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sasfunclust-package Sparse and smooth functional data clustering

Description

Implements the sparse and smooth functional clustering (SaS-Funclust) method (Centofanti et al. (2021) <arXiv:2103.15224>) that aims to classify a sample of curves into homogeneous groups while jointly detecting the most informative portions of domain.

Details

Package: sasfunclust Type: Package Version: 1.0.0.9000 Date: 2021-04-04 License: GPL-3

Author(s)

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References

Centofanti, F., Lepore, A., & Palumbo, B. (2021). Sparse and Smooth Functional Data Clustering. *arXiv* preprint arXiv:2103.15224.

See Also

```
sasfclust, sasfclust_cv
```

Examples

```
library(sasfunclust)
train<-simulate_data("Scenario I",n_i=20,var_e = 1,var_b = 0.5^2)
lambda_s_seq=10^seq(-4,-3)
lambda_l_seq=10^seq(-1,0)
G_seq=2
mod_cv<-sasfclust_cv(X=train$X,grid=train$grid,G_seq=G_seq,
lambda_l_seq = lambda_l_seq,lambda_s_seq =lambda_s_seq,maxit = 5,K_fold = 2,q=10)
plot(mod_cv)
mod<-sasfclust(X=train$X,grid=train$grid,G=mod_cv$G_opt,
lambda_l = mod_cv$lambda_l_opt,lambda_s = mod_cv$lambda_s_opt,maxit = 5,q=10)</pre>
```

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```
print(mod$clus$classes)
plot(mod)
```

plot.sasfclust

Plot the results of the Sas-funclust method

Description

This function provides plots of the estimated cluster mean functions and of the classified curves when applied to the output of sasfclust, whereas provides the cross-validation plots when applied to the output of sasfclust_cv. In the latter case the first plot displays the CV values as a function of G, lambda_s and lambda_l; the second plot displays the CV values as a function of lambda_s and lambda_l for G fixed at its optimal value; the third plot displays the CV values as a function of lambda_l for G and lambda_s fixed at their optimal value.

Usage

```
## S3 method for class 'sasfclust_cv'
plot(x, ...)
## S3 method for class 'sasfclust'
plot(x, ...)
```

Arguments

x The output of either sasfclust or sasfclust_cv.

.. No additional parameters, called for side effects.

Value

No return value, called for side effects.

Examples

```
library(sasfunclust)
train<-simulate_data("Scenario I",n_i=20,var_e = 1,var_b = 0.5^2)
lambda_s_seq=10^seq(-4,-3)
lambda_l_seq=10^seq(-1,0)
G_seq=2
mod_cv<-sasfclust_cv(X=train$X,grid=train$grid,G_seq=G_seq,
lambda_l_seq = lambda_l_seq,lambda_s_seq = lambda_s_seq,maxit = 20,K_fold = 2,q=10)
plot(mod_cv)
mod<-sasfclust(X=train$X,grid=train$grid,lambda_s = 10^-6,lambda_l = 10,G = 2,maxit = 20,q=10)
plot(mod)</pre>
```

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sasfclust

Sparse and Smooth Functional Data Clustering

Description

Sparse and smooth functional clustering (SaS-Funclust) allows to cluster a sample of curves into homogeneous groups while jointly detecting the most informative portion of domain. (Centofanti et al., 2021).

Usage

