

Package ‘ICSOutlier’

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Type Package

Title Outlier Detection Using Invariant Coordinate Selection

Version 0.4-0

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Depends R (>= 3.0.0), methods, ICS (>= 1.4-0), moments

Imports graphics, grDevices, mvtnorm, parallel

Suggests ICSClust, REPPlab, testthat (>= 3.0.0)

Description Multivariate outlier detection is performed using invariant coordinates where the package offers different methods to choose the appropriate components. ICS is a general multivariate technique with many applications in multivariate analysis. ICSOutlier offers a selection of functions for automated detection of outliers in the data based on a fitted ICS object or by specifying the dataset and the scatters of interest. The current implementation targets data sets with only a small percentage of outliers.

License GPL (>= 2)

NeedsCompilation no

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ICSOutlier-package	<i>Outlier Detection Using Invariant Coordinate Selection</i>
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Description

Multivariate outlier detection is performed using invariant coordinates where the package offers different methods to choose the appropriate components. ICS is a general multivariate technique with many applications in multivariate analysis. ICSOutlier offers a selection of functions for automated detection of outliers in the data based on a fitted ICS object or by specifying the dataset and the scatters of interest. The current implementation targets data sets with only a small percentage of outliers.

Details

The DESCRIPTION file:

Package:	ICSOutlier
Type:	Package
Title:	Outlier Detection Using Invariant Coordinate Selection
Version:	0.4-0
Date:	2023-12-13
Authors@R:	c(person("Klaus", "Nordhausen", email = "klausnordhausenR@gmail.com", role = c("aut", "cre"), co
Author:	Klaus Nordhausen [aut, cre] (< https://orcid.org/0000-0002-3758-8501 >), Aurore Archimbaud [aut]
Maintainer:	Klaus Nordhausen <klausnordhausenR@gmail.com>
Depends:	R (>= 3.0.0), methods, ICS (>= 1.4-0), moments

```
Imports:      graphics, grDevices, mvtnorm, parallel
Suggests:    ICSClust, REPPlab, testthat (>= 3.0.0)
Description:  Multivariate outlier detection is performed using invariant coordinates where the package offers diff
License:      GPL (>= 2)
NeedsCompilation: no
Packaged:    2023-09-18 08:47:44 UTC; admin
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Roxygen:      list(markdown = TRUE)
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```

Index of help topics:

HTP	Production Measurements of High-Tech Parts - Full Rank Case
HTP2	Production Measurements of High-Tech Parts - Singular Case
HTP3	Production Measurements of High-Tech Parts - Nearly Singular Case
ICSOutlier-package	Outlier Detection Using Invariant Coordinate Selection
ICS_outlier	Outlier Detection Using ICS
comp.norm.test	Selection of Nonnormal Invariant Components Using Marginal Normality Tests
comp.simu.test	Selection of Nonnormal Invariant Components Using Simulations
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print.icsOut	Vector of Outlier Indicators
summary.ICS_Out	Summary of an 'ICS_Out' Object Summarizes an 'ICS_Out' object in an informative way.
summary.icsOut	Summarize a icsOut object

Author(s)

Klaus Nordhausen [aut, cre] (<<https://orcid.org/0000-0002-3758-8501>>), Aurore Archimbaud [aut] (<<https://orcid.org/0000-0002-6511-9091>>), Anne Ruiz-Gazen [aut] (<<https://orcid.org/0000-0001-8970-8061>>)

Maintainer: Klaus Nordhausen <klausnordhausenR@gmail.com>

References

Archimbaud, A., Nordhausen, K. and Ruiz-Gazen, A. (2018), ICS for multivariate outlier detection with application to quality control. Computational Statistics & Data Analysis, 128:184-199. ISSN 0167-9473. doi:[10.1016/j.csda.2018.06.011](https://doi.org/10.1016/j.csda.2018.06.011).

Archimbaud, A., Nordhausen, K. and Ruiz-Gazen, A. (2018), ICSOutlier: Unsupervised Outlier Detection for Low-Dimensional Contamination Structure. The R Journal, 10:234-250. doi:[10.32614/RJ2018034](https://doi.org/10.32614/RJ2018034).

comp.norm.test	<i>Selection of Nonnormal Invariant Components Using Marginal Normality Tests</i>
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Description

Identifies invariant coordinates that are non normal using univariate normality tests.

Usage

```
comp.norm.test(object, test = "agostino.test", type = "smallprop", level = 0.05,
  adjust = TRUE)
```

Arguments

object	object of class ics2 where both S1 and S2 are specified as functions. The sample size and the dimension of interest are also obtained from the object.
test	name of the normality test to be used. Possibilities are "jarque.test", "anscombe.test", "bonett.test", "agostino.test", "shapiro.test". Default is "agostino.test".
type	currently the only option is "smallprop". See details.
level	the initial level used to make a decision based on the test p-values. See details.
adjust	logical. If TRUE, the quantiles levels are adjusted. Default is TRUE. See details.

Details

Currently the only available type is "smallprop" which detects which of the components follow a univariately normal distribution. It starts from the first component and stops when a component is detected as gaussian. Five tests for univariate normality are available.

If adjust = FALSE all tests are performed at the same level. This leads however often to too many components. Therefore some multiple testing adjustments might be useful. The current default adjusts the level for the jth component as level/j.

Note that the function is seldomly called directly by the user but internally by [ics.outlier](#).

Value

A list containing:

index	integer vector indicating the indices of the selected components.
test	string with the name of the normality test used.
criterion	vector of the p-values from the marginal normality tests for each component.
levels	vector of the levels used for the decision for each component.
adjust	logical. TRUE if adjusted.
type	type used.

Note

Function `comp.norm.test` reached the end of its lifecycle, please use `comp_norm_test` instead. In future versions, `comp.norm.test` will be deprecated and eventually removed.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

References

Archimbaud, A., Nordhausen, K. and Ruiz-Gazen, A. (2018), *ICS for multivariate outlier detection with application to quality control*. *Computational Statistics & Data Analysis*, 128:184-199. ISSN 0167-9473. <<https://doi.org/10.1016/j.csda.2018.06.011>>.

See Also

[ics2](#), [comp.simu.test](#), [jarque.test](#), [anscombe.test](#), [bonett.test](#), [agostino.test](#), [shapiro.test](#)

Examples

