# Package 'adamethods'

October 12, 2022

October 12, 2022
Type Package
Title Archetypoid Algorithms and Anomaly Detection
Version 1.2.1
<b>Date</b> 2020-08-04
Author Guillermo Vinue, Irene Epifanio
Maintainer Guillermo Vinue <guillermo.vinue@uv.es></guillermo.vinue@uv.es>
<b>Description</b> Collection of several algorithms to obtain archetypoids with small and large databases, and with both classical multivariate data and functional data (univariate and multivariate). Some of these algorithms also allow to detect anomalies (outliers). Please see Vinue and Epifanio (2020) <doi:10.1007 s11634-020-00412-9="">.</doi:10.1007>
License GPL (>= 2)
<pre>URL https://www.r-project.org</pre>
<b>Depends</b> R (>= $3.4.0$ )
<b>Imports</b> Anthropometry, archetypes, FNN, foreach, graphics, nnls, parallel, stats, tolerance, univOutl, utils
Suggests doParallel, fda
LazyData true
RoxygenNote 6.1.1
NeedsCompilation no
Repository CRAN
<b>Date/Publication</b> 2020-08-04 12:30:14 UTC
R topics documented:
adalara2adalara_no_paral5archetypoids_funct8archetypoids_funct_multiv9archetypoids_funct_multiv_robust11

2 adalara

	archetypoids_funct_robust	13
	archetypoids_norm_frob	15
	archetypoids_robust	16
	bisquare_function	17
	do_ada	18
	do_ada_robust	20
	do_alphas_rss	22
	do_alphas_rss_multiv	23
	do_clean	26
	do_clean_multiv	27
	do_fada	28
	do_fada_multiv	31
	do_fada_multiv_robust	33
	do_fada_robust	35
	do_knno	37
	do_outl_degree	38
	fadalara	39
	fadalara_no_paral	42
	<del></del>	45
	frobenius_norm	46
		47
	frobenius_norm_funct_multiv	48
		49
	frobenius_norm_funct_robust	50
	frobenius_norm_robust	51
	int_prod_mat	52
	int_prod_mat_funct	53
	int_prod_mat_sq	54
		54
	outl_toler	55
	stepArchetypesRawData_funct	56
	stepArchetypesRawData_funct_multiv	
	stepArchetypesRawData_funct_multiv_robust	
	stepArchetypesRawData_funct_robust	61
		63
	stepArchetypesRawData_robust	64
Index		66
adala	ra Multivariate parallel archetypoid algorithm for large applications	
	(ADALARA)	

adalara 3

## **Description**

The ADALARA algorithm is based on the CLARA clustering algorithm. This is the parallel version of the algorithm to try to get faster results. It allows to detect anomalies (outliers). There are two different methods to detect them: the adjusted boxplot (default and most reliable option) and tolerance intervals. If needed, tolerance intervals allow to define a degree of outlierness.

## Usage

#### **Arguments**

data Data matrix. Each row corresponds to an observation and each column corre-

sponds to a variable. All variables are numeric. The data must have row names

so that the algorithm can identify the archetypoids in every sample.

N Number of samples.

m Sample size of each sample.

numArchoid Number of archetypes/archetypoids.

numRep For each numArchoid, run the archetype algorithm numRep times. huge Penalization added to solve the convex least squares problems.

prob Probability with values in [0,1].

type\_alg String. Options are 'ada' for the non-robust adalara algorithm and 'ada\_rob' for

the robust adalara algorithm.

compare Boolean argument to compute the robust residual sum of squares if type\_alg =

"ada" and the non-robust if type\_alg = "ada\_rob".

vect\_tol Vector with the tolerance values. Default c(0.95, 0.9, 0.85). Needed if method='toler'.

alpha Significance level. Default 0.05. Needed if method='toler'.

outl\_degree Type of outlier to identify the degree of outlierness. Default c("outl\_strong",

"outl\_semi\_strong", "outl\_moderate"). Needed if method='toler'.

method Method to compute the outliers. Options allowed are 'adjbox' for using adjusted

boxplots for skewed distributions, and 'toler' for using tolerance intervals.

frame Boolean value to indicate whether the frame is computed (Mair et al., 2017) or

not. The frame is made up of a subset of extreme points, so the archetypoids are only computed on the frame. Low frame densities are obtained when only small portions of the data were extreme. However, high frame densities reduce

this speed-up.

#### Value

A list with the following elements:

- · cases Optimal vector of archetypoids.
- · rss Optimal residual sum of squares.
- outliers: Outliers.

4 adalara

#### Author(s)

Guillermo Vinue, Irene Epifanio

#### References

Eugster, M.J.A. and Leisch, F., From Spider-Man to Hero - Archetypal Analysis in R, 2009. *Journal of Statistical Software* **30(8)**, 1-23, https://doi.org/10.18637/jss.v030.i08

Hubert, M. and Vandervieren, E., An adjusted boxplot for skewed distributions, 2008. *Computational Statistics and Data Analysis* **52(12)**, 5186-5201, https://doi.org/10.1016/j.csda. 2007.11.008

Kaufman, L. and Rousseeuw, P.J., Clustering Large Data Sets, 1986. *Pattern Recognition in Practice*, 425-437.

Mair, S., Boubekki, A. and Brefeld, U., Frame-based Data Factorizations, 2017. Proceedings of the 34th International Conference on Machine Learning, Sydney, Australia, 1-9.

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

Vinue, G., Anthropometry: An R Package for Analysis of Anthropometric Data, 2017. *Journal of Statistical Software* **77(6)**, 1-39, https://doi.org/10.18637/jss.v077.i06

#### See Also

```
do_ada, do_ada_robust, adalara_no_paral
```

```
## Not run:
library(Anthropometry)
library(doParallel)
# Prepare parallelization (including the seed for reproducibility):
no_cores <- detectCores() - 1</pre>
cl <- makeCluster(no_cores)</pre>
registerDoParallel(cl)
clusterSetRNGStream(cl, iseed = 1)
# Load data:
data(mtcars)
data <- mtcars
n <- nrow(data)</pre>
# Arguments for the archetype/archetypoid algorithm:
# Number of archetypoids:
k <- 3
numRep <- 2
huge <- 200
# Size of the random sample of observations:
m <- 10
```

adalara\_no\_paral 5

```
# Number of samples:
N \leftarrow floor(1 + (n - m)/(m - k))
prob <- 0.75
# ADALARA algorithm:
preproc <- preprocessing(data, stand = TRUE, percAccomm = 1)</pre>
data1 <- as.data.frame(preproc$data)</pre>
adalara_aux <- adalara(data1, N, m, k, numRep, huge, prob,
                        "ada_rob", FALSE, method = "adjbox", frame = FALSE)
#adalara_aux <- adalara(data1, N, m, k, numRep, huge, prob,</pre>
                         "ada_rob", FALSE, vect_tol = c(0.95, 0.9, 0.85), alpha = 0.05,
#
                     outl_degree = c("outl_strong", "outl_semi_strong", "outl_moderate"),
#
                         method = "toler", frame = FALSE)
# Take the minimum RSS, which is in the second position of every sublist:
adalara <- adalara_aux[which.min(unlist(sapply(adalara_aux, function(x) x[2])))][[1]]
adalara
# End parallelization:
stopCluster(cl)
## End(Not run)
```

adalara\_no\_paral

Multivariate non-parallel archetypoid algorithm for large applications (ADALARA)

# Description

The ADALARA algorithm is based on the CLARA clustering algorithm. This is the non-parallel version of the algorithm. It allows to detect anomalies (outliers). There are two different methods to detect them: the adjusted boxplot (default and most reliable option) and tolerance intervals. If needed, tolerance intervals allow to define a degree of outlierness.

#### Usage

6 adalara\_no\_paral

## **Arguments**

data Data matrix. Each row corresponds to an observation and each column corre-

sponds to a variable. All variables are numeric. The data must have row names

so that the algorithm can identify the archetypoids in every sample.

seed Integer value to set the seed. This ensures reproducibility.

N Number of samples.

m Sample size of each sample.

numArchoid Number of archetypes/archetypoids.

numRep For each numArchoid, run the archetype algorithm numRep times.

huge Penalization added to solve the convex least squares problems.

prob Probability with values in [0,1].

type\_alg String. Options are 'ada' for the non-robust adalara algorithm and 'ada\_rob' for

the robust adalara algorithm.

compare Boolean argument to compute the robust residual sum of squares if type\_alg =

"ada" and the non-robust if type\_alg = "ada\_rob".

verbose Display progress? Default TRUE.

vect\_tol Vector the tolerance values. Default c(0.95, 0.9, 0.85). Needed if method='toler'.

alpha Significance level. Default 0.05. Needed if method='toler'.

outl\_degree Type of outlier to identify the degree of outlierness. Default c("outl\_strong",

"outl\_semi\_strong", "outl\_moderate"). Needed if method='toler'.

method Method to compute the outliers. Options allowed are 'adjbox' for using adjusted

boxplots for skewed distributions, and 'toler' for using tolerance intervals.

frame Boolean value to indicate whether the frame is computed (Mair et al., 2017) or

not. The frame is made up of a subset of extreme points, so the archetypoids are only computed on the frame. Low frame densities are obtained when only small portions of the data were extreme. However, high frame densities reduce

this speed-up.

# Value

A list with the following elements:

- · cases Optimal vector of archetypoids.
- rss Optimal residual sum of squares.
- outliers: Outliers.

#### Author(s)

Guillermo Vinue, Irene Epifanio

adalara\_no\_paral 7

#### References

Eugster, M.J.A. and Leisch, F., From Spider-Man to Hero - Archetypal Analysis in R, 2009. *Journal of Statistical Software* **30(8)**, 1-23, https://doi.org/10.18637/jss.v030.i08

Hubert, M. and Vandervieren, E., An adjusted boxplot for skewed distributions, 2008. *Computational Statistics and Data Analysis* **52(12)**, 5186-5201, https://doi.org/10.1016/j.csda. 2007.11.008

Kaufman, L. and Rousseeuw, P.J., Clustering Large Data Sets, 1986. *Pattern Recognition in Practice*, 425-437.

Mair, S., Boubekki, A. and Brefeld, U., Frame-based Data Factorizations, 2017. Proceedings of the 34th International Conference on Machine Learning, Sydney, Australia, 1-9.

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

Vinue, G., Anthropometry: An R Package for Analysis of Anthropometric Data, 2017. *Journal of Statistical Software* **77(6)**, 1-39, https://doi.org/10.18637/jss.v077.i06

#### See Also

```
do_ada, do_ada_robust, adalara
```

```
## Not run:
library(Anthropometry)
# Load data:
data(mtcars)
data <- mtcars
n <- nrow(data)</pre>
# Arguments for the archetype/archetypoid algorithm:
# Number of archetypoids:
k <- 3
numRep <- 2
huge <- 200
# Size of the random sample of observations:
# Number of samples:
N \leftarrow floor(1 + (n - m)/(m - k))
prob <- 0.75
# ADALARA algorithm:
preproc <- preprocessing(data, stand = TRUE, percAccomm = 1)</pre>
data1 <- as.data.frame(preproc$data)</pre>
res_adalara <- adalara_no_paral(data1, 1, N, m, k,
                                  numRep, huge, prob, "ada_rob", FALSE, TRUE,
```

8 archetypoids\_funct

archetypoids\_funct

Archetypoid algorithm with the functional Frobenius norm

# **Description**

Archetypoid algorithm with the functional Frobenius norm to be used with functional data.

