Package ‘kml’

December 13, 2023

Type Package
Title K-Means for Longitudinal Data
Version 2.4.6.1
Date 2023-02-11
Description An implementation of k-means specifically design
to cluster longitudinal data. It provides facilities to deal with missing
value, compute several quality criterion (Calinski and Harabatz,
Ray and Turie, Davies and Bouldin, BIC, ...) and propose a graphical
interface for choosing the 'best' number of clusters.
License GPL (>= 2)
LazyData no
URL https://www.r-project.org
Depends methods,clv,longitudinalData (>= 2.4)
Encoding UTF-8
NeedsCompilation yes
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R topics documented:

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Descrption

This package is a implementation of k-means for longitudinal data (or trajectories). Here is an overview of the package. For the description of the algorithm, see kml.

Details

Package: kml
Type: Package
Version: 2.4.1
Date: 2016-02-02
License: GPL (>= 2)
LazyData: yes
Depends: methods,clv,longitudinalData(>= 2.1.2)
URL: http://www.r-project.org
URL: http://christophe.genolini.free.fr/kml

Overview

To cluster data, Kml go through three steps, each of which is associated to some functions:

1. Data preparation
2. Building "optimal" partition
3. Exporting results
1. Data preparation

KML works on object of class `ClusterLongData`. Data preparation therefore simply consists in transforming data into an object `ClusterLongData`. This can be done via function `clusterLongData`. It converts a data.frame or a matrix into a `ClusterLongData`.

Instead of working on real data, one can also work on artificial data. Such data can be created with `generateArtificialLongData` (gald in short).

2. Building "optimal" partition

Once an object of class `ClusterLongData` has been created, the algorithm `kml` can be run.

Starting with a `ClusterLongData`, `kml` built a `Partition`. A object of class `Partition` is a partition of trajectories into subgroups. It also contains some information like the percentage of trajectories contained in each group or some quality criterion.

`kml` is a "hill-climbing" algorithm. The specificity of this kind of algorithm is that it always converges towards a maximum, but one cannot know whether it is a local or a global maximum. It offers no guarantee of optimality. To maximize one's chances of getting a quality `Partition`, it is better to run the hill climbing algorithm several times, then to choose the best solution. By default, `kml` executes the hill climbing algorithm 20 times and chooses the `Partition` maximizing the determinant of the matrix between.

Likewise, it is not possible to know beforehand the optimum number of clusters. On the other hand, afterwards, it is possible to calculate clues that will enable us to choose. In the end, `kml` tests by default 2, 3, 4, 5 et 6 clusters, 20 times each.

3. Exporting results

When `kml` has constructed some `Partition`, the user can examine them one by one and choose to export some. This can be done via function `choice`. `choice` opens a graphic windows showing various information including the trajectories clustered by a specific `Partition`.

When some `Partition` has been selected (the user can select more than 1), it is possible to save them. The clusters are therefore exported towards the file name-cluster.csv. Criteria are exported towards name-criteres.csv. The graphs are exported according to their extension.

It is also possible to extract a partition from the object `ClusterLongData` using the function `getClusters`.

See Also

Classes: `ClusterLongData`, `Partition`
Methods: `clusterLongData`, `kml`, `choice`
Plot: `plot(ClusterLongData)`

Examples

```r
### Move to tempdir
wd <- getwd()
setwd(tempdir()); getwd()
```
### 1. Data Preparation

data(epipageShort)
names(epipageShort)

cldSDQ <- cld(epipageShort, timeInData=3:6, time=c(3,4,5,8))

### 2. Building "optimal" clusteration (with only 3 redrawings)

kml(cldSDQ, nbRedrawing=3, toPlot="both")

### 3. Exporting results

### To check the best's cluster numbers

plotAllCriterion(cldSDQ)

# To see the best partition

try(choice(cldSDQ))

### 4. Further analysis

epipageShort$clust <- getClusters(cldSDQ, 4)

summary(glm(gender~clust, data=epipageShort, family="binomial"))

### Go back to current dir

setwd(wd)

---

affectFuzzyIndiv \(~ Function: affectFuzzyIndiv ~\)

**Description**

Given some longitudinal data (trajectories) and k cluster's centers, affectFuzzyIndiv compute the matrix of individual membership (according to the algorithm fuzzy k-means).

**Usage**

affectFuzzyIndiv(traj, clustersCenter, fuzzyfier=1.25)

**Arguments**

- **traj** [matrix]: longitudinal data. Each line is an individual, each column is a time measurement.
- **clustersCenter** [matrix]: cluster's centers. Each line is a cluster's center, each column is a time measurement.
- **fuzzyfier** [numeric]: value of the fuzzyfier used to compute individual's memberships.

**Details**

Given a matrix of clusters center clustersCenter (each line is a cluster center), the function affectFuzzyIndiv compute for each individual and each cluster a "membership".

affectFuzzyIndiv used with `calculTrajFuzzyMean` simulates one fuzzy k-means step.
**Value**

Matrix of the membership. Each line is an individual, column are for clusters.

**Examples**

```r
# Some LongitudinalData
traj <- gald()$"traj"

# 4 clusters centers
center <- traj[runif(4,1,nrow(traj)),]

# Affectation of each individual
affectFuzzyIndiv(traj,center)
```

---

**Description**

Given some longitudinal data (trajectories) and k clusters' centers, `affectIndiv` and `affectIndivC` affect each individual to the cluster whose centre is the closest.

**Usage**

```r
affectIndiv(traj, clustersCenter, distance = function(x,y){dist(rbind(x, y))})
affectIndivC(traj, clustersCenter)
```

**Arguments**

- `traj` [matrix(numeric)]: longitudinal data. Each line is an individual, each column is a time measurement.
- `clustersCenter` [matrix(numeric)]: clusters centre. Each line is a cluster center, each column is a time measurement.
- `distance` [numeric <- function(trajectory, trajectory)]: use to estimate the distance between an individual and a clusters center.

