

Package ‘TFunHDDC’

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Type Package

Title Clustering of Functional Data via Mixtures of t-Distributions

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Description Extension of 'funHDDC' Schmutz et al. (2018) [doi:10.1007/s00180-020-00958-4](https://doi.org/10.1007/s00180-020-00958-4) for cases including outliers by fitting t-distributions for robust groups. 'TFunHDDC' can cluster univariate or multivariate data produced by the 'fda' package for data using a b-splines or Fourier basis.

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contaminatedTriangles *contaminatedTriangles*

Description

Simulated triangle data produced as an example of mild contaminated data with behavioural outliers.

Value

fd	A functional data object representing the fitted triangle data.
groupd	Group classifications for each curve as a ordinary behavioral group (1,2,3, or 4) or outlier (4 as outliers to group 1 and 6 as outliers for group 3).

Author(s)

Cristina Anton and Iain Smith

References

- Cristina Anton, Iain Smith Model-based clustering of functional data via mixtures of t distributions. Advances in Data Analysis and Classification (to appear).

fitNOxBenchmark *fitNOxBenchmark*

Description

Extract NOx data from fda.usc

Usage

```
fitNOxBenchmark(nbasis=15)
```

Arguments

nbasis The number of basis functions to fit to the simulated data.

Details

Open NOx data from the poblenou data set of [fda.usc](http://fda.usc.edu). Fit the data to a given number of basis functions and adjust classes for festive days into just weekdays and weekends.

Value

fd A functional data object representing the fitted NOx data.
 groupd Group classifications for each curve as a curve representing a weekday or week-end/festive day.

Author(s)

Cristina Anton and Iain Smith

References

- Febrero-Bande M, Galeano P, Gonzalez-Manteiga W (2008) Outlier detection in functional data by depth measures, with application to identify abnormal nox levels. *Environmetrics* 19:331-345. doi.org/10.1002/env.878.
- Cristina Anton, Iain Smith Model-based clustering of functional data via mixtures of t distributions. *Advances in Data Analysis and Classification* (to appear).

See Also

[plotNOx](#)

Examples

```
# Univariate Contaminated Data
data1<-fitNOxBenchmark(15)
plotNOx(data1)
```

genModelFD

genModelFD

Description

Generate functional data with coefficients distributed according to a finite mixture of contaminated normal distributions such that for the k th cluster we have the multivariate contaminated normal distribution with density

$$f(\gamma_i; \theta_k) = \alpha_k \phi(\gamma_i; \mu_k, \Sigma_k) + (1 - \alpha_k) \phi(\gamma_i; \mu_k, \eta_k \Sigma_k)$$

where $\alpha_k \in (0.5, 1)$ represents the proportion of uncontaminated data, $\eta_k > 1$ is the inflation coefficient due to outliers, and $\phi(\gamma_i; \mu_k, \Sigma_k)$ is the density for the multivariate normal distribution $N(\mu_k, \Sigma_k)$.

Usage

```
genModelFD(ncurves=1000, nsplines=35, alpha=c(0.9,0.9,0.9),
            eta=c(10, 5, 15))
```

Arguments

ncurves	The number of curves total for the simulation.
nsplines	The number of splines to fit to the simulated data.
alpha	The proportion of uncontaminated data in each group.
eta	The inflation coefficient that measures the increase in variability due to the outliers.

Details

The data are generate from the model $FCLM[a_k, b_k, \mathbf{Q}_k, d_k, \alpha_k, \eta_k]$. The number of clusters is fixed to $K = 3$ and the mixing proportions are equal $\pi_1 = \pi_2 = \pi_3 = 1/3$. We consider the following values of the parameters

Group 1: $d = 5, a = 150, b = 5, \mu = (1, 0, 50, 100, 0, \dots, 0)$

Group 2: $d = 20, a = 15, b = 8, \mu = (0, 0, 80, 0, 40, 2, 0, \dots, 0)$

Group 3: $d = 10, a = 30, b = 10, \mu = (0, \dots, 0, 20, 0, 80, 0, 0, 100),$

where d is the intrinsic dimension of the subgroups, μ is the mean vector of size 70, a is the values of the d -first diagonal elements of \mathbf{D} , and b the value of the last $70 - d$ - elements. Curves as smoothed using 35 Fourier basis functions.