## Usage

```
archetypoids_funct(numArchoid, data, huge = 200, ArchObj, PM)
```

## **Arguments**

numArchoid Number of archetypoids.

data Data matrix. Each row corresponds to an observation and each column corre-

sponds to a variable. All variables are numeric.

huge Penalization added to solve the convex least squares problems.

ArchObj The list object returned by the stepArchetypesRawData\_funct function.

PM Penalty matrix obtained with eval.penalty.

## Value

A list with the following elements:

- cases: Final vector of archetypoids.
- rss: Residual sum of squares corresponding to the final vector of archetypoids.
- archet\_ini: Vector of initial archetypoids.
- alphas: Alpha coefficients for the final vector of archetypoids.
- resid: Matrix with the residuals.

## Author(s)

Irene Epifanio

#### References

Epifanio, I., Functional archetype and archetypoid analysis, 2016. *Computational Statistics and Data Analysis* **104**, 24-34, https://doi.org/10.1016/j.csda.2016.06.007

#### See Also

archetypoids

# **Examples**

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- t(growth$hgtm)</pre>
# Create basis:
basis_fd <- create.bspline.basis(c(1,ncol(hgtm)), 10)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
temp_points <- 1:ncol(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = growth$hgtm, basisobj = basis_fd)</pre>
data_archs <- t(temp_fd$coefs)</pre>
lass <- stepArchetypesRawData_funct(data = data_archs, numArch = 3,</pre>
                                       numRep = 5, verbose = FALSE,
                                       saveHistory = FALSE, PM)
af <- archetypoids_funct(3, data_archs, huge = 200, ArchObj = lass, PM)</pre>
str(af)
## End(Not run)
```

archetypoids\_funct\_multiv

Archetypoid algorithm with the functional multivariate Frobenius norm

## Description

Archetypoid algorithm with the functional multivariate Frobenius norm to be used with functional data.

## Usage

```
archetypoids_funct_multiv(numArchoid, data, huge = 200, ArchObj, PM)
```

# **Arguments**

numArchoid Number of archetypoids.

data Data matrix. Each row corresponds to an observation and each column corre-

sponds to a variable. All variables are numeric.

huge Penalization added to solve the convex least squares problems.

ArchObj The list object returned by the stepArchetypesRawData\_funct function.

PM Penalty matrix obtained with eval.penalty.

#### Value

A list with the following elements:

• cases: Final vector of archetypoids.

• rss: Residual sum of squares corresponding to the final vector of archetypoids.

• archet\_ini: Vector of initial archetypoids.

• alphas: Alpha coefficients for the final vector of archetypoids.

• resid: Matrix with the residuals.

## Author(s)

Irene Epifanio

## References

Epifanio, I., Functional archetype and archetypoid analysis, 2016. *Computational Statistics and Data Analysis* **104**, 24-34, https://doi.org/10.1016/j.csda.2016.06.007

## See Also

archetypoids

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- growth$hgtm
hgtf <- growth$hgtf[,1:39]

# Create array:
nvars <- 2
data.array <- array(0, dim = c(dim(hgtm), nvars))
data.array[,,1] <- as.matrix(hgtm)
data.array[,,2] <- as.matrix(hgtf)
rownames(data.array) <- 1:nrow(hgtm)
colnames(data.array) <- colnames(hgtm)
str(data.array)</pre>
```

```
# Create basis:
nbasis <- 10
basis_fd <- create.bspline.basis(c(1,nrow(hgtm)), nbasis)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
temp_points <- 1:nrow(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = data.array, basisobj = basis_fd)</pre>
X <- array(0, dim = c(dim(t(temp_fd$coefs[,,1])), nvars))</pre>
X[,,1] \leftarrow t(temp_fd\$coef[,,1])
X[,,2] \leftarrow t(temp_fd\$coef[,,2])
# Standardize the variables:
Xs <- X
Xs[,,1] <- scale(X[,,1])
Xs[,,2] \leftarrow scale(X[,,2])
lass <- stepArchetypesRawData_funct_multiv(data = Xs, numArch = 3,</pre>
                                               numRep = 5, verbose = FALSE,
                                               saveHistory = FALSE, PM)
afm <- archetypoids_funct_multiv(3, Xs, huge = 200, ArchObj = lass, PM)</pre>
str(afm)
## End(Not run)
```

archetypoids\_funct\_multiv\_robust

Archetypoid algorithm with the functional multivariate robust Frobenius norm

# **Description**

Archetypoid algorithm with the functional multivariate robust Frobenius norm to be used with functional data.

# Usage

```
archetypoids_funct_multiv_robust(numArchoid, data, huge = 200, ArchObj, PM, prob)
```

# **Arguments**

numArchoid	Number of archetypoids.
data	Data matrix. Each row corresponds to an observation and each column corresponds to a variable. All variables are numeric.
huge	Penalization added to solve the convex least squares problems.
ArchObj	The list object returned by the stepArchetypesRawData_funct function.

```
PM Penalty matrix obtained with eval.penalty.

prob Probability with values in [0,1].
```

#### Value

A list with the following elements:

- cases: Final vector of archetypoids.
- rss: Residual sum of squares corresponding to the final vector of archetypoids.
- archet\_ini: Vector of initial archetypoids.
- alphas: Alpha coefficients for the final vector of archetypoids.
- resid: Matrix with the residuals.

#### Author(s)

Irene Epifanio

#### References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

#### See Also

```
archetypoids
```

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- growth$hgtm
hgtf <- growth$hgtf[,1:39]</pre>
# Create array:
nvars <- 2
data.array <- array(0, dim = c(dim(hgtm), nvars))</pre>
data.array[,,1] <- as.matrix(hgtm)</pre>
data.array[,,2] <- as.matrix(hgtf)</pre>
rownames(data.array) <- 1:nrow(hgtm)</pre>
colnames(data.array) <- colnames(hgtm)</pre>
str(data.array)
# Create basis:
nbasis <- 10
basis_fd <- create.bspline.basis(c(1,nrow(hgtm)), nbasis)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
```

```
temp_points <- 1:nrow(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = data.array, basisobj = basis_fd)</pre>
X <- array(0, dim = c(dim(t(temp_fd$coefs[,,1])), nvars))</pre>
X[,,1] \leftarrow t(temp_fd\$coef[,,1])
X[,,2] \leftarrow t(temp_fdscoef[,,2])
# Standardize the variables:
Xs <- X
Xs[,,1] \leftarrow scale(X[,,1])
Xs[,,2] \leftarrow scale(X[,,2])
lass <- stepArchetypesRawData_funct_multiv_robust(data = Xs, numArch = 3,</pre>
                                                       numRep = 5, verbose = FALSE,
                                                       saveHistory = FALSE, PM, prob = 0.8,
                                                       nbasis, nvars)
afmr <- archetypoids_funct_multiv_robust(3, Xs, huge = 200, ArchObj = lass, PM, 0.8)
str(afmr)
## End(Not run)
```

archetypoids\_funct\_robust

Archetypoid algorithm with the functional robust Frobenius norm

# Description

Archetypoid algorithm with the functional robust Frobenius norm to be used with functional data.

# Usage

```
archetypoids_funct_robust(numArchoid, data, huge = 200, ArchObj, PM, prob)
```

#### **Arguments**

numArchoid	Number of archetypoids.
data	Data matrix. Each row corresponds to an observation and each column corresponds to a variable. All variables are numeric.
huge	Penalization added to solve the convex least squares problems.
ArchObj	The list object returned by the $stepArchetypesRawData\_funct\_robust$ function.
PM	Penalty matrix obtained with eval.penalty.
prob	Probability with values in [0,1].

#### Value

A list with the following elements:

- cases: Final vector of archetypoids.
- rss: Residual sum of squares corresponding to the final vector of archetypoids.
- archet\_ini: Vector of initial archetypoids.
- alphas: Alpha coefficients for the final vector of archetypoids.
- resid: Matrix with the residuals.

# Author(s)

Irene Epifanio

#### References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

#### See Also

archetypoids

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- t(growth$hgtm)</pre>
# Create basis:
basis_fd <- create.bspline.basis(c(1,ncol(hgtm)), 10)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
temp_points <- 1:ncol(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = growth$hgtm, basisobj = basis_fd)</pre>
data_archs <- t(temp_fd$coefs)</pre>
lass <- stepArchetypesRawData_funct_robust(data = data_archs, numArch = 3,</pre>
                                              numRep = 5, verbose = FALSE,
                                              saveHistory = FALSE, PM, prob = 0.8)
afr <- archetypoids_funct_robust(3, data_archs, huge = 200, ArchObj = lass, PM, 0.8)
str(afr)
## End(Not run)
```

archetypoids\_norm\_frob

Archetypoid algorithm with the Frobenius norm

## Description

This function is the same as archetypoids but the 2-norm is replaced by the Frobenius norm. Thus, the comparison with the robust archetypoids can be directly made.

#### **Usage**

```
archetypoids_norm_frob(numArchoid, data, huge = 200, ArchObj)
```

#### **Arguments**

numArchoid Number of archetypoids.

data Data matrix. Each row corresponds to an observation and each column corre-

sponds to a variable. All variables are numeric.

huge Penalization added to solve the convex least squares problems.

ArchObj The list object returned by the stepArchetypesRawData\_norm\_frob function.

#### Value

A list with the following elements:

- cases: Final vector of archetypoids.
- rss: Residual sum of squares corresponding to the final vector of archetypoids.
- archet\_ini: Vector of initial archetypoids.
- alphas: Alpha coefficients for the final vector of archetypoids.
- resid: Matrix with the residuals.

## Author(s)

Irene Epifanio

#### References

Eugster, M.J.A. and Leisch, F., From Spider-Man to Hero - Archetypal Analysis in R, 2009. *Journal of Statistical Software* **30(8)**, 1-23, https://doi.org/10.18637/jss.v030.i08

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

Vinue, G., Epifanio, I., and Alemany, S., Archetypoids: a new approach to define representative archetypal data, 2015. *Computational Statistics and Data Analysis* 87, 102-115, https://doi.org/10.1016/j.csda.2015.01.018

Vinue, G., Anthropometry: An R Package for Analysis of Anthropometric Data, 2017. *Journal of Statistical Software* **77(6)**, 1-39, https://doi.org/10.18637/jss.v077.i06

16 archetypoids\_robust

## See Also

archetypoids

## **Examples**

archetypoids\_robust

Archetypoid algorithm with the robust Frobenius norm

## **Description**

Robust version of the archetypoid algorithm with the Frobenius form.