**Details**

Given a matrix of clusters center `clustersCenter` (each line is a cluster center), the function `affectIndiv` affect each individual of the matrix `traj` to the closest clusters (according to `distance`). `affectIndivC` does the same but assume that the distance is the Euclidean distance. `affectIndivC` is writen in C (and is therefor much faster).

`affectIndiv` used with `calculTrajMean` simulates one k-means step.
Value

Object of class **Partition**.

Examples

```
# affectIndiv

### Some trajectories
traj <- gald()$"traj"

### 4 clusters centers
center <- traj[runif(4,1,nrow(traj)),]

### Affectation of each individual
system.time(part <- affectIndiv(traj,center))
system.time(part <- affectIndivC(traj,center))
```

---

**calculTrajFuzzyMean**  ~ Function: calculTrajFuzzyMean ~

**Description**

Given some longitudinal data and a group’s membership, `calculFuzzyMean` computes the mean trajectories of each cluster.

**Usage**

```
calculTrajFuzzyMean(traj, fuzzyClust)
```

**Arguments**

- `traj`  
  [matrix]: longitudinal data. Each line is an individual, each column is a time measurement.

- `fuzzyClust`  
  [matrix(numeric)]: membership matrix of each individual.

**Details**

Given a matrix of individual membership, the function `calculTrajFuzzyMean` compute the mean trajectory of each clusters.

`affectFuzzyIndiv` used with `calculTrajFuzzyMean` simulates one fuzzy k-means step.

**Value**

A matrix with k line and t column containing k clusters centers. Each line is a center, each column is a time measurement.
Examples

### calculTrajFuzzyMean

### Some LongitudinalData
traj <- gald()$"traj"

### 4 clusters centers
center <- traj[runif(4,1,nrow(traj)),]

### Affectation of each individual
membership <- affectFuzzyIndiv(traj,center)

### Computation of the mean's trajectories
calculTrajFuzzyMean(traj,membership)

calculTrajMean ~ Functions: calculTrajMean & calculTrajMeanC ~

Description

Given some longitudinal data and a cluster affection, calculTrajMean and calculTrajMeanC compute the mean trajectories of each cluster.

Usage

calculTrajMean(traj, clust, centerMethod = function(x){mean(x, na.rm =TRUE)})
calculTrajMeanC(traj, clust)

Arguments

<table>
<thead>
<tr>
<th>Argument</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>traj</td>
<td>[matrix(numeric)]: longitudinal data. Each line is an individual, each column is a time measurement.</td>
</tr>
<tr>
<td>clust</td>
<td>[vector(numeric)]: affectation of each individual.</td>
</tr>
<tr>
<td>centerMethod</td>
<td>[trajectory &lt;- function(matrix(numeric))]: function that compute the mean trajectory of a group of trajectories.</td>
</tr>
</tbody>
</table>

Details

Given a vector of affection to a cluster, the function calculTrajMean compute the "central" trajectory of each clusters. The "center" can be define using the argument centerMethod. calculTrajMeanC does the same but assume that the center definition is the classic "mean". calculTrajMeanC is written in C (and is therefore much faster).

affectIndiv used with calculTrajMean simulates one k-means step.
Value
A matrix with k line and t column containing k clusters centers. Each line is a center, each column is a time measurement.

Examples

### calculMean

```r
### Some trajectories
traj <- gald()$traj

### A cluster affectation
clust <- initializePartition(3,200,"randomAll")

### Computation of the cluster's centers
system.time(centers <- calculTrajMean(traj,clust))
system.time(centers <- calculTrajMeanC(traj,clust))
```

choice ~ Function: choice ~

Description
choice lets the user choose some Partition he wants to export.

Usage

```r
choice(object, typeGraph = "bmp")
```

Arguments

- **object** [ClusterLongData]: Object containing the trajectories and all the Partition found by kml.
- **typeGraph** [character]: for every selected Partition, choice export some graphs. typeGraph set the format that will be used. Possible formats are the ones available for savePlot.

Details

choice is a function that lets the user see the Partition found by kml. At first, choice opens a graphics window (for Linux user, the windows should be explicitly open using `x11(type = "Xlib")`). On the left side, all the Partition contain in Object are ploted by a number (the number of cluster of the Partition). The level of the number is proportionnal to a quality criteria (like Calinski & Harabatz). One Partition is 'active', it is the one marked by a black dot.

On the right side, the trajectories of Object are drawn, according to the active Partition. From there, choice offers numerous options:
**Arrow** Change the active Partition.

**Space** Select/unselect a Partition (the selected Partition are surrounded by a circle).

**Return** Export all the selected Partition, then quit the function choice.

'**e**' Change the display (Trajectories alone / quality criterion alone / both)

'**d**' Change actif criterion.

'**c**' Sort the Partition according to the actif criterion.

'**r**' Change the trajectories’ style.

'**f**' Change the means trajectories’s style.

'**g/t**' Change the symbol size.

'**y/h**' Change the number of symbols.

When 'return' is pressed (or 'm' using Linux), the selected Partition are exported. Exporting is done in a specific named `objectName-Cx-y` where x is the number of cluster and y is the order in the sublist. Four files are created:

- `objectName-Cx-y-Clusters.csv` Table with two columns. The first is the identifier of each trajectory (idAll); the second holds the cluster's affectation of the trajectory.

- `objectName-Cx-y-Detail.csv` Table containing information about the clusteration (percentage of individual in each cluster, various qualities criterion, algorithm used to find the partition and convergence time.)

- `objectName-Cx-y-Traj.bmp` Graph representing the trajectories. All the parameters set during the visualization (color of the trajectories, symbols used, mean color) are used for the export. Note that the 'typeGraph' argument can be used to export the graph in a format different than 'bmp'.

- `objectName-Cx-y-TrajMean.bmp` Graph representing the means trajectories of each clusters. All the parameters set during the visualization (color of the trajectories, symbols used, mean color) are used for the export.