Value

fd	A functional data object representing the simulated data.
groupd	Group classifications for each curve.

Author(s)

Cristina Anton and Iain Smith

References

- Amovin-Assagba M, Gannaz I, Jacques J (2022) Outlier detection in multivariate functional data through a contaminated mixture model. *Comput Stat Data Anal* 174. - Cristina Anton, Iain Smith Model-based clustering of functional data via mixtures of t distributions. *Advances in Data Analysis and Classification* (to appear).

Examples

```
# Univariate Contaminated Data
data <- genModelFD(ncurves=300, nsplines=35, alpha=c(0.9,0.9,0.9),
                  eta=c(10, 7, 17))
plot(data$fd, col = data$groupd)
c1m <- data$groupd
```

genTriangles	<i>genTriangles</i>
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Description

Generate contaminated triangle data. Groups 1, 2, 3, and 4 are separable over the two dimensions of functional data. Groups 5 and 6 contain the contaminated curves of groups 1 and 3 respectively.

Usage

```
genTriangles()
```

Details

Group 1:

$$X_1(t) = U + (0.6 - U)H_1(t) + \epsilon_1(t)$$

$$X_2(t) = U + (0.5 - U)H_1(t) + \epsilon_1(t)$$

$$\text{Contaminated } X_1(t) = \sin(t) + (0.6 - U)H_1(t) + \epsilon_2(t)$$

$$\text{Contaminated } X_2(t) = \sin(t) + (0.5 - U)H_1(t) + \epsilon_2(t)$$

Group 2:

$$X_1(t) = U + (0.6 - U)H_2(t) + \epsilon_1(t)$$

$$X_2(t) = U + (0.5 - U)H_2(t) + \epsilon_1(t)$$

Group 3:

$$X_1(t) = U + (0.5 - U)H_1(t) + \epsilon_1(t)$$

$$X_2(t) = U + (0.6 - U)H_2(t) + \epsilon_1(t)$$

$$\text{Contaminated } X_1(t) = \sin(t) + (0.5 - U)H_1(t) + \epsilon_3(t)$$

$$\text{Contaminated } X_2(t) = \sin(t) + (0.6 - U)H_2(t) + \epsilon_3(t)$$

Group 4:

$$X_1(t) = U + (0.5 - U)H_2(t) + \epsilon_1(t)$$

$X_2(t) = U + (0.6 - U)H_1(t) + \epsilon_1(t)$. Here $t \in [1, 21]$, $H_1(t) = (6 - |t - 7|)_+$, and $H_2(t) = (6 - |t - 15|)_+$, with $(\cdot)_+$ representing the positive part. $U \sim \mathcal{U}(0, 0.1)$, and $\epsilon_1(t) \sim N(0, 0.5)$, $\epsilon_2(t) \sim N(0, 2)$, $\epsilon_3(t) \sim \text{Cauchy}(0, 4)$ are mutually independent white noises and independent of U . We simulate 100 curves for each group, groups 1 and 3 consisting of 80 ordinary curves and 20 contaminated curves. Curves are smoothed using a 25 cubic B-spline basis.

Value

fd	List of functional data objects representing the two dimensions of triangle data.
groupd	Group classification for each curve

Author(s)

Cristina Anton and Iain Smith

References

- C.Bouveyron and J.Jacques (2011), Model-based Clustering of Time Series in Group-specific Functional Subspaces, *Advances in Data Analysis and Classification*, vol. 5 (4), pp. 281-300, <doi:10.1007/s11634-011-0095-6>
- Schmutz A, Jacques J, Bouveyron C, et al (2020) Clustering multivariate functional data in group-specific functional subspaces. *Comput Stat* 35:1101-1131
- Cristina Anton, Iain Smith Model-based clustering of functional data via mixtures of t distributions. *Advances in Data Analysis and Classification* (to appear).