## Usage

```
archetypoids_robust(numArchoid, data, huge = 200, ArchObj, prob)
```

## **Arguments**

numArchoid Number of archetypoids.

data Data matrix. Each row corresponds to an observation and each column corre-

sponds to a variable. All variables are numeric.

huge Penalization added to solve the convex least squares problems.

ArchObj The list object returned by the stepArchetypesRawData\_robust function.

prob Probability with values in [0,1].

## Value

A list with the following elements:

- cases: Final vector of archetypoids.
- rss: Residual sum of squares corresponding to the final vector of archetypoids.

bisquare\_function 17

- archet\_ini: Vector of initial archetypoids.
- alphas: Alpha coefficients for the final vector of archetypoids.
- resid: Matrix with the residuals.

# Author(s)

Irene Epifanio

#### References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

#### See Also

```
archetypoids_norm_frob
```

# **Examples**

bisquare\_function

Bisquare function

# **Description**

This function belongs to the bisquare family of loss functions. The bisquare family can better cope with extreme outliers.

## Usage

```
bisquare_function(resid, prob, ...)
```

18 do\_ada

# **Arguments**

resid Vector of residuals, computed from the  $m \times n$  residuals data matrix.

probProbability with values in [0,1].Additional possible arguments.

#### Value

Vector of real numbers.

## Author(s)

Irene Epifanio

## References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

# **Examples**

```
resid <- c(2.47, 11.85)
bisquare_function(resid, 0.8)</pre>
```

do\_ada

Run the whole classical archetypoid analysis with the Frobenius norm

# **Description**

This function executes the entire procedure involved in the archetypoid analysis. Firstly, the initial vector of archetypoids is obtained using the archetypal algorithm and finally, the optimal vector of archetypoids is returned.

# Usage

do\_ada

## **Arguments**

subset Data to obtain archetypes. In ADALARA this is a subset of the entire data

frame.

numArchoid Number of archetypes/archetypoids.

numRep For each numArch, run the archetype algorithm numRep times. huge Penalization added to solve the convex least squares problems.

compare Boolean argument to compute the robust residual sum of squares to compare

these results with the ones provided by do\_ada\_robust.

vect\_tol Vector the tolerance values. Default c(0.95, 0.9, 0.85). Needed if method='toler'.

alpha Significance level. Default 0.05. Needed if method='toler'.

outl\_degree Type of outlier to identify the degree of outlierness. Default c("outl\_strong",

"outl\_semi\_strong", "outl\_moderate"). Needed if method='toler'.

method Method to compute the outliers. Options allowed are 'adjbox' for using adjusted

boxplots for skewed distributions, and 'toler' for using tolerance intervals.

prob If compare=TRUE, probability with values in [0,1].

#### Value

A list with the following elements:

- cases: Final vector of archetypoids.
- alphas: Alpha coefficients for the final vector of archetypoids.
- rss: Residual sum of squares corresponding to the final vector of archetypoids.
- rss\_rob: If compare=TRUE, this is the residual sum of squares using the robust Frobenius norm. Otherwise, NULL.
- resid: Vector with the residuals.
- outliers: Outliers.

## Author(s)

Guillermo Vinue, Irene Epifanio

## References

Eugster, M.J.A. and Leisch, F., From Spider-Man to Hero - Archetypal Analysis in R, 2009. *Journal of Statistical Software* **30(8)**, 1-23, https://doi.org/10.18637/jss.v030.i08

Vinue, G., Epifanio, I., and Alemany, S., Archetypoids: a new approach to define representative archetypal data, 2015. *Computational Statistics and Data Analysis* **87**, 102-115, https://doi.org/10.1016/j.csda.2015.01.018

Vinue, G., Anthropometry: An R Package for Analysis of Anthropometric Data, 2017. *Journal of Statistical Software* **77(6)**, 1-39, https://doi.org/10.18637/jss.v077.i06

## See Also

stepArchetypesRawData\_norm\_frob, archetypoids\_norm\_frob

20 do\_ada\_robust

## **Examples**

```
library(Anthropometry)
data(mtcars)
#data <- as.matrix(mtcars)</pre>
data <- mtcars
k <- 3
numRep <- 2
huge <- 200
preproc <- preprocessing(data, stand = TRUE, percAccomm = 1)</pre>
suppressWarnings(RNGversion("3.5.0"))
set.seed(2018)
res_ada <- do_ada(preproc$data, k, numRep, huge, FALSE, method = "adjbox")</pre>
str(res_ada)
res_ada1 <- do_ada(preproc$data, k, numRep, huge, FALSE,
                   vect_tol = c(0.95, 0.9, 0.85), alpha = 0.05,
                    outl_degree = c("outl_strong", "outl_semi_strong",
                                     "outl_moderate"), method = "toler")
str(res_ada1)
res_ada2 <- do_ada(preproc$data, k, numRep, huge, TRUE, method = "adjbox", prob = 0.8)
str(res_ada2)
```

do\_ada\_robust

Run the whole robust archetypoid analysis with the robust Frobenius norm

# **Description**

This function executes the entire procedure involved in the robust archetypoid analysis. Firstly, the initial vector of archetypoids is obtained using the robust archetypal algorithm and finally, the optimal vector of robust archetypoids is returned.

## Usage

# **Arguments**

subset Data to obtain archetypes. In ADALARA this is a subset of the entire data

frame.

numArchoid Number of archetypes/archetypoids.

do\_ada\_robust 21

For each numArch, run the archetype algorithm numRep times. numRep Penalization added to solve the convex least squares problems. huge Probability with values in [0,1]. prob compare Boolean argument to compute the non-robust residual sum of squares to compare these results with the ones provided by do\_ada. Vector the tolerance values. Default c(0.95, 0.9, 0.85). Needed if method='toler'. vect\_tol alpha Significance level. Default 0.05. Needed if method='toler'. outl\_degree Type of outlier to identify the degree of outlierness. Default c("outl\_strong", "outl\_semi\_strong", "outl\_moderate"). Needed if method='toler'. Method to compute the outliers. Options allowed are 'adjbox' for using adjusted method

boxplots for skewed distributions, and 'toler' for using tolerance intervals.

#### Value

A list with the following elements:

- cases: Final vector of archetypoids.
- alphas: Alpha coefficients for the final vector of archetypoids.
- rss: Residual sum of squares corresponding to the final vector of archetypoids.
- rss\_non\_rob: If compare=TRUE, this is the residual sum of squares using the non-robust Frobenius norm. Otherwise, NULL.
- resid Vector of residuals.
- outliers: Outliers.

## Author(s)

Guillermo Vinue, Irene Epifanio

# References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

#### See Also

stepArchetypesRawData\_robust, archetypoids\_robust

```
## Not run:
library(Anthropometry)
data(mtcars)
#data <- as.matrix(mtcars)
data <- mtcars
k <- 3</pre>
```

do\_alphas\_rss

do\_alphas\_rss

Alphas and RSS of every set of archetypoids

## Description

In the ADALARA algorithm, every time that a set of archetypoids is computed using a sample of the data, the alpha coefficients and the associated residual sum of squares (RSS) for the entire data set must be computed.

## Usage

#### **Arguments**

data Data matrix with all the observations.

subset Data matrix with a sample of the data observations.

huge Penalization added to solve the convex least squares problems.

k\_subset Archetypoids obtained from subset.
rand\_obs Sample observations that form subset.
alphas\_subset Alpha coefficients related to k\_subset.

type\_alg String. Options are 'ada' for the non-robust multivariate adalara algorithm,

'ada\_rob' for the robust multivariate adalara algorithm, 'fada' for the non-robust

fda fadalara algorithm and 'fada\_rob' for the robust fda fadalara algorithm.

PM Penalty matrix obtained with eval.penalty. Needed when type\_alg = 'fada'

or type\_alg = 'fada\_rob'.

prob Probability with values in [0,1]. Needed when type\_alg = 'ada\_rob' or type\_alg

= 'fada\_rob'.

do\_alphas\_rss\_multiv 23

# Value

A list with the following elements:

- rss Real number of the residual sum of squares.
- resid\_rss Matrix with the residuals.
- alphas Matrix with the alpha values.

#### Author(s)

Guillermo Vinue

#### See Also

```
archetypoids_norm_frob
```

# **Examples**

```
data(mtcars)
data <- mtcars
n <- nrow(data)</pre>
m <- 10
k <- 3
numRep <- 2
huge <- 200
suppressWarnings(RNGversion("3.5.0"))
set.seed(1)
rand_obs_si <- sample(1:n, size = m)</pre>
si <- data[rand_obs_si,]</pre>
ada_si <- do_ada(si, k, numRep, huge, FALSE)</pre>
k_si <- ada_si$cases
alphas_si <- ada_si$alphas</pre>
colnames(alphas_si) <- rownames(si)</pre>
rss_si <- do_alphas_rss(data, si, huge, k_si, rand_obs_si, alphas_si, "ada")</pre>
str(rss_si)
```

 ${\tt do\_alphas\_rss\_multiv} \quad \textit{Alphas and RSS of every set of multivariate archetypoids}$ 

# **Description**

In the ADALARA algorithm, every time that a set of archetypoids is computed using a sample of the data, the alpha coefficients and the associated residual sum of squares (RSS) for the entire data set must be computed.

24 do\_alphas\_rss\_multiv

## Usage

## Arguments

data Data matrix with all the observations.

subset Data matrix with a sample of the data observations.

huge Penalization added to solve the convex least squares problems.

k\_subset Archetypoids obtained from subset.
rand\_obs Sample observations that form subset.
alphas\_subset Alpha coefficients related to k\_subset.

type\_alg String. Options are 'ada' for the non-robust multivariate adalara algorithm,

'ada\_rob' for the robust multivariate adalara algorithm, 'fada' for the non-robust fda fadalara algorithm and 'fada\_rob' for the robust fda fadalara algorithm.

PM Penalty matrix obtained with eval.penalty. Needed when type\_alg = 'fada'

or type\_alg = 'fada\_rob'.

prob Probability with values in [0,1]. Needed when type\_alg = 'ada\_rob' or type\_alg

= 'fada\_rob'.

nbasis Number of basis.

nvars Number of variables.

## Value

A list with the following elements:

- rss Real number of the residual sum of squares.
- resid\_rss Matrix with the residuals.
- alphas Matrix with the alpha values.