```
Z <- rmvnorm(1000, rep(0, 6))
# Add 20 outliers on the first component
Z[1:20, 1] <- Z[1:20, 1] + 10
pairs(Z)
icsZ <- ics2(Z)
# The shift located outliers can be displayed in one dimension
comp.norm.test(icsZ)
# Only one invariant component is non normal and selected.
comp.norm.test(icsZ, test = "bo")

# Example with no outlier
Z0 <- rmvnorm(1000, rep(0, 6))
pairs(Z0)
icsZ0 <- ics2(Z0)
# Should select no component
comp.norm.test(icsZ0, level = 0.01)$index
```

comp.simu.test

*Selection of Nonnormal Invariant Components Using Simulations***Description**

Identifies invariant coordinates that are nonnormal using simulations under a standard multivariate normal model for a specific data setup and scatter combination.

Usage

```
comp.simu.test(object, m = 10000, type = "smallprop", level = 0.05,
  adjust = TRUE, ncores = NULL, iseed = NULL, pkg = "ICSOutlier",
  qtype = 7, ...)
```

Arguments

object	object of class <code>ics2</code> where both <code>S1</code> and <code>S2</code> are specified as functions. The sample size and the dimension of interest are also obtained from the object.
m	number of simulations. Note that since extreme quantiles are of interest <code>m</code> should be large.
type	currently the only type option is "smallprop". See details.
level	the initial level used to make a decision. The cut-off values are the (1-level)th quantile of the eigenvalues obtained from simulations. See details.
adjust	logical. If TRUE, the quantiles levels are adjusted. Default is TRUE. See details.
ncores	number of cores to be used. If NULL or 1, no parallel computing is used. Otherwise makeCluster with type = "PSOCK" is used.
iseed	If parallel computation is used the seed passed on to clusterSetRNGStream . Default is NULL which means no fixed seed is used.
pkg	When using parallel computing, a character vector listing all the packages which need to be loaded on the different cores via require . Must be at least "ICSOutlier" and must contain the packages needed to compute the scatter matrices.
qtype	specifies the quantile algorithm used in quantile .
...	further arguments passed on to the function quantile .

Details

Based on simulations it detects which of the components follow a univariately normal distribution. More precisely it identifies the observed eigenvalues larger than the ones coming from normal distributed data. `m` standard normal data sets are simulated using the same data size and scatters as specified in the `ics2` object. The cut-off values are determined based on a quantile of these simulated eigenvalues.

As the eigenvalues, aka generalized kurtosis values, of ICS are ordered it is natural to perform the comparison in a specific order depending on the purpose. Currently the only available type is

"smallprop" so starting with the first component, the observed eigenvalues are successively compared to these cut-off values. The procedure stops when an eigenvalue is below the corresponding cut-off, so when a normal component is detected.

If `adjust = FALSE` all eigenvalues are compared to the same $(1 - \text{level})$ th level of the quantile. This leads however often to too many selected components. Therefore some multiple testing adjustment might be useful. The current default adjusts the quantile for the j th component as $1 - \text{level}/j$.

Note that depending on the data size and scatters used this can take a while and so it is more efficient to parallelize computations. Note also that the function is seldomly called directly by the user but internally by `ics.outlier`.

Value

A list containing:

<code>index</code>	integer vector indicating the indices of the selected components.
<code>test</code>	string "simulation".
<code>criterion</code>	vector of the cut-off values for all the eigenvalues.
<code>levels</code>	vector of the levels used to derive the cut-offs for each component.
<code>adjust</code>	logical. TRUE if adjusted.
<code>type</code>	type used.
<code>m</code>	number of iterations m used in the simulations.

Note

Function `comp.simu.test` reached the end of its lifecycle, please use `comp_simu_test()` instead. In future versions, `comp.simu.test` will be deprecated and eventually removed.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

References

Archimbaud, A., Nordhausen, K. and Ruiz-Gazen, A. (2018), *ICS for multivariate outlier detection with application to quality control*. *Computational Statistics & Data Analysis*, 128:184-199. ISSN 0167-9473. <<https://doi.org/10.1016/j.csda.2018.06.011>>.

See Also

`ics2`, `comp.norm.test`

Examples

```
# For a real analysis use larger values for m and more cores if available

set.seed(123)
Z <- rmvnorm(1000, rep(0, 6))
# Add 20 outliers on the first component
```

```

Z[1:20, 1] <- Z[1:20, 1] + 10
pairs(Z)
icsZ <- ics2(Z)
# For demo purpose only small m value, should select the first component
comp.simu.test(icsZ, m = 400, ncores = 1)

## Not run:
# For using two cores
# For demo purpose only small m value, should select the first component
comp.simu.test(icsZ, m = 500, ncores = 2, iseed = 123)

# For using several cores and for using a scatter function from a different package
# Using the parallel package to detect automatically the number of cores
library(parallel)
# ICS with MCD estimates and the usual estimates
# Need to create a wrapper for the CovMcd function to return first the location estimate
# and the scatter estimate secondly.
library(rrcov)
myMCD <- function(x,...){
  mcd <- CovMcd(x,...)
  return(list(location = mcd@center, scatter = mcd@cov))
}
icsZmcd <- ics2(Z, S1 = myMCD, S2 = MeanCov, S1args = list(alpha = 0.75))
# For demo purpose only small m value, should select the first component
comp.simu.test(icsZmcd, m = 500, ncores = detectCores()-1,
               pkg = c("ICSOutlier", "rrcov"), iseed = 123)