See Also

[plotTriangles](#)

Examples

```
# Multivariate Contaminated Triangles
conTrig <- genTriangles()
cls = conTrig$groupd
plotTriangles(conTrig)
```

plotNOx

plotNOx

Description

Plot data returned by [fitNOxBenchmark](#) as lines coloured according to the assigned clusters.

Usage

```
plotNOx(fdn)
```

Arguments

`fdn` List with an element *fd* given the functional data, and an element *groupd* given the classes; usually returned from the function [fitNOxBenchmark](#).

Value

No return value, used for side effects.

Author(s)

Cristina Anton and Iain Smith

See Also

[fitNOxBenchmark](#)

Examples

```
# Univariate Contaminated Data
data1<-fitNOxBenchmark(15)
plotNOx(data1)
```

`plotTriangles` *plotTriangles*

Description

Plot data returned by [genTriangles](#) as lines coloured according to the assigned clusters.

Usage

```
plotTriangles(fdt)
```

Arguments

`fdt` List with an element *fd* given the functional data, and an element *groupd* given the classes, as returned from the function [genTriangles](#).

Value

No return value, used for side effects.

Author(s)

Cristina Anton and Iain Smith

See Also

[genTriangles](#)

Examples

```
conTrig <- genTriangles()
plotTriangles(conTrig)
```

predict.tfunHDDC *predict.tfunHDDC: Predicting Function for t-funHDDC Objects*

Description

Provides the matrix of classification probabilities and the classification vector for inputted observations assuming the model provided by the `tfunHDDC` object.

Usage

```
## S3 method for class 'tfunHDDC'
predict(object, data=NULL, ...)
```

Arguments

<code>object</code>	An object of class <code>tfunHDDC</code>
<code>data</code>	Data frame (univariate functional data) or a list (multivariate functional data) of new observations on the same variables used in the fitting of the <code>tfunHDDC</code> object. If <code>NULL</code> , then the observations used in the fitting of the <code>tfunHDDC</code> object are inputted.
<code>...</code>	Arguments to be passed to other functions.

Value

<code>t</code>	Matrix of classification probabilities
<code>class</code>	Vector of maximum a posteriori classifications

Author(s)

Cristina Anton, Iain Smith

References

-Andrews JL, McNicholas PD (2012) Model-based clustering, classification, and discriminant analysis via mixtures of multivariate t-distributions: The teigen family. *Stat Comput* 22:1021-1029. <doi.org/10.1007/s11222-011-9272-x>

-Andrews JL, Wickins JR, Boers NM, et al (2018) An R package for modelbased clustering and classification via the multivariate t distribution. *Journal of Statistical Software* 83(7):1-32

- Cristina Anton, Iain Smith (2024) Model-based clustering of functional data via mixtures of *t* distributions. *Advances in Data Analysis and Classification* 18(3): 563-595.

See Also

`tfunHDDC`

Examples

```

set.seed(1027)
#simulataed univariate data

data = genModelFD(ncurves=300, nsplines=35, alpha=c(0.9,0.9,0.9),
                  eta=c(10, 7, 17))

plot(data$fd, col = data$groupd)

clm = data$groupd

model1=c("AkjBkQkDk", "AkjBQkDk", "AkBkQkDk", "ABkQkDk", "AkBQkDk", "ABQkDk")

#####classification example with predictions

training=c(1:50,101:150, 201:250)

test=c(51:100,151:200, 251:300)

known1=clm[training]

t4<-tfunHDDC(data$fd[training],K=3,threshold=0.2,init="kmeans",nb.rep=1,
             dfconstr="no", dfupdate="numeric", model=model1[1],known=known1,
             itermax = 10)

if (!is.null(t4$class)) {
  table(clm[training], t4$class)

p1<-predict.tfunHDDC(t4,data$fd[test] )

if (!is.null(p1$class)) table(clm[test], p1$class)
}

#####NOX data

data1=fitNOxBenchmark(15)

plotNOx(data1)

###example for prediction

training=c(1:50)

test=c(51:115)

known1=data1$groupd[training]

t1<-tfunHDDC(data1$fd[training],K=2,threshold=0.6,init="kmeans",nb.rep=10,
             dfconstr="no", model=c("AkjBkQkDk", "AkjBQkDk", "AkBkQkDk",
             "ABkQkDk", "AkBQkDk", "ABQkDk"),known=known1)

if (!is.null(t1$class)) {