#### Author(s)

Guillermo Vinue

## See Also

```
archetypoids_norm_frob
```

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- growth$hgtm
hgtf <- growth$hgtf[,1:39]</pre>
```

```
# Create array:
nvars <- 2
data.array <- array(0, dim = c(dim(hgtm), nvars))</pre>
data.array[,,1] <- as.matrix(hgtm)</pre>
data.array[,,2] <- as.matrix(hgtf)</pre>
rownames(data.array) <- 1:nrow(hgtm)</pre>
colnames(data.array) <- colnames(hgtm)</pre>
str(data.array)
# Create basis:
nbasis <- 10
basis_fd <- create.bspline.basis(c(1,nrow(hgtm)), nbasis)</pre>
PM <- eval.penalty(basis_fd)</pre>
# Make fd object:
temp_points <- 1:nrow(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = data.array, basisobj = basis_fd)</pre>
X <- array(0, dim = c(dim(t(temp_fd$coefs[,,1])), nvars))</pre>
X[,,1] \leftarrow t(temp_fd\$coef[,,1])
X[,,2] \leftarrow t(temp_fdscoef[,,2])
# Standardize the variables:
Xs <- X
Xs[,,1] \leftarrow scale(X[,,1])
Xs[,,2] \leftarrow scale(X[,,2])
# We have to give names to the dimensions to know the
# observations that were identified as archetypoids.
dimnames(Xs) <- list(paste("Obs", 1:dim(hgtm)[2], sep = ""),</pre>
                       1:nbasis,
                       c("boys", "girls"))
n \leftarrow dim(Xs)[1]
# Number of archetypoids:
k <- 3
numRep <- 20
huge <- 200
# Size of the random sample of observations:
m <- 15
# Number of samples:
N \leftarrow floor(1 + (n - m)/(m - k))
Ν
prob <- 0.75
data_alg <- Xs
nbasis <- dim(data_alg)[2] # number of basis.</pre>
nvars <- dim(data_alg)[3] # number of variables.</pre>
n <- nrow(data_alg)</pre>
suppressWarnings(RNGversion("3.5.0"))
set.seed(1)
rand_obs_si <- sample(1:n, size = m)</pre>
```

do\_clean

do\_clean

Cleaning outliers

# Description

Cleaning of the most remarkable outliers. This improves the performance of the archetypoid algorithm since it is not affected by spurious points.

# Usage

```
do_clean(data, num_pts, range = 1.5, out_perc = 80)
```

# **Arguments**

data	Data frame with (temporal) points in the rows and observations in the columns.
num_pts	Number of temporal points.
range	Same parameter as in function boxplot. A value of 1.5 is enough to detect amplitude and shift outliers, while a value of 3 is needed to detect isolated outliers.
out_perc	Minimum number of temporal points (in percentage) to consider the observation as an outlier. Needed when range=1.5.

## Value

Numeric vector with the outliers.

# Author(s)

Irene Epifanio

## See Also

boxplot

do\_clean\_multiv 27

# **Examples**

```
data(mtcars)
data <- mtcars
num_pts <- ncol(data)
do_clean(t(data), num_pts, 1.5, 80)</pre>
```

do\_clean\_multiv

Cleaning multivariate functional outliers

# Description

Cleaning of the most remarkable multivariate functional outliers. This improves the performance of the archetypoid algorithm since it is not affected by spurious points.

# Usage

```
do_clean_multiv(data, num_pts, range = 1.5, out_perc = 80, nbasis, nvars)
```

# Arguments

data	Data frame with (temporal) points in the rows and observations in the columns.
num_pts	Number of temporal points.
range	Same parameter as in function boxplot. A value of 1.5 is enough to detect amplitude and shift outliers, while a value of 3 is needed to detect isolated outliers.
out_perc	Minimum number of temporal points (in percentage) to consider the observation as an outlier. Needed when range=1.5.
nbasis	Number of basis.
nvars	Number of variables.

## Value

List with the outliers for each variable.

# Author(s)

Irene Epifanio

## See Also

boxplot

28 do\_fada

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- growth$hgtm
hgtf <- growth$hgtf[,1:39]</pre>
# Create array:
nvars <- 2
data.array <- array(0, dim = c(dim(hgtm), nvars))</pre>
data.array[,,1] <- as.matrix(hgtm)</pre>
data.array[,,2] <- as.matrix(hgtf)</pre>
rownames(data.array) <- 1:nrow(hgtm)</pre>
colnames(data.array) <- colnames(hgtm)</pre>
str(data.array)
# Create basis:
nbasis <- 10
basis_fd <- create.bspline.basis(c(1,nrow(hgtm)), nbasis)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
temp_points <- 1:nrow(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = data.array, basisobj = basis_fd)</pre>
X <- array(0, dim = c(dim(t(temp_fd$coefs[,,1])), nvars))</pre>
X[,,1] \leftarrow t(temp_fd\$coef[,,1])
X[,,2] \leftarrow t(temp_fdscoef[,,2])
# Standardize the variables:
Xs <- X
Xs[,,1] <- scale(X[,,1])
Xs[,,2] <- scale(X[,,2])
x1 <- t(Xs[,,1])
for (i in 2:nvars) {
x12 <- t(Xs[,,i])
x1 \leftarrow rbind(x1, x12)
data_all \leftarrow t(x1)
num_pts <- ncol(data_all) / nvars</pre>
range <- 3
outl <- do_clean_multiv(t(data_all), num_pts, range, out_perc, nbasis, nvars)
outl
## End(Not run)
```

do\_fada 29

do_fada	Run the whole functional archetypoid analysis with the Frobenius
	norm

## **Description**

This function executes the entire procedure involved in the functional archetypoid analysis. Firstly, the initial vector of archetypoids is obtained using the functional archetypal algorithm and finally, the optimal vector of archetypoids is returned.

## Usage

# **Arguments**

_	
subset	Data to obtain archetypes. In fadalara this is a subset of the entire data frame.
numArchoid	Number of archetypes/archetypoids.
numRep	For each numArch, run the archetype algorithm numRep times.
huge	Penalization added to solve the convex least squares problems.
compare	Boolean argument to compute the robust residual sum of squares to compare these results with the ones provided by do_fada_robust.
PM	Penalty matrix obtained with eval.penalty.
vect_tol	Vector the tolerance values. Default $c(0.95, 0.9, 0.85)$ . Needed if method='toler'
alpha	Significance level. Default 0.05. Needed if method='toler'.
outl_degree	Type of outlier to identify the degree of outlierness. Default c("outl_strong", "outl_semi_strong", "outl_moderate"). Needed if method='toler'.
method	Method to compute the outliers. Options allowed are 'adjbox' for using adjusted boxplots for skewed distributions, and 'toler' for using tolerance intervals.
prob	If compare=TRUE, probability with values in [0,1].

#### Value

A list with the following elements:

- cases: Final vector of archetypoids.
- alphas: Alpha coefficients for the final vector of archetypoids.
- rss: Residual sum of squares corresponding to the final vector of archetypoids.
- rss\_rob: If compare\_robust=TRUE, this is the residual sum of squares using the robust Frobenius norm. Otherwise, NULL.
- resid: Vector of residuals.
- outliers: Outliers.

do\_fada

#### Author(s)

Guillermo Vinue, Irene Epifanio

#### References

Epifanio, I., Functional archetype and archetypoid analysis, 2016. *Computational Statistics and Data Analysis* **104**, 24-34, https://doi.org/10.1016/j.csda.2016.06.007

#### See Also

stepArchetypesRawData\_funct, archetypoids\_funct

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- t(growth$hgtm)</pre>
# Create basis:
basis_fd <- create.bspline.basis(c(1,ncol(hgtm)), 10)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
temp_points <- 1:ncol(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = growth$hgtm, basisobj = basis_fd)</pre>
data_archs <- t(temp_fd$coefs)</pre>
suppressWarnings(RNGversion("3.5.0"))
set.seed(2018)
res_fada <- do_fada(subset = data_archs, numArchoid = 3, numRep = 5, huge = 200,
                    compare = FALSE, PM = PM, method = "adjbox")
str(res_fada)
suppressWarnings(RNGversion("3.5.0"))
set.seed(2018)
res_fada1 <- do_fada(subset = data_archs, numArchoid = 3, numRep = 5, huge = 200,
                     compare = FALSE, PM = PM,
                      vect_tol = c(0.95, 0.9, 0.85), alpha = 0.05,
                     outl_degree = c("outl_strong", "outl_semi_strong", "outl_moderate"),
                     method = "toler")
str(res_fada1)
res_fada2 <- do_fada(subset = data_archs, numArchoid = 3, numRep = 5, huge = 200,
                     compare = TRUE, PM = PM, method = "adjbox", prob = 0.8)
str(res_fada2)
## End(Not run)
```

do\_fada\_multiv 31

do_fada_multiv	Run the whole archetypoid analysis with the functional multivariate Frobenius norm
----------------	--

# **Description**

This function executes the entire procedure involved in the functional archetypoid analysis. Firstly, the initial vector of archetypoids is obtained using the functional archetypal algorithm and finally, the optimal vector of archetypoids is returned.

# Usage

# **Arguments**

subset	Data to obtain archetypes. In fadalara this is a subset of the entire data frame.
numArchoid	Number of archetypes/archetypoids.
numRep	For each numArch, run the archetype algorithm numRep times.
huge	Penalization added to solve the convex least squares problems.
compare	Boolean argument to compute the robust residual sum of squares to compare these results with the ones provided by do_fada_robust.
PM	Penalty matrix obtained with eval.penalty.
method	Method to compute the outliers. So far the only option allowed is 'adjbox' for using adjusted boxplots for skewed distributions. The use of tolerance intervals might also be explored in the future for the multivariate case.
prob	If compare=TRUE, probability with values in [0,1].

#### Value

A list with the following elements:

- cases: Final vector of archetypoids.
- alphas: Alpha coefficients for the final vector of archetypoids.
- rss: Residual sum of squares corresponding to the final vector of archetypoids.
- rss\_rob: If compare\_robust=TRUE, this is the residual sum of squares using the robust Frobenius norm. Otherwise, NULL.
- resid: Vector of residuals.
- outliers: Outliers.

## Author(s)

Guillermo Vinue, Irene Epifanio

32 do\_fada\_multiv

## References

Epifanio, I., Functional archetype and archetypoid analysis, 2016. *Computational Statistics and Data Analysis* **104**, 24-34, https://doi.org/10.1016/j.csda.2016.06.007

#### See Also

stepArchetypesRawData\_funct\_multiv, archetypoids\_funct\_multiv

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- growth$hgtm
hgtf <- growth$hgtf[,1:39]</pre>
# Create array:
nvars <- 2
data.array <- array(0, dim = c(dim(hgtm), nvars))</pre>
data.array[,,1] <- as.matrix(hgtm)</pre>
data.array[,,2] <- as.matrix(hgtf)</pre>
rownames(data.array) <- 1:nrow(hgtm)</pre>
colnames(data.array) <- colnames(hgtm)</pre>
str(data.array)
# Create basis:
nbasis <- 10
basis_fd <- create.bspline.basis(c(1,nrow(hgtm)), nbasis)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
temp_points <- 1:nrow(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = data.array, basisobj = basis_fd)</pre>
X <- array(0, dim = c(dim(t(temp_fd$coefs[,,1])), nvars))</pre>
X[,,1] \leftarrow t(temp_fd\$coef[,,1])
X[,,2] \leftarrow t(temp_fd\$coef[,,2])
# Standardize the variables:
Xs <- X
Xs[,,1] \leftarrow scale(X[,,1])
Xs[,,2] <- scale(X[,,2])
suppressWarnings(RNGversion("3.5.0"))
set.seed(2018)
res_fada <- do_fada_multiv(subset = Xs, numArchoid = 3, numRep = 5, huge = 200,
                             compare = FALSE, PM = PM, method = "adjbox")
str(res_fada)
## End(Not run)
```

do\_fada\_multiv\_robust Run the whole archetypoid analysis with the functional multivariate robust Frobenius norm

# **Description**

This function executes the entire procedure involved in the functional archetypoid analysis. Firstly, the initial vector of archetypoids is obtained using the functional archetypal algorithm and finally, the optimal vector of archetypoids is returned.