This four file are created for each selected Partition. In addition, two 'global' graphes are created:

- `objectName-criterionActif.bmp` Graph presenting the values of the criterionActifall for all the Partition.

- `objectName-criterionAll.bmp` For each cluster’s number, the first Partition is considered. This graph presents on a single display the values of all the criterion for each first Partition. It is helpfull to compare the various qualities criterion.

**Value**

For each selected Partition, four files are saved, plus two global files.

**See Also**

Overview: [kml-package](#)

Classes: [ClusterLongData, Partition](#)

Methods: [kml](#)

Plot: [plot](#)
Examples

```r
### Move to tempdir
wd <- getwd()
setwd(tempdir()); getwd()

### Creation of artificial data
cld1 <- gald(25)

### Clusterisation
kml(cld1,3:5,nbRedrawing=2,toPlot=’both’)

### Selection of the clustering we want
# (note that ”try” is for compatibility with CRAN only,
# you probably can use ”choice(cld1)”)
try(choice(cld1))

### Go back to current dir
setwd(wd)
```

---

**clusterLongData**  

~ Function: clusterLongData (or cld) ~

---

Description

clusterLongData (or cld in short) is the constructor for `ClusterLongData` object.

Usage

```r
clusterLongData(traj, idAll, time, timeInData, varNames, maxNA)
cld(traj, idAll, time, timeInData, varNames, maxNA)
```

Arguments

- **traj**  
  [matrix(numeric)] or [data.frame]: structure containning the trajectories. Each line is the trajectory of an individual. The columns refer to the time during which measures were made.

- **idAll**  
  [vector(character)]: single identifier for each trajectory (ie each individual). Note that the identifiers are of type character (that allow to deal identifiers like XUK32-612, identifiers that our favorite epidemiologists are so good at providing). If idAll are numeric, they are converted into characters.

- **time**  
  [vector(numeric)]: time at which measures were made.

- **timeInData**  
  [vector(numeric)]: precise the column containing the trajectories.

- **varNames**  
  [character]: name of the variable being measured.

- **maxNA**  
  [numeric]: maximum number of NA that are tolerates on a trajectory. If a trajectory has more missing than maxNA, then it is remove from the analysis.
Details

classClusterLongData construct a object of class ClusterLongData. Two cases can be distinguished:

**traj is an array:** lines are individual. Column are time of measurement.
  - If `idAll` is missing, the individuals are labelled i1, i2, i3,...
  - If `timeInData` is missing, all the column are used (`timeInData=1:ncol(traj)`).

**If traj is a data.frame:** lines are individual. Column are time of measurement.
  - If `idAll` is missing, then the first column of the data.frame is used for `idAll`
  - If `timeInData` is missing and `idAll` is missing, then all the columns but the first are used for `timeInData` (the first is omitted since it is already used for `idAll`): `idAll=traj[,1], timeInData=2:ncol(traj)`.
  - If `timeInData` is missing but `idAll` is not missing, then all the column including the first are used for `timeInData`: `timeInData=1:ncol(traj)`.

Value

An object of class ClusterLongData.

Author

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References

[1] C. Genolini and B. Falissard
"KmL: k-means for longitudinal data"
Computational Statistics, vol 25(2), pp 317-328, 2010

"KmL: A package to cluster longitudinal data"
Computer Methods and Programs in Biomedicine, 104, pp e112-121, 2011

See Also

Overview: kml-package
Classes: ClusterLongData
Methods: choice, kml
Plot: plot(ClusterLongData)

Examples

```
### From matrix
### Small data
```
mat <- matrix(c(1,NA,3,2,3,6,1,8,10),3,3,dimnames=list(c(101,102,104),c("T2","T4","T8")))
clusterLongData(mat)
(ld1 <- clusterLongData(traj=mat,idAll=as.character(c(101,102,104)),time=c(2,4,8),varNames="V"))
plot(ld1)

### Big data
mat <- matrix(runif(1051*325),1051,325)
(ld2 <- clusterLongData(traj=mat,idAll=paste("I-",1:1051,sep=""),time=(1:325)+0.5,varNames="R"))

### From data.frame

### Basic
clusterLongData(dn)

### Selecting some times
(ld3 <- clusterLongData(dn,timeInData=c(1,2,4),varNames=c("Hyp")))

### Excluding trajectories with more than 1 NA
(ld3 <- clusterLongData(dn,maxNA=1))

ClusterLongData-class ~ Class: ClusterLongData ~

Description
ClusterLongData is an object containing trajectories and associated Partition

Objects from the Class

kml is an algorithm that builds a set of Partition from longitudinal data. ClusterLongData is the object containing the original longitudinal data and all the Partition that kml finds.

When created, an ClusterLongData object simply contains initial data (the trajectories). After the execution of kml, it contains the original data and the Partition which has just been calculated by kml.

Note that if kml is executed several times, every new Partition is added to the original ones, no pre-existing Partition is erased.

Slots
idAll [vector(character)]: Single identifier for each of the trajectory (each individual). Useful for exporting clusters.
idFewNA [vector(character)]: Restriction of idAll to the trajectories that does not have 'too many' missing value. See maxNA for details.
time [numeric]: Time at which measures are made.
ClusterLongData-class

varNames [character]: Name of the variable measured.

traj [matrix(numeric)]: Contains the longitudinal data. Each line is the trajectories of an individual. Each column is the time at which measures are made.

dimTraj [vector2(numeric)]: size of the matrix traj (ie dimTraj=c(length(idFewNA),length(time))).

maxNA [numeric] or [vector(numeric)]: Individual whose trajectories contain 'too many' missing value are exclude from traj and will no be use in the analysis. Their identifier is preserved in idAll but not in idFewNA. 'too many' is define by maxNA: a trajectory with more missing than maxNA is exclude.

reverse [matrix(numeric)]: if the trajectories are scale using the function scale, the 'scaling parameters' (probably mean and standard deviation) are saved in reverse. This is usefull to restaura the original data after a scaling operation.

criterionActif [character]: Store the criterion name that will be used by functions that need a single criterion (like plotCriterion or ordered).

initializationMethod [vector(character)]: list all the initialization method that has already been used to find some Partition (usefull to not run several time a deterministic method).

sorted [logical]: are the Partition curently hold in the object sorted in decreasing order?

c1 [list(Partition)]: list of Partition with 1 clusters.
c2 [list(Partition)]: list of Partition with 2 clusters.
c3 [list(Partition)]: list of Partition with 3 clusters.
...
c26 [list(Partition)]: list of Partition with 26 clusters.