## End(Not run)

# Example with no outlier
Z0 <- rmvnorm(1000, rep(0, 6))
pairs(Z0)
icsZ0 <- ics2(Z0)
#Should select no component
comp.simu.test(icsZ0, m = 400, level = 0.01, ncores = 1)

```

comp_norm_test

Selection of Nonnormal Invariant Components Using Marginal Normality Tests

Description

Identifies invariant coordinates that are non normal using univariate normality tests.

Usage

```

comp_norm_test(
  object,
  test = "agostino.test",
  type = "smallprop",

```

```

    level = 0.05,
    adjust = TRUE
  )

```

Arguments

object	object of class "ICS" where both S1 and S2 are specified as functions. The sample size and the dimension of interest are also obtained from the object.
test	name of the normality test to be used. Possibilities are "jarque.test", "anscombe.test", "bonett.test", "agostino.test", "shapiro.test". Default is "agostino.test".
type	currently the only option is "smallprop". See details.
level	the initial level used to make a decision based on the test p-values. See details.
adjust	logical. If TRUE, the quantiles levels are adjusted. Default is TRUE. See details.

Details

Currently the only available type is "smallprop" which detects which of the components follow a univariately normal distribution. It starts from the first component and stops when a component is detected as gaussian. Five tests for univariate normality are available. See [normal_crit\(\)](#) function for more general cases.

If adjust = FALSE all tests are performed at the same level. This leads however often to too many components. Therefore some multiple testing adjustments might be useful. The current default adjusts the level for the jth component as level/j.

Note that the function is seldomly called directly by the user but internally by [ICS_outlier\(\)](#).

Value

A list containing:

- index: integer vector indicating the indices of the selected components.
- test: string with the name of the normality test used.
- criterion: vector of the p-values from the marginal normality tests for each component.
- levels: vector of the levels used for the decision for each component.
- adjust: logical. TRUE if adjusted.
- type: type used

Author(s)

Aurore Archimbaud and Klaus Nordhausen

References

Archimbaud, A., Nordhausen, K. and Ruiz-Gazen, A. (2018), ICS for multivariate outlier detection with application to quality control. Computational Statistics & Data Analysis, 128:184-199. ISSN 0167-9473. doi:[10.1016/j.csda.2018.06.011](https://doi.org/10.1016/j.csda.2018.06.011).

See Also

[ICS\(\)](#), [comp_simu_test\(\)](#), [jarque.test\(\)](#), [anscombe.test\(\)](#), [bonett.test\(\)](#), [bonett.test\(\)](#), [shapiro.test\(\)](#)

Examples

```
Z <- rmvnorm(1000, rep(0, 6))
# Add 20 outliers on the first component
Z[1:20, 1] <- Z[1:20, 1] + 10
pairs(Z)
icsZ <- ICS(Z)
# The shift located outliers can be displayed in one dimension
comp_norm_test(icsZ)
# Only one invariant component is non normal and selected.
comp_norm_test(icsZ, test = "bonett.test")

# Example with no outlier
Z0 <- rmvnorm(1000, rep(0, 6))
pairs(Z0)
icsZ0 <- ICS(Z0)
# Should select no component
comp_norm_test(icsZ0, level = 0.01)$index
```

comp_simu_test

Selection of Nonnormal Invariant Components Using Simulations

Description

Identifies invariant coordinates that are nonnormal using simulations under a standard multivariate normal model for a specific data setup and scatter combination.

Usage

```
comp_simu_test(
  object,
  S1 = NULL,
  S2 = NULL,
  S1_args = list(),
  S2_args = list(),
  m = 10000,
  type = "smallprop",
  level = 0.05,
  adjust = TRUE,
  n_cores = NULL,
  iseed = NULL,
  pkg = "ICSOutlier",
  q_type = 7,
  ...
)
```

Arguments

object	object of class "ICS" where both S1 and S2 are specified as functions. The sample size and the dimension of interest are also obtained from the object. It is also natural to expect that the invariant coordinate are centered.
S1	an object of class "ICS_scatter" or a function that contains the location vector and scatter matrix as location and scatter components.
S2	an object of class "ICS_scatter" or a function that contains the location vector and scatter matrix as location and scatter components.
S1_args	a list containing additional arguments for S1.
S2_args	a list containing additional arguments for S2.
m	number of simulations. Note that since extreme quantiles are of interest m should be large.
type	currently the only type option is "smallprop". See details.
level	the initial level used to make a decision. The cut-off values are the (1-level)th quantile of the eigenvalues obtained from simulations. See details.
adjust	logical. If TRUE, the quantiles levels are adjusted. Default is TRUE. See details.
n_cores	number of cores to be used. If NULL or 1, no parallel computing is used. Otherwise makeCluster with type = "PSOCK" is used.
iseed	If parallel computation is used the seed passed on to clusterSetRNGStream . Default is NULL which means no fixed seed is used.
pkg	When using parallel computing, a character vector listing all the packages which need to be loaded on the different cores via require . Must be at least "ICSOutlier" and must contain the packages needed to compute the scatter matrices.
q_type	specifies the quantile algorithm used in quantile .
...	further arguments passed on to the function quantile .

Details

Based on simulations it detects which of the components follow a univariately normal distribution. More precisely it identifies the observed eigenvalues larger than the ones coming from normal distributed data. m standard normal data sets are simulated using the same data size and scatters as specified in the "ICS" object. The cut-off values are determined based on a quantile of these simulated eigenvalues.

As the eigenvalues, aka generalized kurtosis values, of ICS are ordered it is natural to perform the comparison in a specific order depending on the purpose. Currently the only available type is "smallprop" so starting with the first component, the observed eigenvalues are successively compared to these cut-off values. The procedure stops when an eigenvalue is below the corresponding cut-off, so when a normal component is detected.

If `adjust = FALSE` all eigenvalues are compared to the same (1-level)th level of the quantile. This leads however often to too many selected components. Therefore some multiple testing adjustment might be useful. The current default adjusts the quantile for the j th component as $1 - \text{level}/j$.

Note that depending on the data size and scatters used this can take a while and so it is more efficient to parallelize computations. Note also that the function is seldomly called directly by the user but internally by [ICS_outlier\(\)](#).

Value

A list containing:

- index: integer vector indicating the indices of the selected components.
- test: string "simulation".
- criterion: vector of the cut-off values for all the eigenvalues.
- levels: vector of the levels used for the decision for each component.
- adjust: logical. TRUE if adjusted.
- type: type used
- m: number of iterations m used in the simulations.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

References

Archimbaud, A., Nordhausen, K. and Ruiz-Gazen, A. (2018), ICS for multivariate outlier detection with application to quality control. Computational Statistics & Data Analysis, 128:184-199. ISSN 0167-9473. doi:[10.1016/j.csda.2018.06.011](https://doi.org/10.1016/j.csda.2018.06.011).

See Also

[ICS\(\)](#), [comp_norm_test\(\)](#)

Examples