# Usage

#### **Arguments**

subset	Data to obtain archetypes. In fadalara this is a subset of the entire data frame.
numArchoid	Number of archetypes/archetypoids.
numRep	For each numArch, run the archetype algorithm numRep times.
huge	Penalization to solve the convex least squares problem, see archetypoids.
prob	Probability with values in [0,1].
compare	Boolean argument to compute the non-robust residual sum of squares to compare these results with the ones provided by do_fada.
PM	Penalty matrix obtained with eval.penalty.
method	Method to compute the outliers. So far the only option allowed is 'adjbox' for using adjusted boxplots for skewed distributions. The use of tolerance intervals might also be explored in the future for the multivariate case.

#### Value

A list with the following elements:

- cases: Final vector of archetypoids.
- alphas: Alpha coefficients for the final vector of archetypoids.
- rss: Residual sum of squares corresponding to the final vector of archetypoids.
- rss\_non\_rob: If compare=TRUE, this is the residual sum of squares using the non-robust Frobenius norm. Otherwise, NULL.
- resid Vector of residuals.
- outliers: Outliers.
- local\_rel\_imp Matrix with the local (casewise) relative importance (in percentage) of each variable for the outlier identification. Only for the multivariate case. It is relative to the outlier observation itself. The other observations are not considered for computing this importance. This procedure works because the functional variables are in the same scale, after standardizing. Otherwise, it couldn't be interpreted like that.

• margi\_rel\_imp Matrix with the marginal relative importance of each variable (in percentage) for the outlier identification. Only for the multivariate case. In this case, the other points are considered, since the value of the outlier observation is compared with the remaining points.

## Author(s)

Guillermo Vinue, Irene Epifanio

#### References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

#### See Also

stepArchetypesRawData\_funct\_multiv\_robust, archetypoids\_funct\_multiv\_robust

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- growth$hgtm
hgtf <- growth$hgtf[,1:39]</pre>
# Create array:
nvars <- 2
data.array <- array(0, dim = c(dim(hgtm), nvars))</pre>
data.array[,,1] <- as.matrix(hgtm)</pre>
data.array[,,2] <- as.matrix(hgtf)</pre>
rownames(data.array) <- 1:nrow(hgtm)</pre>
colnames(data.array) <- colnames(hgtm)</pre>
str(data.array)
# Create basis:
nbasis <- 10
basis_fd <- create.bspline.basis(c(1,nrow(hgtm)), nbasis)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
temp_points <- 1:nrow(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = data.array, basisobj = basis_fd)</pre>
X <- array(0, dim = c(dim(t(temp_fd$coefs[,,1])), nvars))</pre>
X[,,1] \leftarrow t(temp_fd\$coef[,,1])
X[,,2] \leftarrow t(temp_fd\$coef[,,2])
# Standardize the variables:
Xs <- X
Xs[,,1] \leftarrow scale(X[,,1])
Xs[,,2] \leftarrow scale(X[,,2])
```

do\_fada\_robust 35

do\_fada\_robust

Run the whole archetypoid analysis with the functional robust Frobenius norm

# **Description**

This function executes the entire procedure involved in the functional archetypoid analysis. Firstly, the initial vector of archetypoids is obtained using the functional archetypal algorithm and finally, the optimal vector of archetypoids is returned.

# Usage

# Arguments

subset	Data to obtain archetypes. In fadalara this is a subset of the entire data frame.
numArchoid	Number of archetypes/archetypoids.
numRep	For each numArch, run the archetype algorithm numRep times.
huge	Penalization added to solve the convex least squares problems.
prob	Probability with values in [0,1].
compare	Boolean argument to compute the non-robust residual sum of squares to compare these results with the ones provided by do_fada.
PM	Penalty matrix obtained with eval.penalty.
vect_tol	Vector the tolerance values. Default $c(0.95, 0.9, 0.85)$ . Needed if method='toler'
alpha	Significance level. Default 0.05. Needed if method='toler'.
outl_degree	Type of outlier to identify the degree of outlierness. Default c("outl_strong", "outl_semi_strong", "outl_moderate"). Needed if method='toler'.
method	Method to compute the outliers. Options allowed are 'adjbox' for using adjusted

boxplots for skewed distributions, and 'toler' for using tolerance intervals.

36 do\_fada\_robust

#### Value

A list with the following elements:

- cases: Final vector of archetypoids.
- alphas: Alpha coefficients for the final vector of archetypoids.
- rss: Residual sum of squares corresponding to the final vector of archetypoids.
- rss\_non\_rob: If compare=TRUE, this is the residual sum of squares using the non-robust Frobenius norm. Otherwise, NULL.
- resid: Vector of residuals.
- outliers: Outliers.

# Author(s)

Guillermo Vinue, Irene Epifanio

#### References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

## See Also

 $step Archetypes Raw Data\_funct\_robust, archetypoids\_funct\_robust$ 

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- t(growth$hgtm)</pre>
# Create basis:
basis_fd <- create.bspline.basis(c(1,ncol(hgtm)), 10)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
temp_points <- 1:ncol(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = growth$hgtm, basisobj = basis_fd)</pre>
data_archs <- t(temp_fd$coefs)</pre>
suppressWarnings(RNGversion("3.5.0"))
set.seed(2018)
res_fada_rob <- do_fada_robust(subset = data_archs, numArchoid = 3, numRep = 5, huge = 200,
                                 prob = 0.75, compare = FALSE, PM = PM, method = "adjbox")
str(res_fada_rob)
suppressWarnings(RNGversion("3.5.0"))
set.seed(2018)
res_fada_rob1 <- do_fada_robust(subset = data_archs, numArchoid = 3, numRep = 5, huge = 200,</pre>
```

do\_knno

do\_knno

kNN for outlier detection

# Description

Ramaswamy et al. proposed the k-nearest neighbors outlier detection method (kNNo). Each point's anomaly score is the distance to its kth nearest neighbor in the data set. Then, all points are ranked based on this distance. The higher an example's score is, the more anomalous it is.

# Usage

```
do_knno(data, k, top_n)
```

# Arguments

data Data observations.

k Number of neighbors of a point that we are interested in.

top\_n Total number of outliers we are interested in.

### Value

Vector of outliers.

#### Author(s)

Guillermo Vinue

#### References

Ramaswamy, S., Rastogi, R. and Shim, K. Efficient Algorithms for Mining Outliers from Large Data Sets. SIGMOD'00 Proceedings of the 2000 ACM SIGMOD international conference on Management of data, 2000, 427-438.

```
data(mtcars)
data <- as.matrix(mtcars)
outl <- do_knno(data, 3, 2)
outl
data[outl,]</pre>
```

do\_outl\_degree

do_outl_degree
----------------

# **Description**

Classification of outliers according to their degree of outlierness. They are classified using the tolerance proportion. For instance, outliers from a 95

### Usage

# Arguments

vect\_tol Vector the tolerance values. Default c(0.95, 0.9, 0.85).

resid\_vect Vector of n residuals, where n was the number of rows of the data matrix.

alpha Significance level. Default 0.05.

outl\_degree Type of outlier to identify the degree of outlierness. Default c("outl\_strong",

"outl\_semi\_strong", "outl\_moderate").

### Value

List with the type outliers.

# Author(s)

Guillermo Vinue

### See Also

```
outl_toler
```

```
do_outl_degree(0.95, 1:100, 0.05, "outl_strong")
```

fadalara 39

fadalara	Functional parallel archetypoid algorithm for large applications (FADALARA)

# Description

The FADALARA algorithm is based on the CLARA clustering algorithm. This is the parallel version of the algorithm. It allows to detect anomalies (outliers). In the univariate case, there are two different methods to detect them: the adjusted boxplot (default and most reliable option) and tolerance intervals. In the multivariate case, only adjusted boxplots are used. If needed, tolerance intervals allow to define a degree of outlierness.

# Usage

# Arguments

data	Data matrix. Each row corresponds to an observation and each column corresponds to a variable. All variables are numeric. The data must have row names so that the algorithm can identify the archetypoids in every sample.
N	Number of samples.
m	Sample size of each sample.
numArchoid	Number of archetypes/archetypoids.
numRep	For each numArch, run the archetype algorithm numRep times.
huge	Penalization added to solve the convex least squares problems.
prob	Probability with values in [0,1].
type_alg	String. Options are 'fada' for the non-robust fadalara algorithm, whereas 'fada_rob' is for the robust fadalara algorithm.
compare	Boolean argument to compute the robust residual sum of squares if type_alg = "fada" and the non-robust if type_alg = "fada_rob".
PM	Penalty matrix obtained with eval.penalty.
vect_tol	Vector the tolerance values. Default $c(0.95, 0.9, 0.85)$ . Needed if method='toler'.
alpha	Significance level. Default 0.05. Needed if method='toler'.
outl_degree	Type of outlier to identify the degree of outlierness. Default c("outl_strong", "outl_semi_strong", "outl_moderate"). Needed if method='toler'.
method	Method to compute the outliers. Options allowed are 'adjbox' for using adjusted boxplots for skewed distributions, and 'toler' for using tolerance intervals. The tolerance intervals are only computed in the univariate case, i.e., method='toler' only valid if multiv=FALSE.

40 fadalara

multiv

Multivariate (TRUE) or univariate (FALSE) algorithm.

frame

Boolean value to indicate whether the frame is computed (Mair et al., 2017) or not. The frame is made up of a subset of extreme points, so the archetypoids are only computed on the frame. Low frame densities are obtained when only small portions of the data were extreme. However, high frame densities reduce this speed-up.

#### Value

A list with the following elements:

- · cases Vector of archetypoids.
- rss Optimal residual sum of squares.
- · outliers: Outliers.
- alphas: Matrix with the alpha coefficients.
- local\_rel\_imp Matrix with the local (casewise) relative importance (in percentage) of each variable for the outlier identification. Only for the multivariate case. It is relative to the outlier observation itself. The other observations are not considered for computing this importance. This procedure works because the functional variables are in the same scale, after standardizing. Otherwise, it couldn't be interpreted like that.
- margi\_rel\_imp Matrix with the marginal relative importance of each variable (in percentage)
  for the outlier identification. Only for the multivariate case. In this case, the other points are
  considered, since the value of the outlier observation is compared with the remaining points.