```
sasfclust(
  X = NULL
  timeindex = NULL,
  curve = NULL,
  grid = NULL,
  q = 30,
  lambda_l = 10,
  lambda_s = 10,
  G = 2,
  tol = 10^-7,
 maxit = 50,
  par_LQA = list(eps_diff = 1e-06, MAX_iter_LQA = 200, eps_LQA = 1e-05),
  plot = F,
  trace = F,
  init = "kmeans",
  varcon = "diagonal",
  lambda_s_ini = NULL
)
```

Arguments

For functional data observed over a regular grid: a matrix of where the rows must correspond to argument values and columns to replications. For functional data observed over an irregular grid: a vector of length $\sum_{i=1}^{N} n_i$, with N the number of curves, where the entries from $\sum_{i=1}^{k-1} (n_i+1)$ to $\sum_{i=1}^{k} n_i$ are elements representing the observations for curve k.

timeindex

A vector of length $\sum_{i=1}^{N} n_i$. The entries from $\sum_{i=1}^{k-1} (n_i+1)$ to $\sum_{i=1}^{k} n_i$ provide the locations on grid of curve k. So for example, if the kth curve is observed at time points t_l, t_m of the grid then the entries from $\sum_{i=1}^{k-1} (n_i+1)$ to $\sum_{i=1}^{k} n_i$ would be l, m, being $n_k = 2$. If X is a matrix, timeindex is ignored.

curve

A vector of length $\sum_{i=1}^{N} n_i$. The entries from $\sum_{i=1}^{k-1} (n_i + 1)$ to $\sum_{i=1}^{k} n_i$ are equal to k. If X is a matrix, curve is ignored.

grid

The vector of time points where the curves are sampled. For Functional data observed over an irregular grid, timeindex and grid provide the time points for each curve.

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The dimension of the set of B-spline functions. q lambda_1 Tuning parameter of the functional adaptive pairwise fusion penalty (FAPFP). lambda_s Tuning parameter of the smoothness penalty. G The number of clusters. tol The tolerance for the stopping condition of the expectation conditional maximization (ECM) algorithms. The algorithm stops when the log-likelihood difference between two consecutive iterations is less or equal than tol. maxit The maximum number of iterations allowed in the ECM algorithm. par_LQA A list of parameters for the local quadratic approximation (LQA) in the ECM algorithm. eps_diff is the lower bound for the coefficient mean differences, values below eps_diff are set to zero. MAX_iter_LQA is the maximum number of iterations allowed in the LQA. eps_LQA is the tolerance for the stopping condition of LQA. plot If TRUE, the estimated cluster means are plotted at each iteration of the ECM algorithm. Default is FALSE. trace If TRUE, information are shown at each iteration of the ECM algorithm. Default is FALSE. init It is the way to initialize the ECM algorithm. There are three ways of initialization: "kmeans", "model-based", and "hierarchical", that provide initialization through the k-means algorithm, model-based clustering based on parameterized finite Gaussian mixture model, and hierarchical clustering, respectively. Default is "kmeans". varcon A vector of character strings indicating the type of coefficient covariance matrix. Three values are allowed: "full", "diagonal", and "equal". "full" means unrestricted cluster coefficient covariance matrices allowed to be different among clusters. "diagonal" means diagonal cluster coefficient covariance matrices that are equal among clusters. "equal" means diagonal cluster coefficient covariance matrices, with equal diagonal entries, that are equal among clusters. Default is "diagonal". lambda_s_ini The tuning parameter used to obtain the functional data through smoothing Bsplines before applying the initialization algorithm. If NULL a Generalized

Value

A list containing the following arguments: mod that is a list composed by

 data: A list containing the vectorized form of X, timeindex, and curve. For functional data observed over a regular grid timeindex and curve are trivially obtained.

cross validation procedure is used as described in Ramsay (2005). Default is

- parameters: A list containing all the estimated parameters.
- vars: A list containing results from the Expectation step of the ECM algorithm.
- FullS: The matrix of B-spline computed over grid.

NULL.

• grid: The vector of time points where the curves are sampled.

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 W: The basis roughness penalty matrix containing the inner products of pairs of basis function second derivatives.

- AW_vec: Vectorized version of the diagonal matrix used in the approximation of FAPFP.
- P_tot: Sparse Matrix used to compute all the pairwise comparisons in the FAPFP.
- lambda_s: Tuning parameter of the smoothness penalty.
- lambda_1: Tuning parameter of the FAPFP.

A list, named clus, containing the following arguments:

- classes: The vector of cluster membership.
- po_pr: Posterior probabilities of cluster membership.

mean_fd The estimated cluster mean functions.

class A label for the output type.

References

Centofanti, F., Lepore, A., & Palumbo, B. (2021). Sparse and Smooth Functional Data Clustering. *arXiv preprint arXiv:2103.15224*.

Ramsay, J., Ramsay, J., & Silverman, B. W. (2005). Functional Data Analysis. Springer Science & Business Media.

See Also