Extends

Class LongData, directly. Class ListPartition, directly.

Construction

Class ClusterizLongData objects can be constructed via function clusterLongData that turn a data.frame or a matrix into a ClusterLongData. Note that some artificial data can be generated using gald.

Methods

object['xxx'] Get the value of the field xxx. Inherit from LongData and ListPartition.

object['xxx']<-value Set the field xxx to value. xxx. Inherit from ListPartition.

plot Display the ClusterLongData according to a Partition.

Special thanks

Special thanks to Boris Hejblum for debugging the '[' and '[<-' operators (the previous version was not compatible with the matrix package, which is used by lme4).
See Also

Overview: kml-package
Classes: Partition, LongData, ListPartition
Methods: clusterLongData, kml, choice
Plot: plot(ClusterLongData), plotCriterion

Examples

### Move to tempdir
wd <- getwd()
setwd(tempdir()); getwd()

################
### Creation of some trajectories
traj <- matrix(c(1,2,3,1,4, 3,6,1,8,10, 1,2,1,3,2, 4,2,5,6,3, 4,3,4,4,4, 7,6,5,5,4),6)

myCld <- clusterLongData(
  traj=traj,
  idAll=as.character(c(100,102,103,109,115,123)),
  time=c(1,2,4,8,15),
  varNames="P",
  maxNA=3
)

################
### get and set
myCld["idAll"]
myCld["varNames"]
myCld["traj"]

################
### Creation of a Partition
part2 <- partition(clusters=rep(1:2,3),myCld)
part3 <- partition(clusters=rep(1:3,2),myCld)

################
### Adding a clusterization to a clusterizLongData
myCld["add"] <- part2
myCld["add"] <- part3
myCld

### Go back to current dir
setwd(wd)
Description

A subset of the longitudinal study EPIPAGE.

Usage

data(epipageShort)

Format

id          unique identifier for each patient.
gender      Male or Female.
sdq3        score of the Strengths and Difficulties Questionnaire at 3 years old.
sdq4        score of the Strengths and Difficulties Questionnaire at 4 years old.
sdq5        score of the Strengths and Difficulties Questionnaire at 5 years old.
sdq8        score of the Strengths and Difficulties Questionnaire at 8 years old.

Details

The EPIPAGE cohort, funded by INSERM and the French general health authority, is a multi-regional French follow-up survey of severely premature children. It included more than 4000 children born at less than 33 weeks gestational age, and two control samples of children, respectively born at 33-34 weeks of gestational age and born full term. The general objectives were to study short and long term motor, cognitive and behavioural outcomes in these children, and to determine the impact of medical practice, care provision and organization of perinatal care, environment, family circle and living conditions on child health and development. About 2600 children born severely premature and 400 and 600 controls respectively were followed up to the age of 5 years and then to the age of 8.

The SDQ is a behavioral questionnaire for children and adolescents ages 4 through 16 years old. It measures the severity of the disability (higher score indicate higher disability).

The database belongs to the INSERM unit U953 (P.Y. Ancel). which has agreed to include the variable SDQ in the library.

References


Examples

data(epipageShort)
str(epipageShort)

---

Algorithm fuzzy kml: Fuzzy k-means for Longitudinal data

Description

fuzzyKmlSlow is a new implementation of fuzzy k-means for longitudinal data (or trajectories).

Usage

fuzzyKmlSlow(traj, clusterAffectation, toPlot = "traj",
             fuzzyfier = 1.25, parAlgo = parALGO())

Arguments

traj [matrix(numeric)]: Matrix holding the longitudinal data
clusterAffectation [vector(numeric)]: Initial starting condition
toPlot [character]: if "traj", then the trajectories are plot. If "none", there is no graphical display (faster).
fuzzyfier [numeric]: value of the fuzzy k-means algorithm fuzzyfier.
parAlgo [ParKml]: default parameters for the algorithm.

Details

fuzzyKmlSlow is a new implementation of fuzzy k-means for longitudinal data (or trajectories). To date, it is written in R (and not in C, this explain the "slow")

Value

The matrix of the individual membership.

See Also

kml

Examples

### Data generation
traj <- gald(25)["traj"]
partInit <- initializePartition(3,100,"kmeans--",traj)

### fuzzy Kml
partResult <- fuzzyKmlSlow(traj,partInit)
generateArtificialLongData

~ Function: generateArtificialLongData (or gald) ~

Description

This function builds up an artificial longitudinal data set (single variable-trajectory) and turn it into an object of class ClusterLongData.