```
# For a real analysis use larger values for m and more cores if available
set.seed(123)
Z <- rmvnorm(1000, rep(0, 6))
# Add 20 outliers on the first component
Z[1:20, 1] <- Z[1:20, 1] + 10
pairs(Z)
icsZ <- ICS(Z)
# For demo purpose only small m value, should select the first component
comp_simu_test(icsZ, S1 = ICS_cov, S2 = ICS_cov4, m = 400, n_cores = 1)

## Not run:
# For using two cores
# For demo purpose only small m value, should select the first component
comp_simu_test(icsZ, S1 = ICS_cov, S2 = ICS_cov4, m = 500, n_cores = 2, iseed = 123)
# For using several cores and for using a scatter function from a different package
# Using the parallel package to detect automatically the number of cores
library(parallel)
# ICS with MCD estimates and the usual estimates
library(ICSclust)
icsZmcd <- ICS(Z, S1 = ICS_mcd_raw, S2 = ICS_cov, S1_args = list(alpha = 0.75))
# For demo purpose only small m value, should select the first component
comp_simu_test(icsZmcd, S1 = ICS_mcd_raw, S2 = ICS_cov,
```

```

S1_args = list(alpha = 0.75, location = TRUE),
m = 500, ncores = detectCores()-1,
             pkg = c("ICSOutlier", "ICSClust"), iseed = 123)

## End(Not run)
# Example with no outlier
Z0 <- rmvnorm(1000, rep(0, 6))
pairs(Z0)
icsZ0 <- ICS(Z0)
# Should select no component
comp_simu_test(icsZ0, S1 = ICS_cov, S2 = ICS_cov4, m = 400, level = 0.01, n_cores = 1)

```

dist.simu.test	<i>Cut-Off Values Using Simulations for the Detection of Extreme ICS Distances</i>
----------------	--

Description

Computes the cut-off values for the identification of the outliers based on the squared ICS distances. It uses simulations under a multivariate standard normal model for a specific data setup and scatters combination.

Usage

```
dist.simu.test(object, index, m = 10000, level = 0.025, ncores = NULL,
               iseed = NULL, pkg = "ICSOutlier", qtype = 7, ...)
```

Arguments

object	object of class <code>ics2</code> where both <code>S1</code> and <code>S2</code> are specified as functions. The sample size and the dimension of interest are also obtained from the object.
index	integer vector specifying which components are used to compute the ics.distances .
m	number of simulations. Note that extreme quantiles are of interest and hence <code>m</code> should be large.
level	the (1-level(s))th quantile(s) used to choose the cut-off value(s). Usually just one number between 0 and 1. However a vector is also possible.
ncores	number of cores to be used. If <code>NULL</code> or 1, no parallel computing is used. Otherwise makeCluster with type = "PSOCK" is used.
iseed	If parallel computation is used the seed passed on to clusterSetRNGStream . Default is <code>NULL</code> which means no fixed seed is used.
pkg	When using parallel computing, a character vector listing all the packages which need to be loaded on the different cores via require . Must be at least "ICSOutlier" and must contain the packages needed to compute the scatter matrices.
qtype	specifies the quantile algorithm used in quantile .
...	further arguments passed on to the function quantile .

Details

The function extracts basically the dimension of the data from the `ics2` object and simulates `m` times, from a multivariate standard normal distribution, the squared ICS distances with the components specified in `index`. The resulting value is then the mean of the `m` corresponding quantiles of these distances at level `1-level`.

Note that depending on the data size and scatters used this can take a while and so it is more efficient to parallelize computations.

Note that the function is seldomly called directly by the user but internally by `ics.outlier`.

Value

A vector with the values of the `(1-level)`th quantile.

Note

Function `dist.simu.test` reached the end of its lifecycle, please use `dist_simu_test` instead. In future versions, `dist.simu.test` will be deprecated and eventually removed.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

References

Archimbaud, A., Nordhausen, K. and Ruiz-Gazen, A. (2018), ICS for multivariate outlier detection with application to quality control. *Computational Statistics & Data Analysis*, 128:184-199. ISSN 0167-9473. <<https://doi.org/10.1016/j.csda.2018.06.011>>.

See Also

`ics2`, `ics.distances`

Examples

```
# For a real analysis use larger values for m and more cores if available

Z <- rmvnorm(1000, rep(0, 6))
Z[1:20, 1] <- Z[1:20, 1] + 10
A <- matrix(rnorm(36), ncol = 6)
X <- tcrossprod(Z, A)

pairs(X)
icsX <- ics2(X)

icsX.dist.1 <- ics.distances(icsX, index = 1)
CutOff <- dist.simu.test(icsX, 1, m = 500, ncores = 1)