```
sasfclust_cv
```

Examples

```
library(sasfunclust)
train<-simulate_data("Scenario I",n_i=20,var_e = 1,var_b = 0.5^2)
mod<-sasfclust(X=train$X,grid=train$grid,lambda_s = 10^-6,lambda_l =10,G = 2,maxit = 5,q=10)
plot(mod)</pre>
```

sasfclust_cv

Cross-validation for sasfclust

Description

K-fold cross-validation procedure to choose the number of clusters and the tuning parameters for the sparse and smooth functional clustering (SaS-Funclust) method (Centofanti et al., 2021).

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Usage

```
sasfclust_cv(
 X = NULL
  timeindex = NULL,
  curve = NULL,
 grid = NULL,
 q = 30,
  lambda_l_seq = 10^seq(-1, 2),
  lambda_s_seq = 10^seq(-5, -3),
  G_{seq} = 2,
  tol = 10^{-7},
 maxit = 50,
 par_LQA = list(eps_diff = 1e-06, MAX_iter_LQA = 200, eps_LQA = 1e-05),
 plot = FALSE,
  trace = FALSE,
  init = "kmeans",
  varcon = "diagonal",
 lambda_s_ini = NULL,
 K_fold = 5,
 X_{test} = NULL
 grid_test = NULL,
 m1 = 1,
 m2 = 0,
 m3 = 1,
 ncores = 1
)
```

Arguments

Χ

For functional data observed over a regular grid: a matrix of where the rows must correspond to argument values and columns to replications. For functional data observed over an irregular grid: a vector of length $\sum_{i=1}^N n_i$, with N the number of curves, where the entries from $\sum_{i=1}^{k-1} (n_i+1)$ to $\sum_{i=1}^k n_i$ are elements representing the observations for curve k.

timeindex

A vector of length $\sum_{i=1}^{N} n_i$. The entries from $\sum_{i=1}^{k-1} (n_i+1)$ to $\sum_{i=1}^{k} n_i$ provide the locations on grid of curve k. So for example, if the kth curve is observed at time points t_l, t_m of the grid then the entries from $\sum_{i=1}^{k-1} (n_i+1)$ to $\sum_{i=1}^{k} n_i$ would be l, m, being $n_k = 2$. If X is a matrix, timeindex is ignored.

curve

A vector of length $\sum_{i=1}^{N} n_i$. The entries from $\sum_{i=1}^{k-1} (n_i + 1)$ to $\sum_{i=1}^{k} n_i$ are equal to k. If X is a matrix, curve is ignored.

grid

The vector of time points where the curves are sampled. For Functional data observed over an irregular grid, timeindex and grid provide the time points for each curve.

q

The dimension of the set of B-spline functions.

lambda_l_seq

Sequence of tuning parameter of the functional adaptive pairwise fusion penalty (FAPFP).

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lambda_s_seq Sequence of tuning parameter of the smoothness penalty. Sequence of number of clusters. G_seq tol The tolerance for the stopping condition of the expectation conditional maximization (ECM) algorithms. The algorithm stops when the log-likelihood difference between two consecutive iterations is less or equal than tol. The maximum number of iterations allowed in the ECM algorithm. maxit A list of parameters for the local quadratic approximation (LQA) in the ECM par_LQA algorithm. eps_diff is the lower bound for the coefficient mean differences, values below eps_diff are set to zero. MAX_iter_LQA is the maximum number of iterations allowed in the LQA. eps_LQA is the tolerance for the stopping condition of LQA. plot If TRUE, the estimated cluster means are plotted at each iteration of the ECM algorithm. Default is FALSE. If TRUE, information are shown at each iteration of the ECM algorithm. Default trace is FALSE. It is the way to initialize the ECM algorithm. There are three ways of initialinit ization: "kmeans", "model-based", and "hierarchical", that provide initialization through the k-means algorithm, model-based clustering based on parameterized finite Gaussian mixture model, and hierarchical clustering, respectively. Default is "kmeans". A vector of character strings indicating the type of coefficient covariance mavarcon trix. Three values are allowed: "full", "diagonal", and "equal". "full" means unrestricted cluster coefficient covariance matrices allowed to be different among clusters. "diagonal" means diagonal cluster coefficient covariance matrices that are equal among clusters. "equal" means diagonal cluster coefficient covariance matrices, with equal diagonal entries, that are equal among clusters. Default is "diagonal". lambda_s_ini The tuning parameter used to obtain the functional data through smoothing Bsplines before applying the initialization algorithm. If NULL a Generalized cross validation procedure is used as described in Ramsay (2005). Default is NULL. K_fold Number of folds. Default is 5. X_{test} Only for functional data observed over a regular grid, a matrix where the rows must correspond to argument values and columns to replications of the test set. Default in NULL. grid_test The vector of time points where the test set curves are sampled. Default is NULL. The m-standard deviation rule parameter to choose G for each lambda_s and m1 lambda_1. m2 The m-standard deviation rule parameter to choose lambda_s fixed G for each

The m-standard deviation rule parameter to choose lambda_1 fixed G and lambda_s.

If ncores>1, then parallel computing is used, with ncores cores. Default is 1.

lambda_1.

m3

ncores

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Value

A list containing the following arguments:

G_opt: The optimal number of clusters.

lambda_l_opt: The optimal tuning parameter of the FAPFP.

lambda_s_opt: The optimal tuning parameter of the smoothness penalty.

comb_list: The combinations of G,lambda_s and lambda_l explored.

CV: The cross-validation values obtained for each combination of G,lambda_s and lambda_1.

CV_sd: The standard deviations of the cross-validation values.

zeros: Fraction of domain over which the estimated cluster means are fused.

ms: The m-standard deviation rule parameters.

class: A label for the output type.

References

Centofanti, F., Lepore, A., & Palumbo, B. (2021). Sparse and Smooth Functional Data Clustering. *arXiv preprint arXiv:2103.15224*.

Ramsay, J., Ramsay, J., & Silverman, B. W. (2005). Functional Data Analysis. Springer Science & Business Media.

See Also

sasfclust

Examples