```

```

table(data1$groupd[training], t1$class)

p1<-predict.tfunHDDC(t1,data1$fd[test] )

if (!is.null(p1$class)) table(data1$groupd[test], p1$class)
}

```

tfunHDDC

tfunHDDC: Function for Model-Based Clustering of Functional Data with Outliers Using the t-Distribution.

Description

tfunHDDC is an adaptation of funHDDC (Schmutz et al., 2018) that uses t-distributions for robust clustering in the presence of outliers.

Usage

```

tfunHDDC(data, K=1:10, model="AkjBkQkDk", known=NULL, dfstart=50, dfupdate="approx",
  dfconstr="no", threshold=0.1, itermax=200, eps=1e-6, init='random',
  criterion="bic", d_select="Cattell", init.vector=NULL,
  show=TRUE, mini.nb=c(5, 10), min.individuals=2, mc.cores=1, nb.rep=2,
  keepAllRes=TRUE, kmeans.control = list(), d_max=100, d_range=2,
  verbose = TRUE)

```

Arguments

data	In the univariate case: a functional data object produced by the fda package. In the multivariate case: a list of functional data objects.
K	The number of clusters or list of clusters to try, for example K=2:10.
dfstart	The df (degrees of freedom) to which we initialize the t-distribution.
dfupdate	Either "numeric", or "approx". The default is "approx" indicating a closed form approximation be used. Alternatively, "numeric" can be specified which makes use of uniroot .
dfconstr	"yes" when df (degrees of freedom) for the t-distribution should be the same between all clusters; "no" when df may be different between clusters.
model	The chosen model among 'AkjBkQkDk', 'AkjBQkDk', 'AkBkQkDk', 'ABkQkDk', 'AkBQkDk', 'ABQkDk'. 'AkjBkQkDk' is the default. We can test multiple models at the same time with the command c(). For example c("AkjBkQkDk","AkjBQkDk").
threshold	The threshold of the Cattell' scree-test used for selecting the group-specific intrinsic dimensions.
known	A vector of known classifications that can be numeric or NA. It is optional for clustering. For classification, curves with unknown classification should be given the value NA within known (see the examples below). Must be the same length as the number of curves in the data set.