Usage

gald(nbEachClusters=50, time=0:10, varNames="V",
   meanTrajectories=list(function(t){0},function(t){t},
   function(t){10-t},function(t){-0.4*t^2+4*t}),
   personalVariation=function(t){rnorm(1,0,2)},
   residualVariation=function(t){rnorm(1,0,2)},
   decimal=2, percentOfMissing=0)

generateArtificialLongData(nbEachClusters=50, time=0:10, varNames="V",
   meanTrajectories=list(function(t){0},function(t){t},
   function(t){10-t},function(t){-0.4*t^2+4*t}),
   personalVariation=function(t){rnorm(1,0,2)},
   residualVariation=function(t){rnorm(1,0,2)},
   decimal=2, percentOfMissing=0)

Arguments

nbEachClusters [numeric] or [vector(numeric)]: number of trajectories that each cluster must contain. If a single number is given, it is duplicated for all groups.
time [vector(numeric)]: time at which measures are made.
varNames [character]: name of the variable.
meanTrajectories [list(function)]: lists the functions define the average trajectories of each cluster.
personalVariation [function] or [list(function)]: lists the functions defining the personal variation between an individual and the mean trajectories of its cluster. Note that these function should be constant function (the personal variation can not evolve with time). If a single function is given, it is duplicated for all groups (see detail).
residualVariation [function] or [list(function)]: lists the functions generating the noise of each trajectory within its own cluster. If a single function is given, it is duplicated for all groups (see detail).
decimal [numeric]: number of decimals used to round up values.
generateArtificialLongData

percentOfMissing

[numeric]: percentage (between 0 and 1) of missing data generated in each cluster. If a single value is given, it is duplicated for all groups. The missing values are Missing Completly At Random (MCAR).

Details

generateArtificialLongData (gald in short) is a function that contruct a set of artificial longitudinal data. Each individual is considered as belonging to a group. This group follows a theoretical trajectory, function of time. These functions (one per group) are given via the argument meanTrajectories.

Within a group, the individual undergoes individual variations. Individual variations are given via the argument residualVariation.

The number of individuals in each group is given by nbEachClusters.

Finally, it is possible to add missing values randomly (MCAR) striking the data thanks to percent0fMissing.

Value

An object of class ClusterLongData.

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References

[1] C. Genolini and B. Falissard
"KmL: k-means for longitudinal data"
Computational Statistics, vol 25(2), pp 317-328, 2010

"KmL: A package to cluster longitudinal data"
Computer Methods and Programs in Biomedicine, 104, pp e112-121, 2011

See Also

ClusterLongData, clusterLongData

Examples

par(ask=TRUE)

#########################
### Default example
getBestPostProba

```r
(ex1 <- generateArtificialLongData())
plot(ex1)
plot(ex1, parTraj=parTRAJ(col=rep(2:5, each=50)))

############################
### Three diverging lines

ex2 <- generateArtificialLongData(meanTrajectories=list(function(t)0, function(t)-t, function(t)t))
plot(ex2, parTraj=parTRAJ(col=rep(2:4, each=50)))

############################
### Three diverging lines with high variance, unbalance groups and missing value

ex3 <- generateArtificialLongData(
  meanTrajectories=list(function(t)0, function(t)-t, function(t)t),
  nbEachClusters=c(100, 30, 10),
  residualVariation=function(t){rnorm(1, 0, 3)},
  percentOfMissing=c(0.25, 0.5, 0.25)
)
part3 <- partition(rep(1:3, c(100, 30, 10)))
plot(ex3, parTraj=parTRAJ(col=rep(2:4, c(100, 30, 10))))

############################
### Four strange functions

ex4 <- generateArtificialLongData(
  nbEachClusters=c(300, 200, 100, 100),
  meanTrajectories=list(function(t){-10+2*t}, function(t){-0.6*t^2+6*t-7.5},
    function(t){10*sin(t)}, function(t){30*dnorm(t, 2, 1.5)}),
  residualVariation=function(t){rnorm(1, 0, 3)},
  time=0:10, decimal=2, percentOfMissing=0.3)
plot(ex4, parTraj=parTRAJ(col=rep(2:5, c(300, 200, 100, 100))))

############################
### To get only longData (if you want some artificial longData
### to deal with another algorithm), use the getteur ["traj"]

ex5 <- gald(nbEachCluster=3, time=1:3)
ex5["traj"]

par(ask=FALSE)
```

getBestPostProba ~ Function: getBestPostProba ~
Description

Given a ClusterLongData object that hold a Partition, this function extract the best posterior probability of each individual.

Usage

getBestPostProba(xCld, nbCluster, clusterRank = 1)

Arguments

xCld [ClusterLongData]: object from who a cluster should be extracted.

nbCluster [integer]: number of cluster of the desired cluster.

clusterRank [integer]: rank of the partition in the clusters list.

Details

Given a ClusterLongData object that hold a Partition, this function extract the best posterior probability of each individual.

Value

A vector of numeric.

See Also

ClusterLongData

Examples

### Move to tempdir
wd <- getwd()
setwd(tempdir()); getwd()

### Creation of an object ClusterLongData
myCld <- gald(20)

### Computation of some partition
kml(myCld, 2:4, 3)

### Extraction the best posterior probabilities
### form the list of partition with 3 clusters of the second clustering
getBestPostProba(myCld, 3, 2)

### Go back to current dir
setwd(wd)
getClusters ~ Function: getClusters ~

Description

This function extract a cluster affectation from an `ClusterLongData` object.

Usage

```r
getClusters(xCld, nbCluster, clusterRank = 1, asInteger = FALSE)
```

Arguments

- `xCld` `[ClusterLongData]`: object from who a cluster should be extracted.
- `nbCluster` `[integer]`: number of cluster of the desired cluster.
- `clusterRank` `[integer]`: rank of the partition in the clusters list.
- `asInteger` `[logical]`: should the cluster be given as a vector of integer ? If FALSE, a vector of LETTERS is return.

Details

This function extract a clusters from an object `ClusterLongData`. It is almost the same as `xCld[paste("c",nbCluster,sep="")][[clusterRank]]` except that the individual with too many missing value (and thus excludes from the analysis) will be noted by some NA values.

Value

A vector of numeric or a LETTER, according to the value of `asInteger`.