# check if outliers are above the cut-off value
plot(icsX.dist.1, col = rep(2:1, c(20, 980)))
abline(h = CutOff)
```

```

library(REPPlab)
data(ReliabilityData)
# The observations 414 and 512 are suspected to be outliers
icsReliability <- ics2(ReliabilityData, S1 = MeanCov, S2 = Mean3Cov4)
# Choice of the number of components with the screeplot: 2
screeplot(icsReliability)
# Computation of the distances with the first 2 components
ics.dist.scree <- ics.distances(icsReliability, index = 1:2)
# Computation of the cut-off of the distances
CutOff <- dist.simu.test(icsReliability, 1:2, m = 50, level = 0.02, ncores = 1)
# Identification of the outliers based on the cut-off value
plot(ics.dist.scree)
abline(h = CutOff)
outliers <- which(ics.dist.scree >= CutOff)
text(outliers, ics.dist.scree[outliers], outliers, pos = 2, cex = 0.9)

## Not run:
# For using three cores
# For demo purpose only small m value, should select the first component
dist.simu.test(icsReliability, 1:2, m = 500, level = 0.02, ncores = 3, iseed = 123)

# For using several cores and for using a scatter function from a different package
# Using the parallel package to detect automatically the number of cores
library(parallel)
# ICS with Multivariate Median and Tyler's Shape Matrix and the usual estimates
library(ICSNP)
icsReliabilityHRMest <- ics2(ReliabilityData, S1 = HR.Mest, S2 = MeanCov,
                           Slargs = list(maxiter = 1000))
# Computation of the cut-off of the distances. For demo purpose only small m value.
dist.simu.test(icsReliabilityHRMest, 1:2, m = 500, level = 0.02, ncores = detectCores()-1,
              pkg = c("ICSOutlier", "ICSNP"), iseed = 123)

## End(Not run)

```

dist_simu_test	<i>Cut-Off Values Using Simulations for the Detection of Extreme ICS Distances</i>
----------------	--

Description

Computes the cut-off values for the identification of the outliers based on the squared ICS distances. It uses simulations under a multivariate standard normal model for a specific data setup and scatters combination.

Usage

```

dist_simu_test(
  object,

```

```

S1 = NULL,
S2 = NULL,
S1_args = list(),
S2_args = list(),
index,
m = 10000,
level = 0.025,
n_cores = NULL,
iseed = NULL,
pkg = "ICSOutlier",
q_type = 7,
...
)

```

Arguments

object	object of class "ICS" where both S1 and S2 are specified as functions. The sample size and the dimension of interest are also obtained from the object. The invariant coordinate are required to be centered.
S1	an object of class "ICS_scatter" or a function that contains the location vector and scatter matrix as location and scatter components.
S2	an object of class "ICS_scatter" or a function that contains the location vector and scatter matrix as location and scatter components.
S1_args	a list containing additional arguments for S1.
S2_args	a list containing additional arguments for S2.
index	integer vector specifying which components are used to compute the ics_distances() .
m	number of simulations. Note that extreme quantiles are of interest and hence m should be large.
level	the (1-level(s))th quantile(s) used to choose the cut-off value(s). Usually just one number between 0 and 1. However a vector is also possible.
n_cores	number of cores to be used. If NULL or 1, no parallel computing is used. Otherwise makeCluster with type = "PSOCK" is used.
iseed	If parallel computation is used the seed passed on to clusterSetRNGStream . Default is NULL which means no fixed seed is used.
pkg	When using parallel computing, a character vector listing all the packages which need to be loaded on the different cores via require . Must be at least "ICSOutlier" and must contain the packages needed to compute the scatter matrices.
q_type	specifies the quantile algorithm used in quantile .
...	further arguments passed on to the function quantile .

Details

The function extracts basically the dimension of the data from the "ICS" object and simulates m times, from a multivariate standard normal distribution, the squared ICS distances with the components specified in `index`. The resulting value is then the mean of the m corresponding quantiles of these distances at level 1-level.

Note that depending on the data size and scatters used this can take a while and so it is more efficient to parallelize computations.

Note that the function is seldomly called directly by the user but internally by `ICS_outlier()`.

Value

A vector with the values of the (1-level)th quantile.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

References

Archimbaud, A., Nordhausen, K. and Ruiz-Gazen, A. (2018), ICS for multivariate outlier detection with application to quality control. Computational Statistics & Data Analysis, 128:184-199. ISSN 0167-9473. doi:[10.1016/j.csda.2018.06.011](https://doi.org/10.1016/j.csda.2018.06.011).

See Also

`ICS()`, `ics_distances()`

Examples

```
# For a real analysis use larger values for m and more cores if available

Z <- rmvnorm(1000, rep(0, 6))
Z[1:20, 1] <- Z[1:20, 1] + 10
A <- matrix(rnorm(36), ncol = 6)
X <- tcrossprod(Z, A)

pairs(X)
icsX <- ICS(X, center = TRUE)

icsX.dist.1 <- ics_distances(icsX, index = 1)
CutOff <- dist_simu_test(icsX, S1 = ICS_cov, S2= ICS_cov4,
                        index = 1, m = 500, ncores = 1)

# check if outliers are above the cut-off value
plot(icsX.dist.1, col = rep(2:1, c(20, 980)))
abline(h = CutOff)

library(REPPlab)
data(ReliabilityData)
# The observations 414 and 512 are suspected to be outliers
icsReliability <- ICS(ReliabilityData, center = TRUE)
# Choice of the number of components with the screeplot: 2
screeplot(icsReliability)
# Computation of the distances with the first 2 components
ics.dist.scree <- ics_distances(icsReliability, index = 1:2)
# Computation of the cut-off of the distances
```