# Author(s)

Guillermo Vinue, Irene Epifanio

#### References

Epifanio, I., Functional archetype and archetypoid analysis, 2016. *Computational Statistics and Data Analysis* **104**, 24-34, https://doi.org/10.1016/j.csda.2016.06.007

Hubert, M. and Vandervieren, E., An adjusted boxplot for skewed distributions, 2008. *Computational Statistics and Data Analysis* **52(12)**, 5186-5201, https://doi.org/10.1016/j.csda. 2007.11.008

Kaufman, L. and Rousseeuw, P.J., Clustering Large Data Sets, 1986. *Pattern Recognition in Practice*, 425-437.

Mair, S., Boubekki, A. and Brefeld, U., Frame-based Data Factorizations, 2017. Proceedings of the 34th International Conference on Machine Learning, Sydney, Australia, 1-9.

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

# See Also

do\_fada, do\_fada\_robust

fadalara 41

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- growth$hgtm</pre>
hgtf <- growth$hgtf[,1:39]</pre>
# Create array:
nvars <- 2
data.array <- array(0, dim = c(dim(hgtm), nvars))</pre>
data.array[,,1] <- as.matrix(hgtm)</pre>
data.array[,,2] <- as.matrix(hgtf)</pre>
rownames(data.array) <- 1:nrow(hgtm)</pre>
colnames(data.array) <- colnames(hgtm)</pre>
str(data.array)
# Create basis:
nbasis <- 10
basis_fd <- create.bspline.basis(c(1,nrow(hgtm)), nbasis)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
temp_points <- 1:nrow(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = data.array, basisobj = basis_fd)</pre>
X <- array(0, dim = c(dim(t(temp_fd$coefs[,,1])), nvars))</pre>
X[,,1] \leftarrow t(temp_fd\$coef[,,1])
X[,,2] \leftarrow t(temp_fd\$coef[,,2])
# Standardize the variables:
Xs <- X
Xs[,,1] <- scale(X[,,1])
Xs[,,2] \leftarrow scale(X[,,2])
# We have to give names to the dimensions to know the
# observations that were identified as archetypoids.
dimnames(Xs) <- list(paste("Obs", 1:dim(hgtm)[2], sep = ""),</pre>
                       1:nbasis,
                       c("boys", "girls"))
n \leftarrow dim(Xs)[1]
# Number of archetypoids:
k <- 3
numRep <- 20
huge <- 200
# Size of the random sample of observations:
# Number of samples:
N \leftarrow floor(1 + (n - m)/(m - k))
prob <- 0.75
data_alg <- Xs
```

42 fadalara\_no\_paral

```
# Parallel:
# Prepare parallelization (including the seed for reproducibility):
library(doParallel)
no_cores <- detectCores() - 1</pre>
no_cores
cl <- makeCluster(no_cores)</pre>
registerDoParallel(cl)
clusterSetRNGStream(cl, iseed = 2018)
res_fl <- fadalara(data = data_alg, N = N, m = m, numArchoid = k, numRep = numRep,
                   huge = huge, prob = prob, type_alg = "fada_rob", compare = FALSE,
                  PM = PM, method = "adjbox", multiv = TRUE, frame = FALSE) # frame = TRUE
stopCluster(cl)
res_fl_copy <- res_fl
res_fl <- res_fl[which.min(unlist(sapply(res_fl, function(x) x[2])))][[1]]</pre>
str(res_fl)
res_fl$cases
res_fl$rss
as.vector(res_fl$outliers)
## End(Not run)
```

fadalara\_no\_paral

Functional non-parallel archetypoid algorithm for large applications (FADALARA)

# **Description**

The FADALARA algorithm is based on the CLARA clustering algorithm. This is the non-parallel version of the algorithm. It allows to detect anomalies (outliers). In the univariate case, there are two different methods to detect them: the adjusted boxplot (default and most reliable option) and tolerance intervals. In the multivariate case, only adjusted boxplots are used. If needed, tolerance intervals allow to define a degree of outlierness.

### **Usage**

### **Arguments**

data

Data matrix. Each row corresponds to an observation and each column corresponds to a variable (temporal point). All variables are numeric. The data must have row names so that the algorithm can identify the archetypoids in every sample.

fadalara\_no\_paral 43

seed Integer value to set the seed. This ensures reproducibility.

N Number of samples.

m Sample size of each sample.

numArchoid Number of archetypes/archetypoids.

numRep For each numArch, run the archetype algorithm numRep times. huge Penalization added to solve the convex least squares problems.

prob Probability with values in [0,1].

type\_alg String. Options are 'fada' for the non-robust fadalara algorithm, whereas 'fada\_rob'

is for the robust fadalara algorithm.

compare Boolean argument to compute the robust residual sum of squares if type\_alg =

"fada" and the non-robust if type\_alg = "fada\_rob".

verbose Display progress? Default TRUE.

PM Penalty matrix obtained with eval.penalty.

vect\_tol Vector the tolerance values. Default c(0.95, 0.9, 0.85). Needed if method='toler'.

alpha Significance level. Default 0.05. Needed if method='toler'.

outl\_degree Type of outlier to identify the degree of outlierness. Default c("outl\_strong",

"outl\_semi\_strong", "outl\_moderate"). Needed if method='toler'.

method Method to compute the outliers. Options allowed are 'adjbox' for using ad-

justed boxplots for skewed distributions, and 'toler' for using tolerance intervals. The tolerance intervals are only computed in the univariate case, i.e.,

method='toler' only valid if multiv = FALSE.

multiv Multivariate (TRUE) or univariate (FALSE) algorithm.

frame Boolean value to indicate whether the frame is computed (Mair et al., 2017) or

not. The frame is made up of a subset of extreme points, so the archetypoids are only computed on the frame. Low frame densities are obtained when only small portions of the data were extreme. However, high frame densities reduce

this speed-up.

### Value

A list with the following elements:

- cases Vector of archetypoids.
- rss Optimal residual sum of squares.
- outliers: Vector of outliers.
- alphas: Matrix with the alpha coefficients.
- local\_rel\_imp Matrix with the local (casewise) relative importance (in percentage) of each variable for the outlier identification. Only for the multivariate case. It is relative to the outlier observation itself. The other observations are not considered for computing this importance. This procedure works because the functional variables are in the same scale, after standardizing. Otherwise, it couldn't be interpreted like that.
- margi\_rel\_imp Matrix with the marginal relative importance of each variable (in percentage) for the outlier identification. Only for the multivariate case. In this case, the other points are considered, since the value of the outlier observation is compared with the remaining points.

44 fadalara\_no\_paral

### Author(s)

Guillermo Vinue, Irene Epifanio

#### References

Epifanio, I., Functional archetype and archetypoid analysis, 2016. *Computational Statistics and Data Analysis* **104**, 24-34, https://doi.org/10.1016/j.csda.2016.06.007

Hubert, M. and Vandervieren, E., An adjusted boxplot for skewed distributions, 2008. *Computational Statistics and Data Analysis* **52(12)**, 5186-5201, https://doi.org/10.1016/j.csda. 2007.11.008

Kaufman, L. and Rousseeuw, P.J., Clustering Large Data Sets, 1986. *Pattern Recognition in Practice*, 425-437.

Mair, S., Boubekki, A. and Brefeld, U., Frame-based Data Factorizations, 2017. Proceedings of the 34th International Conference on Machine Learning, Sydney, Australia, 1-9.

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

#### See Also

fadalara

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- growth$hgtm
hgtf <- growth$hgtf[,1:39]</pre>
# Create array:
nvars <- 2
data.array <- array(0, dim = c(dim(hgtm), nvars))</pre>
data.array[,,1] <- as.matrix(hgtm)</pre>
data.array[,,2] <- as.matrix(hgtf)</pre>
rownames(data.array) <- 1:nrow(hgtm)</pre>
colnames(data.array) <- colnames(hgtm)</pre>
str(data.array)
# Create basis:
nbasis <- 10
basis_fd <- create.bspline.basis(c(1,nrow(hgtm)), nbasis)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
temp_points <- 1:nrow(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = data.array, basisobj = basis_fd)</pre>
X <- array(0, dim = c(dim(t(temp_fd$coefs[,,1])), nvars))</pre>
```

frame\_in\_r 45

```
X[,,1] \leftarrow t(temp_fd\$coef[,,1])
X[,,2] \leftarrow t(temp_fd\$coef[,,2])
# Standardize the variables:
Xs <- X
Xs[,,1] \leftarrow scale(X[,,1])
Xs[,,2] \leftarrow scale(X[,,2])
# We have to give names to the dimensions to know the
# observations that were identified as archetypoids.
dimnames(Xs) <- list(paste("Obs", 1:dim(hgtm)[2], sep = ""),</pre>
                      1:nbasis,
                      c("boys", "girls"))
n \leftarrow dim(Xs)[1]
# Number of archetypoids:
k <- 3
numRep <- 20
huge <- 200
# Size of the random sample of observations:
# Number of samples:
N \leftarrow floor(1 + (n - m)/(m - k))
prob <- 0.75
data_alg <- Xs
seed <- 2018
res_fl \leftarrow fadalara_no_paral(data = data_alg, seed = seed, N = N, m = m,
                              numArchoid = k, numRep = numRep, huge = huge,
                              prob = prob, type_alg = "fada_rob", compare = FALSE,
                              verbose = TRUE, PM = PM, method = "adjbox", multiv = TRUE,
                              frame = FALSE) # frame = TRUE
str(res_fl)
res_fl$cases
res_fl$rss
as.vector(res_fl$outliers)
## End(Not run)
```

frame\_in\_r

Compute archetypes frame

# **Description**

Computing the frame with the approach by Mair et al. (2017).

46 frobenius\_norm

# Usage

```
frame_in_r(X)
```

# Arguments

Χ

Data frame.

# Value

Vector with the observations that belong to the frame.

# Author(s)

Sebastian Mair, code kindly provided by him.

# References

Mair, S., Boubekki, A. and Brefeld, U., Frame-based Data Factorizations, 2017. Proceedings of the 34th International Conference on Machine Learning, Sydney, Australia, 1-9.

# **Examples**

```
## Not run:
X <- mtcars
q <- frame_in_r(X)
H <- X[q,]
q
## End(Not run)</pre>
```

frobenius\_norm

Frobenius norm

# Description

Computes the Frobenius norm.

# Usage

```
frobenius_norm(m)
```

# **Arguments**

m

Data matrix with the residuals. This matrix has the same dimensions as the original data matrix.

frobenius\_norm\_funct 47

### **Details**

Residuals are vectors. If there are p variables (columns), for every observation there is a residual that there is a p-dimensional vector. If there are n observations, the residuals are an n times p matrix.

### Value

Real number.

#### Author(s)

Guillermo Vinue, Irene Epifanio

#### References

Eugster, M.J.A. and Leisch, F., From Spider-Man to Hero - Archetypal Analysis in R, 2009. *Journal of Statistical Software* **30(8)**, 1-23, https://doi.org/10.18637/jss.v030.i08

Vinue, G., Epifanio, I., and Alemany, S., Archetypoids: a new approach to define representative archetypal data, 2015. *Computational Statistics and Data Analysis* 87, 102-115, https://doi.org/10.1016/j.csda.2015.01.018

Vinue, G., Anthropometry: An R Package for Analysis of Anthropometric Data, 2017. *Journal of Statistical Software* **77(6)**, 1-39, https://doi.org/10.18637/jss.v077.i06

# **Examples**

```
mat <- matrix(1:4, nrow = 2)
frobenius_norm(mat)</pre>
```

frobenius\_norm\_funct Functional Frobenius norm

# **Description**

Computes the functional Frobenius norm.