See Also

- `ClusterLongData`

Examples

```r
### Move to tempdir
wd <- getwd()
setwd(tempdir()); getwd()

### Creation of an object ClusterLongData
myCld <- gald(20)

### Computation of some partition
kml(myCld,2:4,3)

### Extraction form the list of partition with 3 clusters
### of the second clustering
getClusters(myCld,3,2)
```
### Go back to current dir
setwd(wd)

---

**kml**  
*Algorithm kml: K-means for Longitudinal data*

---

**Description**

kml is a implementation of k-means for longitudinal data (or trajectories). This algorithm is able to deal with missing value and provides an easy way to re roll the algorithm several times, varying the starting conditions and/or the number of clusters looked for.

Here is the description of the algorithm. For an overview of the package, see kml-package.

**Usage**

```r
kml(object, nbClusters=2:6, nbRedrawing=20, toPlot="none", parAlgo=parALGO())
```

**Arguments**

- `object` [ClusterLongData]: contains trajectories to cluster as well as previous Partition.
- `nbClusters` [vector(numeric)]: Vector containing the number of clusters with which kml must work. By default, nbClusters is 2:6 which indicates that kml must search partitions with respectively 2, then 3, ... up to 6 clusters. Maximum number of cluster is 26.
- `nbRedrawing` [numeric]: Sets the number of time that k-means must be re-run (with different starting conditions) for each number of clusters.
- `toPlot` [character]: either 'traj' for plotting trajectories alone, 'criterion' for plotting criterion alone, 'both' for plotting both or 'none' for not display anything (faster).
- `parAlgo` [ParKml]: parameters used to run the algorithm. They can be change using the function parKml. Option are mainly 'saveFreq', 'maxIt', 'imputationMethod', 'distance' and 'startingCondition'. See ParKml for details.

**Details**

kml works on object of class ClusterLongData. For each number included in nbClusters, kml computes a Partition then stores it in the field cX of the object ClusterLongData according to the number of clusters 'X'. The algorithm starts over as many times as it is told in nbRedrawing. By default, it is executed for 2, 3, 4, 5 and 6 clusters 20 times each, namely 100 times.

When a Partition has been found, it is added to the corresponding slot c1, c2, c3, ... or c26. The sublist cX stores the all Partition with X clusters. Inside a sublist, the Partition can be sorted from the biggest quality criterion to the smallest (the best are stored first, using ordered,ListPartition), or not.
Note that Partition are saved throughout the algorithm. If the user interrupts the execution of kml, the result is not lost. If the user run kml on an object, then running kml again on the same object will add some new Partition to the one already found.

The possible starting conditions are defined in initializePartition.

**Value**

A ClusterLongData object, after having added some Partition to it.

**Optimisation**

Behind kml, there are two different procedures:

1. Fast: when the parameter distance is set to "euclidean" and toPlot is set to 'none' or 'criterion', kml call a C compiled (optimized) procedure.
2. Slow: when the user defines its own distance or if he wants to see the construction of the clusters by setting toPlot to 'traj' or 'both', kml uses a R non compiled programmes.

The C procedure is 25 times faster than the R one.

So we advice to use the R procedure 1/ for trying some new method (like using a new distance) or 2/ to "see" the very first clusters construction, in order to check that every thing goes right. Then it is better to switch to the C procedure (like we do in Example section).

If for a specific use, you need a different distance, feel free to contact the author.

**See Also**

Overview: kml-package

Classes: ClusterLongData, Partition

Methods: clusterLongData, choice

**Examples**

```r
### Move to tempdir
wd <- getwd()
setwd(tempdir()); getwd()

### Generation of some data
cld1 <- generateArtificialLongData(25)

### We suspect 3, 4 or 6 clusters, we want 3 redrawing.
### We want to "see" what happen (so printCal and printTraj are TRUE)
kml(cld1,c(3,4,6),3,toPlot='both')

### 4 seems to be the best. We want 7 more redrawing.
### We don't want to see again, we want to get the result as fast as possible.
kml(cld1,4,10)

### Go back to current dir
setwd(wd)
```
parKml

~ Function: parKml ~

Description

parKml and parALGO are constructor for the object ParKml.

Usage

parKml(saveFreq,maxIt,imputationMethod,distanceName,power,distance,
   centerMethod,startingCond,nbCriterion,scale)

parALGO(saveFreq=100,maxIt=200,imputationMethod="copyMean",
   distanceName="euclidean",power=2,distance=function(){}
   centerMethod=meanNA,startingCond="nearlyAll",nbCriterion=1000,scale=TRUE)

Arguments

saveFreq [numeric]: Long computations can take several days. So it is possible to save
   the object ClusterLongData on which works kml once in a while. saveFreq de-
   fines the frequency of the saving process. The ClusterLongData is saved every
   saveFreq clustering calculations. The object is saved in the file objectName.Rdata
   in the current folder. If saveFreq is set to Inf, the object is never saved.

maxIt [numeric]: Set a limit to the number of iteration if convergence is not reached.

imputationMethod [character]: the calculation of quality criterion can not be done if some value
   are missing. imputationMethod define the method use to impute the missing
   value. See imputation for detail.

distanceName [character]: name of the distance used by k-means. If the distanceName is
   one of "manhattan", "euclidean", "minkowski", "maximum", "canberra" or "bi-
   nary", a compiled optimized version specifically design for trajectories version
   is used. Otherwise, the function define in the slot distance is used.

power [numeric]: If distanceName="minkowski", this define the power that will be
   used.

distance [numeric <- function(trajA,trajB)]: function that computes the distance
   between two trajectories. If no function is specified, the Euclidian distance with
   Gower adjustment (to deal with missing value) is used.

centerMethod [numeric <- function(vector(numeric))]: k-means algorithm computes the
   centers of each cluster. It is possible to personalize the definition of "center" by
   defining a function "centerMethod". This function should take a vector of nu-
   meric as argument and return a single numeric -the center of the vector-.

startingCond [character]: specifies the starting condition. Should be one of "randomAll",
   "randomK", "maxDist", "kmeans++", "kmeans+", "kmeans-" or "kmeans--" (see
   initializePartition for details). It also could take two specifics values: "all"
ParKml-class

stands for c("maxDist","kmeans-") then an alternance of "kmeans-" and "randomK" while "nearlyAll" stands for "kmeans-" then an alternance of "kmeans-" and "randomK".

nbCriterion [numeric]: set the maximum number of quality criterion that are display on the graph (since displaying a high criterion number an slow down the overall process). The default value is 100.

dimCriterias [numeric]: set the maximum number of distances criteria that are display on the graph (since displaying a high criterion number an slow down the overall process). The default value is 100.

scale [logical]: if TRUE, then the data will be automatically scaled (using the function scale with default values) before the execution of k-means on joint trajectories. Then the data will be restore (using the function restoreRealData) just before the end of the function kml3d. This option has no effect on kml.