```

CutOff <- dist_simu_test(icsReliability, S1 = ICS_cov, S2= ICS_cov4,
                        index = 1:2, m = 50, level = 0.02, ncores = 1)
# Identification of the outliers based on the cut-off value
plot(ics.dist.scree)
abline(h = CutOff)
outliers <- which(ics.dist.scree >= CutOff)
text(outliers, ics.dist.scree[outliers], outliers, pos = 2, cex = 0.9)

## Not run:
# For using three cores
# For demo purpose only small m value, should select the first #' component
dist_simu_test(icsReliability, S1 = ICS_cov, S2= ICS_cov4,
               index = 1:2, m = 500, level = 0.02, n_cores = 3, iseed #' = 123)

# For using several cores and for using a scatter function from a different package
# Using the parallel package to detect automatically the number of cores
library(parallel)
# ICS with Cauchy estimates
library(ICSClust)
icsReliabilityMLC <- ICS(ReliabilityData, S1 = ICS_mlc,
                        S1_args = list(location = TRUE),
                        S2 = ICS_cov, center = TRUE)
# Computation of the cut-off of the distances. For demo purpose only small m value.
dist_simu_test(icsReliabilityMLC, S1 = ICS_mlc, S1_args = list(location = TRUE),
               S2 = ICS_cov, index = 1:2, m = 500, level = 0.02,
               n_cores = detectCores()-1, pkg = c("ICSOutlier", "ICSClust"), iseed = 123)

## End(Not run)

```

HTP

Production Measurements of High-Tech Parts - Full Rank Case

Description

The HTP data set contains 902 high-tech parts designed for consumer products characterized by 88 tests. These tests are performed to ensure a high quality of the production. All these 902 parts were considered functional and have been sold. However the two parts 581 and 619 showed defects in use and were returned to the manufacturer by the customer. Therefore these two can be considered as outliers.

Usage

```
data("HTP")
```

Format

A data frame with 902 observations and 88 numeric variables V.1 - V.88.

Source

Anonymized data from a nondisclosed manufacturer.

Examples

```
# HTP data: the observations 581 and 619 are considered as outliers
data(HTP)
outliers <- c(581, 619)
boxplot(HTP)

# Outlier detection using ICS
icsHTP <- ics2(HTP)
# Selection of components based on a Normality Test, for demo purpose only small mDist value,
# but as extreme quantiles are of interest mDist should be much larger.
# Also more cores could be used if available.
icsOutlierDA <- ics.outlier(icsHTP, test = "agostino.test", level.test = 0.05,
                           level.dist = 0.02, mDist = 50, ncores = 1)

icsOutlierDA
summary(icsOutlierDA)
plot(icsOutlierDA)
text(outliers, icsOutlierDA@ics.distances[outliers], outliers, pos = 2, cex = 0.9, col = 2)

## Not run:
# Selection of components based on simulations
# This might take a while to run (around 30 minutes)
icsOutlierPA <- ics.outlier(icsHTP, method = "simulation", level.dist = 0.02,
                           level.test = 0.05, mEig = 10000, mDist = 10000)
icsOutlierPA
summary(icsOutlierPA)
plot(icsOutlierPA)
text(outliers, icsOutlierPA@ics.distances[outliers], outliers, pos = 2, cex = 0.9, col = 2)

## End(Not run)
```

HTP2

Production Measurements of High-Tech Parts - Singular Case

Description

The HTP2 data set contains 457 high-tech parts designed for consumer products characterized by 149 tests. These tests are performed to ensure a high quality of the production. All these 457 parts were considered functional and have been sold. However the part 28 showed defects in use and was returned to the manufacturer by the customer. Therefore this part can be considered as outlier.

Usage

```
data("HTP2")
```

Format

A data frame with 457 rows and 149 variables V.1 - V.149, presenting some collinearity issues.

Source

Anonymized data from a nondisclosed manufacturer.

References

Archimbaud, A., Drmac, Z., Nordhausen, K., Radojic, U. and Ruiz-Gazen, A. (2023) Numerical Considerations and a New Implementation for Invariant Coordinate Selection. *SIAM Journal on Mathematics of Data Science*, **5**(1), 97–121. doi:10.1137/22M1498759.

Examples

```
# HTP2 data: the observation 28 is considered as an outlier
data("HTP2")
outliers <- c(28)
boxplot(HTP2, horizontal = TRUE)
# Outlier detection using ICS
library(ICS)
## Not run:
out <- ICS_outlier(HTP2, ICS_algorithm = "QR",
                  method = "norm_test",
                  test = "agostino.test", level_test = 0.05,
                  level_dist = 0.01, n_dist = 50)

# Here there is a singularity issue. One solution is to first reduce the
# dimension. To ensure higher numerical stability of the subsequent methods
# we suggest to permute the data and to use the QR decomposition instead of
# the regular SVD decomposition.
Xt <- HTP2
# Normalization by the mean
Xt.c <- sweep(HTP2, 2, colMeans(HTP2), "-")

# Permutation by rows
# decreasing by infinity norm: absolute maximum
norm_inf <- apply(Xt.c, 1, function(x) max(abs(x)))
order_rows <- order(norm_inf, decreasing = TRUE)
Xt_row_per <- Xt.c[order_rows,]

# QR decomposition of Xt with column pivoting from LAPACK
qr_Xt <- qr(1/sqrt(nrow(Xt.c)-1)*Xt_row_per, LAPACK = TRUE)

# Estimation of rank q
# R is nxp, but with only zero for rows > p
# the diag of R is already in decreasing order and is a good approximation
# of the rank of X.c. To decide on which singular values are zero we use
# a relative criteria based on previous values.
# R should be pxp
R <- qr.R(qr_Xt)
r_all <- abs(diag(R))
r_ratios <- r_all[2:length(r_all)]/r_all[1:(length(r_all)-1)]
q <- which(r_ratios < max(dim(Xt.c)) *.Machine$double.eps)[1]
q <- ifelse(is.na(q), length(r_all), q)
```