# Usage

```
frobenius_norm_funct(m, PM)
```

### **Arguments**

Data matrix with the residuals. This matrix has the same dimensions as the

original data matrix.

PM Penalty matrix obtained with eval.penalty.

### **Details**

Residuals are vectors. If there are p variables (columns), for every observation there is a residual that there is a p-dimensional vector. If there are n observations, the residuals are an n times p matrix.

#### Value

Real number.

#### Author(s)

Irene Epifanio

### References

Epifanio, I., Functional archetype and archetypoid analysis, 2016. *Computational Statistics and Data Analysis* **104**, 24-34, https://doi.org/10.1016/j.csda.2016.06.007

# **Examples**

```
library(fda)
mat <- matrix(1:9, nrow = 3)
fbasis <- create.fourier.basis(rangeval = c(1, 32), nbasis = 3)
PM <- eval.penalty(fbasis)
frobenius_norm_funct(mat, PM)</pre>
```

```
frobenius_norm_funct_multiv
```

Functional multivariate Frobenius norm

### **Description**

Computes the functional multivariate Frobenius norm.

# Usage

```
frobenius_norm_funct_multiv(m, PM)
```

### **Arguments**

m Data matrix with the residuals. This matrix has the same dimensions as the

original data matrix.

PM Penalty matrix obtained with eval.penalty.

### **Details**

Residuals are vectors. If there are p variables (columns), for every observation there is a residual that there is a p-dimensional vector. If there are n observations, the residuals are an n times p matrix.

# Value

Real number.

### Author(s)

Irene Epifanio

#### References

Epifanio, I., Functional archetype and archetypoid analysis, 2016. *Computational Statistics and Data Analysis* **104**, 24-34, https://doi.org/10.1016/j.csda.2016.06.007

### **Examples**

```
mat <- matrix(1:400, ncol = 20)
PM <- matrix(1:100, ncol = 10)
frobenius_norm_funct_multiv(mat, PM)</pre>
```

frobenius\_norm\_funct\_multiv\_robust

Functional multivariate robust Frobenius norm

# **Description**

Computes the functional multivariate robust Frobenius norm.

### Usage

```
frobenius_norm_funct_multiv_robust(m, PM, prob, nbasis, nvars)
```

# Arguments

m Data matrix with the residuals. This matrix has the same dimensions as the

original data matrix.

PM Penalty matrix obtained with eval.penalty.

prob Probability with values in [0,1].

nbasis Number of basis. nvars Number of variables.

# **Details**

Residuals are vectors. If there are p variables (columns), for every observation there is a residual that there is a p-dimensional vector. If there are n observations, the residuals are an n times p matrix.

### Value

Real number.

#### Author(s)

Irene Epifanio

#### References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

### **Examples**

```
mat <- matrix(1:400, ncol = 20)
PM <- matrix(1:100, ncol = 10)
frobenius_norm_funct_multiv_robust(mat, PM, 0.8, 10, 2)</pre>
```

frobenius\_norm\_funct\_robust

Functional robust Frobenius norm

# **Description**

Computes the functional robust Frobenius norm.

### Usage

```
frobenius_norm_funct_robust(m, PM, prob)
```

# **Arguments**

m Data matrix with the residuals. This matrix has the same dimensions as the

original data matrix.

PM Penalty matrix obtained with eval.penalty.

prob Probability with values in [0,1].

# **Details**

Residuals are vectors. If there are p variables (columns), for every observation there is a residual that there is a p-dimensional vector. If there are n observations, the residuals are an n times p matrix.

# Value

Real number.

frobenius\_norm\_robust 51

### Author(s)

Irene Epifanio

#### References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

# **Examples**

```
library(fda)
mat <- matrix(1:9, nrow = 3)
fbasis <- create.fourier.basis(rangeval = c(1, 32), nbasis = 3)
PM <- eval.penalty(fbasis)
frobenius_norm_funct_robust(mat, PM, 0.8)</pre>
```

frobenius\_norm\_robust Robust Frobenius norm

# **Description**

Computes the robust Frobenius norm.

# Usage

```
frobenius_norm_robust(m, prob)
```

# **Arguments**

m Data matrix with the residuals. This matrix has the same dimensions as the

original data matrix.

prob Probability with values in [0,1].

# **Details**

Residuals are vectors. If there are p variables (columns), for every observation there is a residual that there is a p-dimensional vector. If there are n observations, the residuals are an n times p matrix.

# Value

Real number.

# Author(s)

Irene Epifanio

int\_prod\_mat

### References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

# **Examples**

```
mat <- matrix(1:4, nrow = 2)
frobenius_norm_robust(mat, 0.8)</pre>
```

int\_prod\_mat

Interior product between matrices

# **Description**

Helper function to compute the Frobenius norm.

### Usage

```
int_prod_mat(m)
```

# **Arguments**

m

Data matrix.

### Value

Data matrix.

# Author(s)

Irene Epifanio

### References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

```
mat <- matrix(1:4, nrow = 2)
int_prod_mat(mat)</pre>
```

int\_prod\_mat\_funct 53

int\_prod\_mat\_funct

Interior product between matrices for FDA

# **Description**

Helper function to compute the Frobenius norm in the functional data analysis (FDA) scenario.

# Usage

```
int_prod_mat_funct(m, PM)
```

# **Arguments**

m Data matrix.

PM Penalty matrix obtained with eval.penalty.

### Value

Data matrix.

# Author(s)

Irene Epifanio

# References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

```
library(fda)
mat <- matrix(1:9, nrow = 3)
fbasis <- create.fourier.basis(rangeval = c(1, 32), nbasis = 3)
PM <- eval.penalty(fbasis)
int_prod_mat_funct(mat, PM)</pre>
```

int\_prod\_mat\_sq

Squared interior product between matrices

# Description

Helper function to compute the robust Frobenius norm.

# Usage

```
int_prod_mat_sq(m)
```

# Arguments

m

Data matrix.

### Value

Data matrix.

### Author(s)

Irene Epifanio

# References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

# **Examples**

```
mat <- matrix(1:4, nrow = 2)
int_prod_mat_sq(mat)</pre>
```

int\_prod\_mat\_sq\_funct Squared interior product between matrices for FDA

# **Description**

Helper function to compute the robust Frobenius norm in the functional data analysis (FDA) scenario.

# Usage

```
int_prod_mat_sq_funct(m, PM)
```

outl\_toler 55

# **Arguments**

m Data matrix.

PM Penalty matrix obtained with eval.penalty.

### Value

Data matrix.

#### Author(s)

Irene Epifanio

#### References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

# **Examples**

```
library(fda)
mat <- matrix(1:9, nrow = 3)
fbasis <- create.fourier.basis(rangeval = c(1, 32), nbasis = 3)
PM <- eval.penalty(fbasis)
int_prod_mat_sq_funct(mat, PM)</pre>
```

outl\_toler

Tolerance outliers

#### **Description**

Outliers according to a tolerance interval. This function is used by the archetypoid algorithms to identify the outliers. See the function nptol.int in package tolerance.

# Usage

```
outl_toler(p_tol = 0.95, resid_vect, alpha = 0.05)
```

# **Arguments**

p\_tol The proportion of observations to be covered by this tolerance interval.

resid\_vect Vector of n residuals, where n was the number of rows of the data matrix.

alpha Significance level.

# Value

Vector with the outliers.

### Author(s)

Guillermo Vinue

#### References

Young, D., tolerance: An R package for estimating tolerance intervals, 2010. *Journal of Statistical Software*, **36**(**5**), 1-39, https://doi.org/10.18637/jss.v036.i05

### See Also

```
adalara, fadalara, do_outl_degree
```

# **Examples**

```
outl_toler(0.95, 1:100, 0.05)
```

stepArchetypesRawData\_funct

Archetype algorithm to raw data with the functional Frobenius norm

# Description

This is a slight modification of stepArchetypesRawData to use the functional archetype algorithm with the Frobenius norm.

# Usage

# **Arguments**

data Data to obtain archetypes.

numArch Number of archetypes to compute, from 1 to numArch.

numRep For each numArch, run the archetype algorithm numRep times.

verbose If TRUE, the progress during execution is shown.

saveHistory Save execution steps.

PM Penalty matrix obtained with eval.penalty.

### Value

A list with the archetypes.

# Author(s)

Irene Epifanio

#### References

```
Cutler, A. and Breiman, L., Archetypal Analysis. Technometrics, 1994, 36(4), 338-347, https://doi.org/10.2307/1269949
```

Epifanio, I., Functional archetype and archetypoid analysis, 2016. *Computational Statistics and Data Analysis* **104**, 24-34, https://doi.org/10.1016/j.csda.2016.06.007

Eugster, M.J.A. and Leisch, F., From Spider-Man to Hero - Archetypal Analysis in R, 2009. *Journal of Statistical Software* **30(8)**, 1-23, https://doi.org/10.18637/jss.v030.i08

### **Examples**

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- t(growth$hgtm)</pre>
# Create basis:
basis_fd <- create.bspline.basis(c(1,ncol(hgtm)), 10)</pre>
PM <- eval.penalty(basis_fd)</pre>
# Make fd object:
temp_points <- 1:ncol(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = growth$hgtm, basisobj = basis_fd)</pre>
data_archs <- t(temp_fd$coefs)</pre>
lass <- stepArchetypesRawData_funct(data = data_archs, numArch = 3,</pre>
                                       numRep = 5, verbose = FALSE,
                                       saveHistory = FALSE, PM)
str(lass)
length(lass[[1]])
class(lass[[1]])
class([1]][[5]])
## End(Not run)
```