<code>itermax</code>	The maximum number of iterations.
<code>eps</code>	The threshold of the convergence criterion.
<code>init</code>	A character string. It is the way to initialize the EM algorithm. There are five ways of initialization: “kmeans” (default), “param”, “random”, “mini-em”, “vector”, or “tkmeans”. See details for more information. It can also be directly initialized with a vector containing the prior classes of the observations.
<code>criterion</code>	The criterion used for model selection: bic (default) or icl.
<code>d_select</code>	“Cattell” (default), “BIC”, or “grid”. This parameter selects which method to use to select the intrinsic dimensions of subgroups. “grid” will select <code>d</code> based on the <code>criterion</code> value after running each combination of <code>d1</code> , <code>d2</code> , ..., <code>dK</code> for the groups. <code>d</code> used for each group is based on the values for <code>d_range</code> . “grid” will only work for a single value of <code>K</code> (not a list). See details for more information.
<code>init.vector</code>	A vector of integers or factors. It is a user-given initialization. It should be of the same length as of the data. Only used when <code>init="vector"</code> .
<code>show</code>	Use <code>show = FALSE</code> to settle off the informations that may be printed.
<code>mini.nb</code>	A vector of integers of length two. This parameter is used in the “mini-em” initialization. The first integer sets how many times the algorithm is repeated; the second sets the maximum number of iterations the algorithm will do each time. For example, if <code>init="mini-em"</code> and <code>mini.nb=c(5,10)</code> , the algorithm will be launched 5 times, doing each time 10 iterations; finally the algorithm will begin with the initialization that maximizes the log-likelihood.
<code>min.individuals</code>	This parameter is used to control for the minimum population of a class. If the population of a class becomes strictly inferior to ‘min.individuals’ then the algorithm stops and gives the message: ‘pop<min.indiv.’. Here the meaning of “population of a class” is the sum of its posterior probabilities. The value of ‘min.individuals’ cannot be lower than 2.
<code>mc.cores</code>	Positive integer, default is 1. If <code>mc.cores>1</code> , then parallel computing is used, using <code>mc.cores</code> cores. Warning for Windows users only: the parallel computing can sometimes be slower than using one single core (due to how <code>parLapply</code> works).
<code>nb.rep</code>	A positive integer (default is 1 for kmeans initialization and 20 for random initialization). Each estimation (i.e. combination of (model, <code>K</code> , threshold)) is repeated <code>nb.rep</code> times and only the estimation with the highest log-likelihood is kept.
<code>keepAllRes</code>	Logical. Should the results of all runs be kept? If so, an argument <code>all_results</code> is created in the results. Default is TRUE.
<code>kmeans.control</code>	A list. The elements of this list should match the parameters of the <code>kmeans</code> initialization (see <code>kmeans</code> help for details). The parameters are “iter.max”, “nstart” and “algorithm”. “alpha” is an added parameter for the <code>tkmeans</code> initialization (see <code>tkmeans</code> help for details)
<code>d_max</code>	A positive integer. The maximum number of dimensions to be computed. Default is 100. It means that the intrinsic dimension of any cluster cannot be larger than <code>d_max</code> . It quickens a lot the algorithm for datasets with a large number of variables (e.g. thousands).

d_range	Vector of values to use for the intrinsic dimension for each group when d_select="grid".
verbose	Whether to print progress and approximate timing information as tfunHDDC executes. TRUE (default when running in serial) or FALSE (default when running parallel).

Details

If we choose init="random", the algorithm is run 20 times with the same model options and the solution which maximises the log-likelihood is printed. This explains why sometimes with this initialization it runs a bit slower than with 'kmeans' initialization.

If the warning message: "In tfunHDDC(...) : All models diverged" is printed, it means that the algorithm found less classes than the chosen number (parameter K). Because the EM algorithm is used, it could be because of a bad initialization of the EM algorithm. So we have to restart the algorithm multiple times in order to check if with a new initialization of the EM algorithm the model converges, or if there is no solution with the chosen number K.

The different initializations are:

"mini-em": it is an initialization strategy for which the classes are randomly initialized and the EM algorithm is run for several iterations. This action is repeated a few times (the default is 5 iterations and 10 times). At the end, the initialization chosen is the one which maximises the log-likelihood (see mini.nb for more information about its parameters).

"random": the classes are randomly given using a multinomial distribution

"kmeans": the classes are initialized using the kmeans function (with algorithm="Hartigan-Wong"; nstart=4; iter.max=50); note that the user can use his own arguments for kmeans using the dot-dot-dot argument

"tkmeans": the classes are initialized using the tkmeans function (with same default initialization as kmeans); note that the user can use his own arguments for tkmeans using the dot-dot-dot argument

A prior class "vector": It can also be directly initialized with a vector containing the prior classes of the observations. To do so use init="vector" and provide the vector in the argument init.vector.

Note that the BIC criterion used in this function is to be maximized and is defined as $2*LL-k*log(n)$ where LL is the log-likelihood, k is the number of parameters and n is the number of observations.

There are three methods for selecting the intrinsic dimension using d_select:

"Cattell": Runs a Cattell's scree test to approximate the intrinsic dimension that yields the greatest improvement in clustering.

"BIC": At each iteration we test each value for each group's intrinsic dimension and set the intrinsic dimension that yields the best BIC.

