fqcd$n
m <- curves.fqcd$m
p <- curves.fqcd$p
curves.all <- TG[,,1]
for(i in 2:p) curves.all <- rbind(curves.all,TG[,,i])
curves.fdata <- fdata(mdata = curves.all,delta)
qd <- QuantileDepth(curves.fdata)
windows(20,10)
par(mfrow=c(1,2))
plot(qd, main="Quantiles of TG curves (95%)",col=c("red","blue"),lwd=2,legend = FALSE)
legend(50,80,c("Quantile 2.5%","Quantile 97.5%"),
      col=c("red","blue"),lty=c(1,1),lwd=1,cex=0.7)
```

```
plot(curves.fdata,main="Quantiles of TG curves (95%)",col="gray")
for(i in 1:2)
lines(qd[[i]],col="red",lty = 2,lwd = 2)
legend(50,80,c("Quantiles","TG Curves (105)"),
      col=c("red","gray"),lty=c(1,2),lwd=2,cex=0.7)
par(mfrow=c(1,1))

## End(Not run)
```

QuantileWalter *It provides quantile estimates from FDA point of view.*

Description

It develops a 'lab.fqcs' object to estimate functional quatiles by Walter's method (2011) from a pointwise point of view.

Usage

```
QuantileWalter(x, quantile = 0.95, central = TRUE)
```

Arguments

x	Object of type fdata
quantile	Probability defined in the interval [0,1]
central	Logical argument. If FALSE, functional quantile q is computed. If TRUE, two functional quantiles are obtained, those corresponding to curves (1-q / 2) and q / 2 .

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.

Walter, S. (2011), Defining Quantiles for Functional Data: with an Application to the Reversal of Stock Price Decreases, Department of Math. and Stat. The Uni. of Melbourne.

Examples

```
## Not run:
library(ILS)
data(TG)
delta <- seq(from = 40 ,to = 850 ,length.out = 1000 )
curves.fqcd <- lab.fqcd(TG, argvals = delta)
n <- curves.fqcd$n
m <- curves.fqcd$m
p <- curves.fqcd$p
curves.all <- TG[,,1]
for(i in 2:p) curves.all <- rbind(curves.all,TG[,,i])
```

```
curves.fdata <- fdata(mdata = curves.all,delta)
qw <- QuantileWalter(curves.fdata)
windows(20,10)
par(mfrow=c(1,2))
plot(qw, main="Quantiles of TG curves (95%)",col=c("red","blue"),lwd=2,legend = FALSE)
legend(50,80,c("Quantile 2.5%","Quantile 97.5%"),
      col=c("red","blue"),lty=c(1,1),lwd=1,cex=0.7)
plot(curves.fdata,main="Quantiles of TG curves (95%)",col="gray")
for(i in 1:2)
lines(qw[[i]],col="red",lty = 2,lwd = 2)
legend(50,80,c("Quantiles","TG Curves (105)"),
      col=c("red","gray"),lty=c(1,2),lwd=2,cex=0.7)
par(mfrow=c(1,1))

## End(Not run)
```

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.

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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