```
{\tt stepArchetypesRawData\_funct\_multiv}
```

Archetype algorithm to raw data with the functional multivariate Frobenius norm

# Description

This is a slight modification of stepArchetypesRawData to use the functional archetype algorithm with the multivariate Frobenius norm.

#### Usage

# **Arguments**

data Data to obtain archetypes.

numArch Number of archetypes to compute, from 1 to numArch.

numRep For each numArch, run the archetype algorithm numRep times.

verbose If TRUE, the progress during execution is shown.

saveHistory Save execution steps.

PM Penalty matrix obtained with eval.penalty.

#### Value

A list with the archetypes.

#### Author(s)

Irene Epifanio

#### References

Cutler, A. and Breiman, L., Archetypal Analysis. *Technometrics*, 1994, **36(4)**, 338-347, https://doi.org/10.2307/1269949

Epifanio, I., Functional archetype and archetypoid analysis, 2016. *Computational Statistics and Data Analysis* **104**, 24-34, https://doi.org/10.1016/j.csda.2016.06.007

Eugster, M.J.A. and Leisch, F., From Spider-Man to Hero - Archetypal Analysis in R, 2009. *Journal of Statistical Software* **30(8)**, 1-23, https://doi.org/10.18637/jss.v030.i08

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- growth$hgtm
hgtf <- growth$hgtf[,1:39]</pre>
# Create array:
nvars <- 2
data.array <- array(0, dim = c(dim(hgtm), nvars))</pre>
data.array[,,1] <- as.matrix(hgtm)</pre>
data.array[,,2] <- as.matrix(hgtf)</pre>
rownames(data.array) <- 1:nrow(hgtm)</pre>
colnames(data.array) <- colnames(hgtm)</pre>
str(data.array)
# Create basis:
nbasis <- 10
basis_fd <- create.bspline.basis(c(1,nrow(hgtm)), nbasis)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
```

```
temp_points <- 1:nrow(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = data.array, basisobj = basis_fd)</pre>
X <- array(0, dim = c(dim(t(temp_fd$coefs[,,1])), nvars))</pre>
X[,,1] \leftarrow t(temp_fd\$coef[,,1])
X[,,2] \leftarrow t(temp_fdscoef[,,2])
# Standardize the variables:
Xs <- X
Xs[,,1] <- scale(X[,,1])
Xs[,,2] \leftarrow scale(X[,,2])
lass <- stepArchetypesRawData_funct_multiv(data = Xs, numArch = 3,</pre>
                                               numRep = 5, verbose = FALSE,
                                               saveHistory = FALSE, PM)
str(lass)
length(lass[[1]])
class(lass[[1]])
class([1]][[5]])
## End(Not run)
```

```
step Archetypes Raw Data\_funct\_multiv\_robust
```

Archetype algorithm to raw data with the functional multivariate robust Frobenius norm

# **Description**

This is a slight modification of stepArchetypesRawData to use the functional archetype algorithm with the multivariate Frobenius norm.

# Usage

# **Arguments**

data	Data to obtain archetypes.
numArch	Number of archetypes to compute, from 1 to numArch.
numRep	For each numArch, run the archetype algorithm numRep times.
verbose	If TRUE, the progress during execution is shown.
saveHistory	Save execution steps.
PM	Penalty matrix obtained with eval.penalty.

prob Probability with values in [0,1].

nbasis Number of basis.

nvars Number of variables.

### Value

A list with the archetypes.

# Author(s)

Irene Epifanio

#### References

Cutler, A. and Breiman, L., Archetypal Analysis. *Technometrics*, 1994, **36(4)**, 338-347, https://doi.org/10.2307/1269949

Epifanio, I., Functional archetype and archetypoid analysis, 2016. *Computational Statistics and Data Analysis* **104**, 24-34, https://doi.org/10.1016/j.csda.2016.06.007

Eugster, M.J.A. and Leisch, F., From Spider-Man to Hero - Archetypal Analysis in R, 2009. *Journal of Statistical Software* **30(8)**, 1-23, https://doi.org/10.18637/jss.v030.i08

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- growth$hgtm
hgtf <- growth$hgtf[,1:39]</pre>
# Create array:
nvars <- 2
data.array <- array(0, dim = c(dim(hgtm), nvars))</pre>
data.array[,,1] <- as.matrix(hgtm)</pre>
data.array[,,2] <- as.matrix(hgtf)</pre>
rownames(data.array) <- 1:nrow(hgtm)</pre>
colnames(data.array) <- colnames(hgtm)</pre>
str(data.array)
# Create basis:
nbasis <- 10
basis_fd <- create.bspline.basis(c(1,nrow(hgtm)), nbasis)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
temp_points <- 1:nrow(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = data.array, basisobj = basis_fd)</pre>
```

```
X <- array(0, dim = c(dim(t(temp_fd$coefs[,,1])), nvars))</pre>
X[,,1] \leftarrow t(temp_fd\$coef[,,1])
X[,,2] \leftarrow t(temp_fd\$coef[,,2])
# Standardize the variables:
Xs <- X
Xs[,,1] <- scale(X[,,1])
Xs[,,2] <- scale(X[,,2])
lass <- stepArchetypesRawData_funct_multiv_robust(data = Xs, numArch = 3,</pre>
                                                      numRep = 5, verbose = FALSE,
                                                      saveHistory = FALSE, PM, prob = 0.8,
                                                      nbasis, nvars)
str(lass)
length(lass[[1]])
class(lass[[1]])
class([ass[[1]][[5]])
## End(Not run)
```

 ${\tt stepArchetypesRawData\_funct\_robust}$ 

Archetype algorithm to raw data with the functional robust Frobenius norm

# **Description**

This is a slight modification of stepArchetypesRawData to use the functional archetype algorithm with the functional robust Frobenius norm.

### Usage

# **Arguments**

data Data to obtain archetypes.

numArch Number of archetypes to compute, from 1 to numArch.

numRep For each numArch, run the archetype algorithm numRep times.

verbose If TRUE, the progress during execution is shown.

saveHistory Save execution steps.

PM Penalty matrix obtained with eval.penalty.

prob Probability with values in [0,1].

#### Value

A list with the archetypes.

# Author(s)

Irene Epifanio

#### References

```
Cutler, A. and Breiman, L., Archetypal Analysis. Technometrics, 1994, 36(4), 338-347, https://doi.org/10.2307/1269949
```

Epifanio, I., Functional archetype and archetypoid analysis, 2016. *Computational Statistics and Data Analysis* **104**, 24-34, https://doi.org/10.1016/j.csda.2016.06.007

Eugster, M.J.A. and Leisch, F., From Spider-Man to Hero - Archetypal Analysis in R, 2009. *Journal of Statistical Software* **30(8)**, 1-23, https://doi.org/10.18637/jss.v030.i08

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

```
## Not run:
library(fda)
?growth
str(growth)
hgtm <- t(growth$hgtm)</pre>
# Create basis:
basis_fd <- create.bspline.basis(c(1,ncol(hgtm)), 10)</pre>
PM <- eval.penalty(basis_fd)
# Make fd object:
temp_points <- 1:ncol(hgtm)</pre>
temp_fd <- Data2fd(argvals = temp_points, y = growth$hgtm, basisobj = basis_fd)</pre>
data_archs <- t(temp_fd$coefs)</pre>
lass <- stepArchetypesRawData_funct_robust(data = data_archs, numArch = 3,</pre>
                                              numRep = 5, verbose = FALSE,
                                              saveHistory = FALSE, PM, prob = 0.8)
str(lass)
length(lass[[1]])
class(lass[[1]])
class([1]][[5]])
## End(Not run)
```

stepArchetypesRawData\_norm\_frob

Archetype algorithm to raw data with the Frobenius norm

# **Description**

This is a slight modification of stepArchetypesRawData to use the archetype algorithm with the Frobenius norm.

### **Usage**

# **Arguments**

data Data to obtain archetypes.

numArch Number of archetypes to compute, from 1 to numArch.

numRep For each numArch, run the archetype algorithm numRep times.

verbose If TRUE, the progress during execution is shown.

saveHistory Save execution steps.

### Value

A list with the archetypes.

### Author(s)

Irene Epifanio

# References

Eugster, M.J.A. and Leisch, F., From Spider-Man to Hero - Archetypal Analysis in R, 2009. *Journal of Statistical Software* **30(8)**, 1-23, https://doi.org/10.18637/jss.v030.i08

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

Vinue, G., Epifanio, I., and Alemany, S., Archetypoids: a new approach to define representative archetypal data, 2015. *Computational Statistics and Data Analysis* 87, 102-115, https://doi.org/10.1016/j.csda.2015.01.018

Vinue, G., Anthropometry: An R Package for Analysis of Anthropometric Data, 2017. *Journal of Statistical Software* **77(6)**, 1-39, https://doi.org/10.18637/jss.v077.i06

# See Also

stepArchetypesRawData, stepArchetypes

# **Examples**

stepArchetypesRawData\_robust

Archetype algorithm to raw data with the robust Frobenius norm

# Description

This is a slight modification of stepArchetypesRawData to use the archetype algorithm with the robust Frobenius norm.

# Usage

# Arguments

data Data to obtain archetypes.

numArch Number of archetypes to compute, from 1 to numArch.

numRep For each numArch, run the archetype algorithm numRep times.

verbose If TRUE, the progress during execution is shown.

saveHistory Save execution steps.

prob Probability with values in [0,1].

### Value

A list with the archetypes.

# Author(s)

Irene Epifanio

# References

Moliner, J. and Epifanio, I., Robust multivariate and functional archetypal analysis with application to financial time series analysis, 2019. *Physica A: Statistical Mechanics and its Applications* **519**, 195-208. https://doi.org/10.1016/j.physa.2018.12.036

#### See Also

```
stepArchetypesRawData\_norm\_frob
```

# **Index**

```
adalara, 2, 7, 56
                                                 int_prod_mat, 52
adalara_no_paral, 4, 5
                                                 int_prod_mat_funct, 53
archetypoids, 9, 10, 12, 14-16, 33
                                                 int_prod_mat_sq, 54
archetypoids_funct, 8, 30
                                                 int_prod_mat_sq_funct, 54
archetypoids_funct_multiv, 9, 32
                                                 outl_toler, 38, 55
archetypoids_funct_multiv_robust, 11,
                                                 stepArchetypes, 63
archetypoids_funct_robust, 13, 36
                                                 stepArchetypesRawData, 56, 57, 59, 61, 63,
archetypoids_norm_frob, 15, 17, 19, 23, 24
archetypoids_robust, 16, 21
                                                 stepArchetypesRawData_funct, 8, 10, 11,
                                                          30, 56
bisquare_function, 17
                                                 stepArchetypesRawData_funct_multiv, 32,
boxplot, 26, 27
                                                 stepArchetypesRawData_funct_multiv_robust,
do_ada, 4, 7, 18, 21
do_ada_robust, 4, 7, 19, 20
                                                 stepArchetypesRawData_funct_robust, 13,
do_alphas_rss, 22
do_alphas_rss_multiv, 23
                                                 stepArchetypesRawData_norm_frob, 15, 19,
do_clean, 26
                                                          63, 65
do_clean_multiv, 27
                                                 stepArchetypesRawData_robust, 16, 21, 64
do_fada, 28, 33, 35, 40
do_fada_multiv, 31
do_fada_multiv_robust, 33
do_fada_robust, 29, 31, 35, 40
do_knno, 37
do_outl_degree, 38, 56
eval.penalty, 8, 10, 12, 13, 22, 24, 29, 31,
        33, 35, 39, 43, 47–50, 53, 55, 56, 58,
        59, 61
fadalara, 39, 44, 56
fadalara_no_paral, 42
frame_in_r, 45
frobenius_norm, 46
frobenius_norm_funct, 47
frobenius_norm_funct_multiv, 48
frobenius_norm_funct_multiv_robust, 49
frobenius_norm_funct_robust, 50
frobenius_norm_robust, 51
```