```

# Q should be nxp but we are only interested in nxq
Q1 <- qr.Q(qr_Xt)[,1:q]

# QR decomposition of Rt
R_q <- R[1:q, ]
qr_R <- qr(t(R_q), LAPACK = TRUE)
Tau <- qr.Q(qr_R)[1:q, ]
Omega1 <- qr.R(qr_R)[1:q, 1:q]

# New X tilde
# permutation matrices
# permutation of rows
Pi2 <- data.frame(model.matrix(~ . -1, data = data.frame(row=as.character(order_rows))))
Pi2 <- Pi2[,order(as.numeric(substr(colnames(Pi2), start = 4, stop = nchar(colnames(Pi2)))))]
colnames(Pi2) <- rownames(Xt)

# permutation of cols
Pi3 <- data.frame(model.matrix(~ . -1, data = data.frame(col=as.character( qr_R$pivot))))
Pi3 <- t(Pi3[,order(as.numeric(substr(colnames(Pi3), start = 4, stop = nchar(colnames(Pi3))))))])

X_tilde <- sqrt(nrow(Xt)-1)* Tau %*% t(Pi3) %*% t(Q1)

Xt_tilde <- t(Pi2) %*% t(X_tilde)

# Run ICS_outlier
out <- ICS_outlier(Xt_tilde, ICS_algorithm = "QR",
method = "norm_test",
test = "agostino.test", level_test = 0.01,
level_dist = 0.01, n_dist = 50)

summary(out)
plot(out)
text(outliers, out$ics_distances[outliers], outliers, pos = 2, cex = 0.9, col = 2)

## End(Not run)

```

Description

The HTP3 data set contains 371 high-tech parts designed for consumer products characterized by 33 tests. These tests are performed to ensure a high quality of the production. All these 371 parts were considered functional and have been sold. However the part 32 showed defects in use and was returned to the manufacturer by the customer. Therefore this part can be considered as outlier.

Usage

```
data("HTP3")
```

Format

A data frame with 371 rows and 33 variables V.1 - V.33, presenting some approximate collinearity issues which may cause some numerical inaccuracies.

Source

Anonymized data from a nondisclosed manufacturer.

References

Archimbaud, A., Drmac, Z., Nordhausen, K., Radojcic, U. and Ruiz-Gazen, A. (2023) Numerical Considerations and a New Implementation for Invariant Coordinate Selection. *SIAM Journal on Mathematics of Data Science*, **5**(1), 97–121. doi:[10.1137/22M1498759](https://doi.org/10.1137/22M1498759).

Examples

```
# HTP3 data: the observation 32 is considered as an outlier
data("HTP3")
outliers <- c(32)
boxplot(HTP3)

# Outlier detection using ICS
library(ICS)
out <- ICS_outlier(HTP3, ICS_algorithm = "QR",
                  method = "norm_test",
                  test = "agostino.test", level_test = 0.05,
                  level_dist = 0.01, n_dist = 50)

summary(out)
plot(out)
text(outliers, out$ics_distances[outliers], outliers, pos = 2, cex = 0.9, col = 2)
```

 ics.distances

Squared ICS Distances for Invariant Coordinates

Description

Computes the squared ICS distances, defined as the Euclidian distances of the selected centered components.

Usage

```
ics.distances(object, index = NULL)
```

Arguments

object	object of class ics2 where both S1 and S2 are specified as functions.
index	vector of integers indicating the indices of the components to select.

Details

For outlier detection, the squared ICS distances can be used as a measure of outlierness. Denote as Z the invariant coordinates centered with the location estimate specified in S1 (for details see [ics2](#)). Let Z_k be the k components of Z selected by index, then the ICS distance of the observation i is defined as:

$$ICSD^2(x_i, k) = ||Z_k||^2.$$

Note that if all components are selected, the ICS distances are equivalent to the Mahalanobis distances computed with respect of the first scatter and associated location specified in S1.

Value

A numeric vector containing the squared ICS distances.

Note

Function `ics.distances()` reached the end of its lifecycle, please use [ics_distances](#) instead. In future versions, `ics_distances()` will be deprecated and eventually removed.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

References

Archimbaud, A., Nordhausen, K. and Ruiz-Gazen, A. (2018), *ICS for multivariate outlier detection with application to quality control*. *Computational Statistics & Data Analysis*, 128:184-199. ISSN 0167-9473. <<https://doi.org/10.1016/j.csda.2018.06.011>>.

See Also

[ics2](#), [mahalanobis](#)

Examples

```
Z <- rmvnorm(1000, rep(0, 6))
Z[1:20, 1] <- Z[1:20, 1] + 5
A <- matrix(rnorm(36), ncol = 6)
X <- tcrossprod(Z, A)

pairs(X)
icsX <- ics2(X)

icsX.dist.all <- ics.distances(icsX, index = 1:6)
maha <- mahalanobis(X, center = colMeans(X), cov = cov(X))
# in this case the distances should be the same
plot(icsX.dist.all, maha)
all.equal(icsX.dist.all, maha)

icsX.dist.first <- ics.distances(icsX, index = 1)
plot(icsX.dist.first)
```

ics.outlier

*Outlier Detection Using ICS***Description**

In a multivariate framework outlier(s) are detected using ICS. The function works on an object of class `ics2` and decides automatically about the number of invariant components to use to search for the outliers and the number of outliers detected on these components. Currently the function is restricted to the case of searching outliers only on the first components.

Usage