Details

parKml is the constructor of object ParKml.

Value

An object ParKml.

Examples

### Move to tempdir
wd <- getwd()
setwd(tempdir()); getwd()

### Generation of some data
cld1 <- generateArtificialLongData()

### Setting two different set of option :
(option1 <- parALGO())
(option2 <- parALGO(distanceName="maximum",centerMethod=function(x)median(x,na.rm=TRUE)))

### Running kml We suspect 3, 4 or 5 clusters, we want 3 redrawing.
kml(cld1,3:5,3,toPlot="both",parAlgo=option1)
kml(cld1,3:5,3,toPlot="both",parAlgo=option2)

### Go back to current dir
setwd(wd)
Slots

saveFreq [numeric]: Long computations can take several days. So it is possible to save the object 
ClusterLongData on which works kml once in a while. saveFreq defines the frequency of 
the saving process. The ClusterLongData is saved every saveFreq clustering calculations. 
The object is saved in the file objectName.Rdata in the current folder. If saveFreq is set to 
Inf, the object is never saved.

maxIt: [numeric]: Set a limit to the number of iteration if convergence is not reached.

imputationMethod: [character]: the calculation of quality criterion can not be done if some 
value are missing. imputationMethod define the method use to impute the missing value. 
See imputation for detail.

distanceName: [character]: name of the distance used by k-means. If the distanceName is 
one of "manhattan", "euclidean", "minkowski", "maximum", "canberra" or "binary", a com-
plied optimized version specifically design for trajectories version is used. Otherwise, the 
function define in the slot distance is used.

power: [numeric]: If distanceName="minkowski", this define the power that will be used.

distance: [numeric <- function(trajA, trajB)]: function that computes the distance between 
two trajectories. This field is used only if 'distanceName' is not one of the classical function.

centerMethod: [numeric <- function(vector(numeric))]: k-means algorithm computes the 
centers of each cluster. It is possible to personalize the definition of "center" by defining a 
function "centerMethod". This function should take a vector of numeric as argument and 
return a single numeric -the center of the vector-.

startingCond: [character]: specifies the starting condition. Should be one of "randomAll", 
"randomK", "maxDist", "kmeans++", "kmeans+", "kmeans-" or "kmeans--" (see initializePartition 
for details). It also could take two specifics values: "all" stands for c("maxDist","kmeans-") 
then an alternance of "kmeans-" and "randomK" while "nearlyAll" stands for "kmeans--" then 
an alternance of "kmeans-" and "randomK".

nbCriterion [numeric]: set the maximum number of quality criterion that are display on the 
graph (since displaying a high criterion number an slow down the overall process). The default 
value is 100.

scale [logical]: if TRUE, then the data will be automatically scaled (using the function scale 
with default values) before the execution of k-means on joint trajectories. Then the data will 
be restore (using the function restoreRealData) just before the end of the function kml3d. 
This option has no effect on kml.

Methods

object[’xxx’] Get the value of the field xxx.

Examples

```r
### Move to tempdir
wd <- getwd()
setwd(tempdir()); getwd()

### Building data
```
myCld <- gald()

### Standard kml
kml(myCld,,3,toPlot="both")

### Using median instead of mean
parWithMedian <- parALGO(centerMethod=function(x){median(x, na.rm=TRUE)})
kml(myCld,,3,toPlot="both",parAlgo=parWithMedian)

### Using distance max
parWithMax <- parALGO(distanceName="maximum")
kml(myCld,,3,toPlot="both",parAlgo=parWithMax)

### Go back to current dir
setwd(wd)

---

**plot,ClusterLongData**  ~ Function: plot for ClusterLongData ~

**Description**

plot the trajectories of an object *ClusterLongData* relatively to a *Partition*.

**Usage**

```r
## S4 method for signature 'ClusterLongData,ANY'
plot(x,y=NA,parTraj=parTRAJ(),parMean=parMEAN(),
     addLegend=TRUE, adjustLegend=-0.12,toPlot="both",criterion=x["criterionActif"],
     nbCriterion=1000, ...)
```

**Arguments**

- **x**  
  [ClusterLongData]: Object containing the trajectories to plot.

- **y**  
  [numeric] or [vector(numeric)]: Give the Partition to represent. If y is missing, the Partition with the highest quality criterion (the actif one) is selected. If y is a number, the first Partition of the sublist c-y is selected. If y is a couple of numeric, the y[2]th Partition of the sublist c-y[1] is selected.

- **parTraj**  
  [ParLongData]: Specification of the plotting parameters of the individual trajectories. Fields that can be changes are 'type','col','pch','xlab' and 'ylab'. In addition to the standard possible values, the option col="clusters" can be use to color the individual trajectories according to their clusters (exemple: parTraj=parTRAJ(type="o",col="clusters")). See ParLongData for details.

- **parMean**  
  [ParLongData]: Specification of the plotting parameters of the mean trajectories. Fields that can be changes are 'type','col','pch','pchPeriod' and 'cex'. See ParLongData for details.
toPlot [character]: either 'traj' for plotting trajectories alone, 'criterion' for plotting criterion alone, 'both' for plotting both or 'none' for not display anything (faster).

criterion [character] or [vector(character)]: criterion to display (only if 'toPlot' is 'criterion' or 'both'). If a single criterion is given, it will be display for all the Partition. If several criterion are used, they will be display for the first Partition for each clusters’ numbers.

nbCriterion [numeric]: if a single criterion is given to criterion (and thus is displayed for 'all' the Partition), this slot alows to fix a limit on the number of points that will be display.

addLegend [logical]: should the legend be displayed?

adjustLegend [numeric]: fix the height of the legend

... Some other parameters can be passed to the method (like "xlab" or "ylab".