"grid": Runs every combination of hyperparameters (eg. K=2, threshold = 0.05, model = ...) for every combination of intrinsic dimensions that can be set with the given d_range (with K = 2 and d_range = c(2, 10) it would set (2,2), (2, 10), (10, 2), and (10, 10)). Due to the sharp increase in test cases it is recommended that this mode is run in parallel if possible. Doing an initial short run to approximate the timing with verbose = TRUE is suggested as well.

Value

d	The number of dimensions for each cluster.
a	Values of parameter a for each cluster.

b	Values of parameter b for each cluster.
mu	The mean of each cluster in the original space.
prop	The proportion of individuals in each cluster.
loglik	The maximum of log-likelihood.
loglik_all	The log-likelihood at each iteration.
posterior	The posterior probability for each individual to belong to each cluster.
class	The clustering partition.
BIC	The BIC value.
ICL	The ICL value.
complexity	the number of parameters that are estimated.
all_results	if multiple number of clusters or models are considered, results for each model are stored here
nux	Values for the degrees of freedom of the t-distributions for each group.

Author(s)

Cristina Anton, Iain Smith, and Malcolm Nielsen

References

- Andrews JL and McNicholas PD. “Model-based clustering, classification, and discriminant analysis with the multivariate t -distribution: The t EIGEN family” *Statistics and Computing* 22(5), 1021–1029.
- Andrews JL, McNicholas PD, and Subedi S (2011) “Model-based classification via mixtures of multivariate t -distributions” *Computational Statistics and Data Analysis* 55, 520–529.
- C.Bouveyron and J.Jacques, Model-based Clustering of Time Series in Group-specific Functional Subspaces, *Advances in Data Analysis and Classification*, vol. 5 (4), pp. 281-300, 2011 <doi:10.1007/s11634-011-0095-6>
- Schmutz A, Jacques J, Bouveyron C, et al (2020) Clustering multivariate functional data in group-specific functional subspaces. *Comput Stat* 35:1101-1131
- Cristina Anton, Iain Smith Model-based clustering of functional data via mixtures of t distributions. *Advances in Data Analysis and Classification* (to appear).

See Also

[teigen](#), [kmeans](#), [tkmeans](#), [predict.tfunHDDC](#)

Examples

```
set.seed(1027)
#simulataed univariate data

data = genModelFD(ncurves=300, nsplines=35, alpha=c(0.9,0.9,0.9),
                  eta=c(10, 7, 17))
```

```

plot(data$fd, col = data$groupd)

clm = data$groupd

model1=c("AkjBkQkDk", "AkjBQkDk", "AkBkQkDk", "ABkQkDk", "AkBQkDk", "ABQkDk")

t1<-tfunHDDC(data$fd,K=3,threshold=0.2,init="kmeans",nb.rep=1,dfconstr="no",
             dfupdate="numeric", model=model1[1], itermax=10)

if (!is.null(t1$class)) table(clm, t1$class)

#####example when some classifications are known

known1=rep(NA,1,300)

known1[1]=clm[1]

known1[103]=clm[103]

known1[250]=clm[250]

t2<-tfunHDDC(data$fd,K=3,threshold=0.2,init="kmeans",nb.rep=1,dfconstr="no",
             dfupdate="numeric", model=model1[1],known=known1, itermax=10)
if (!is.null(t2$class)) table(clm, t2$class)

##### example when some classifications are known

known1=rep(NA,1,300)

known1[1:100]=rep(3,1,50)

t3<-tfunHDDC(data$fd,K=3,threshold=0.2,init="kmeans",nb.rep=1,dfconstr="no",
             dfupdate="numeric", model=model1[1],known=known1, itermax=10)

if (!is.null(t3$class)) table(clm, t3$class)

#####multivariate simulated data
set.seed(1027)

conTrig <- genTriangles()

cls = conTrig$groupd # groups 5 and 6 (contaminated) into 1 and 3 respectively

res_s = tfunHDDC(conTrig$fd, K=4, dfconstr="no", dfupdate="numeric",
                model="ABKQKDK", init="kmeans", threshold=0.2, nb.rep=1,
                itermax=10)

if (!is.null(res_s$class)) table(cls, res_s$class)

```

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