```
library(sasfunclust)
train<-simulate_data("Scenario I",n_i=20,var_e = 1,var_b = 0.5^2)
lambda_s_seq=10^seq(-4,-3)
lambda_l_seq=10^seq(-1,0)
G_seq=2
mod_cv<-sasfclust_cv(X=train$X,grid=train$grid,G_seq=G_seq,
lambda_l_seq = lambda_l_seq,lambda_s_seq =lambda_s_seq,maxit = 20,K_fold = 2,q=10)
plot(mod_cv)</pre>
```

simulate_data

Simulate data for functional clustering

Description

Generate synthetic data as in the simulation study of Centofanti et al. (2021).

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Usage

```
simulate_data(
    scenario,
    n_i = 50,
    nbasis = 30,
    length_tot = 50,
    var_e = 1,
    var_b = 1
)
```

Arguments

A character strings indicating the scenario considered. It could be "Scenario I",
"Scenario II", and "Scenario III".

Number of curves in each cluster.

The dimension of the set of B-spline functions.

length_tot

Number of evaluation points.

var_e

Variance of the measurement error.

var_b

Diagonal entries of the coefficient variance matrix, which is assumed to be di-

agonal, with equal diagonal entries, and the same among clusters.

Value

A list containing the following arguments:

X: Observation matrix, where the rows correspond to argument values and columns to replications.

X_fd: Functional observations without measurement error.

mu_fd: True cluster mean function.

grid: The vector of time points where the curves are sampled.

clus: True cluster membership vector.

References

Centofanti, F., Lepore, A., & Palumbo, B. (2021). Sparse and Smooth Functional Data Clustering. *arXiv* preprint arXiv:2103.15224.

Examples

```
library(sasfunclust)
train<-simulate_data("Scenario I",n_i=20,var_e = 1,var_b = 0.5^2)</pre>
```

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