Details

plot the trajectories of an object ClusterLongData relativly to the 'best' Partition, or to the Partition define by y.

Graphical option concerning the individual trajectory (col, type, pch and xlab) can be change using parTraj. Graphical option concerning the cluster mean trajectory (col, type, pch, pchPeriod and cex) can be change using parMean. For more detail on parTraj and parMean, see object of class ParLongData.

See Also

Overview: kml-package
Classes: ClusterLongData
Plot: plot: overview, plotCriterion

Examples

### Move to tempdir
wd <- getwd()
setwd(tempdir()); getwd()

# Construction of the data
ld <- gald()

### Basic plotting
plot(ld)

### Changing graphical parameters 'par'
kml(ld,3:4,1)
### No letters on the mean trajectories
plot(ld,3,parMean=parMEAN(type="l"))

### Only one letter on the mean trajectories
plot(ld,4,parMean=parMEAN(pchPeriod=Inf))

### Color individual according to its clusters (col="clusters")
plot(ld,3,parTraj=parTRAJ(col="clusters"))

### Mean without individual
plot(ld,4,parTraj=parTRAJ(type="n"))

### No mean trajectories (type="n")
### Color individual according to its clusters (col="clusters")
plot(ld,3,parTraj=parTRAJ(col="clusters"),parMean=parMEAN(type="n"))

### Only few trajectories
plot(ld,4,nbSample=10,parTraj=parTRAJ(col='clusters'),parMean=parMEAN(type="n"))

### Go back to current dir
setwd(wd)

---

### Description

`plotMeans` plots the means' trajectories of an object `ClusterLongData` relatively to a `Partition`.

### Usage

```r
# S4 method for signature 'ClusterLongData,ANY'
plotMeans(x, y, parMean=parMEAN(),
          parWin=windowsCut(x["nbVar"], addLegend=TRUE), ...)
```

### Arguments

- `x` [ClusterLongData]: Object containing the trajectories to `plotMeans`.
- `y` [numeric] or [vector(numeric)]: Give the Partition to represent. If `y` is a number, the first Partition of the sublist `c-y` is selected. If `y` is a couple of numeric, the `y[2]`th Partition of the sublist `c-y[1]` is selected (so `y=c(2,3)` select the partition with 2 clusters, the third one).
- `parMean` [ParLongData]: Specification of the plotting parameters of the mean trajectories. Fields that can be changes are 'type','col','pch','pchPeriod' and 'cex'. See `ParLongData` for details.
parWin [parWindows]: Set the graphical display of the windows. See ParWindows for details.

... Some other parameters can be passed to the method.

Details

plotMeans plots the means’ trajectories of an object ClusterLongData relativly to the 'best' Partition, or to the Partition define by y.

Graphical option (col, type, pch, pchPeriod and cex) can be change using parMean. For more detail on parTraj and parMean, see object of class ParLongData.

See Also

Overview: kml-package
Classes : ClusterLongData
PlotMeans : plotMeans: overview, plotCriterion

Examples

### Move to tempdir
wd <- getwd()
setwd(tempdir()); getwd()

##################
### Construction of the data

ld <- gald(10)
kml(ld,3:4,2)

### Basic plotMeansting
plotMeans(ld,3)

### Go back to current dir
setwd(wd)

---

plotTraj,ClusterLongData

~ Function: plotTraj for ClusterLongData ~

Description

plotTraj plot the trajectories of an object ClusterLongData relativly to a Partition.

Usage

```
# S4 method for signature 'ClusterLongData,ANY'
plotTraj(x,y,parTraj=parTRAJ(col="clusters"),
         parWin=windowsCut(x["nbVar"],addLegend=TRUE),nbSample=1000,...)
```
**Arguments**

- **x** [ClusterLongData]: Object containing the trajectories to plotTraj.
- **y** [numeric] or [couple(numeric)]: Give the Partition to represent. If y is missing, the Partition with the highest quality criterion (the actif one) is selected. If y is a number, the first Partition of the sublist c-y is selected. If y is a couple of numeric, the y[2]th Partition of the sublist c-y[1] is selected (so y=c(2,3) select the partition with 2 clusters, the third one).
- **parTraj** [ParLongData]: Specification of the plotting parameters of the individual trajectories. Fields that can be changes are 'type','col','pch','xlab' and 'ylab'. In addition to the standard possible values, the option col="clusters" (the default) can be use to color the individual trajectories according to their clusters (exemple: parTraj=parTRAJ(type="o",col="clusters")). See ParLongData for details.
- **parWin** [parWindows]: Set the graphical display of the windows. See ParWindows for details.
- **nbSample** [numeric]: Graphical display of huge sample can be time consuming. This parameters fixe the maximum number of trajectories (randomly chosen) that will be drawn.
- ... Some other parameters can be passed to the method.

**Details**

plotTraj the trajectories of an object ClusterLongData relativly to the 'best' Partition, or to the Partition define by y.

Graphical option (col, type, pch and xlab) can be change using parTraj. For more detail on parTraj, see object of class ParLongData.

**See Also**

Overview: kml-package  
Classes : ClusterLongData  
PlotTraj : plotTraj: overview, plotCriterion

**Examples**

```r
### Move to tempdir  
wd <- getwd()
setwd(tempdir()); getwd()

########################
### Construction of the data  

ld <- gald()
kml(ld,3:4,1)

### Basic plotTrajting  
plotTraj(ld,3)
```
### Go back to current dir

`setwd(wd)`
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