```
ics.outlier(object, method = "norm.test", test = "agostino.test", mEig = 10000,
  level.test = 0.05, adjust = TRUE, level.dist = 0.025, mDist = 10000,
  type = "smallprop", ncores = NULL, iseed = NULL, pkg = "ICSOutlier",
  qtype = 7, ...)
```

Arguments

object	object of class <code>ics2</code> where both S1 and S2 are specified as functions.
method	name of the method used to select the ICS components involved to compute ICS distances. Options are "norm.test" and "simulation". Depending on the method either <code>comp.norm.test</code> or <code>comp.simu.test</code> are used.
test	name of the marginal normality test to use if method = "norm.test". Possibilities are "jarque.test", "anscombe.test", "bonett.test", "agostino.test", "shapiro.test". Default is "agostino.test".
mEig	number of simulations performed to derive the cut-off values for selecting the ICS components. Only if method = "simulation". See <code>comp.simu.test</code> for details.
level.test	level for the <code>comp.norm.test</code> or <code>comp.simu.test</code> functions. The initial level for selecting the invariant coordinates.
adjust	logical. For selecting the invariant coordinates, the level of the test can be adjusted for each component to deal with multiple testing. See <code>comp.norm.test</code> and <code>comp.simu.test</code> for details. Default is TRUE.
level.dist	level for the <code>dist.simu.test</code> function. The (1-level)th quantile used to determine the cut-off value for the ICS distances.
mDist	number of simulations performed to derive the cut-off value for the ICS distances. See <code>dist.simu.test</code> for details.
type	currently the only option is "smallprop" which means that only the first ICS components can be selected. See <code>comp.norm.test</code> or <code>comp.simu.test</code> for details.

ncores	number of cores to be used in <code>dist.simu.test</code> and <code>comp.simu.test</code> . If NULL or 1, no parallel computing is used. Otherwise <code>makeCluster</code> with type = "PSOCK" is used.
iseed	If parallel computation is used the seed passed on to <code>clusterSetRNGStream</code> . Default is NULL which means no fixed seed is used.
pkg	When using parallel computing, a character vector listing all the packages which need to be loaded on the different cores via <code>require</code> . Must be at least "ICSOutlier" and must contain the packages needed to compute the scatter matrices.
qtype	specifies the quantile algorithm used in <code>quantile</code> .
...	passed on to other methods.

Details

The ICS method has attractive properties for outlier detection in the case of a small proportion of outliers. As for PCA three steps have to be performed: (i) select the components most useful for the detection, (ii) compute distances as outlierness measures for all observation and finally (iii) label outliers using some cut-off value.

This function performs these three steps automatically:

- (i) For choosing the components of interest two methods are proposed: "norm.test" based on some marginal normality tests (see details in `comp.norm.test`) or "simulation" based on a parallel analysis (see details in `comp.simu.test`). These two approaches lie on the intrinsic property of ICS in case of a small proportion of outliers with the choice of S1 "more robust" than S2, which ensures to find outliers on the first components. Indeed when using S1 = MeanCov and S2 = Mean3Cov4, the Invariant Coordinates are ordered according to their classical Pearson kurtosis values in decreasing order. The information to find the outliers should be then contained in the first k nonnormal directions.
- (ii) Then the ICS distances are computed as the Euclidian distances on the selected k centered components Z_k .
- (iii) Finally the outliers are identified based on a cut-off derived from simulations. If the distance of an observation exceeds the expectation under the normal model, this observation is labeled as outlier (see details in `dist.simu.test`).

As a rule of thumb, the percentage of contamination should be limited to 10% in case of a mixture of gaussian distributions and using the default combination of locations and scatters for ICS.

Value

an object of class `icsOut`

Note

Function `ics.outlier` reached the end of its lifecycle, please use `ICS_outlier` instead. In future versions, `ics.outlier` will be deprecated and eventually removed.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

References

Archimbaud, A., Nordhausen, K. and Ruiz-Gazen, A. (2018), ICS for multivariate outlier detection with application to quality control. *Computational Statistics & Data Analysis*, 128:184-199. ISSN 0167-9473. <<https://doi.org/10.1016/j.csda.2018.06.011>>.

Archimbaud, A., Nordhausen, K. and Ruiz-Gazen, A. (2018), ICSOutlier: Unsupervised Outlier Detection for Low-Dimensional Contamination Structure. *The R Journal*, 10:234-250. <[doi:10.32614/RJ-2018-034](https://doi.org/10.32614/RJ-2018-034)>.

See Also

[ics2](#), [comp.norm.test](#), [comp.simu.test](#), [dist.simu.test](#), [icsOut-class](#)

Examples

```
# ReliabilityData example: the observations 414 and 512 are suspected to be outliers
library(REPPlab)
data(ReliabilityData)
icsReliabilityData <- ics2(ReliabilityData, S1 = tM, S2 = MeanCov)
# For demo purpose only small mDist value, but as extreme quantiles
# are of interest mDist should be much larger. Also number of cores used
# should be larger if available
icsOutlierDA <- ics.outlier(icsReliabilityData, level.dist = 0.01, mDist = 50, ncores = 1)
icsOutlierDA
summary(icsOutlierDA)
plot(icsOutlierDA)

## Not run:
# For using several cores and for using a scatter function from a different package
# Using the parallel package to detect automatically the number of cores
library(parallel)
# ICS with MCD estimates and the usual estimates
# Need to create a wrapper for the CovMcd function to return first the location estimate
# and the scatter estimate secondly.
data(HTP)
library(rrcov)
myMCD <- function(x,...){
  mcd <- CovMcd(x,...)
  return(list(location = mcd@center, scatter = mcd@cov))
}
icsHTP <- ics2(HTP, S1 = myMCD, S2 = MeanCov, Slargs = list(alpha = 0.75))
# For demo purpose only small m value, should select the first seven components
icsOutlier <- ics.outlier(icsHTP, mEig = 50, level.test = 0.05, adjust = TRUE,
  level.dist = 0.025, mDist = 50,
  ncores = detectCores()-1, iseed = 123,
  pkg = c("ICSOutlier", "rrcov"))

icsOutlier

## End(Not run)

# Exemple of no direction and hence also no outlier
set.seed(123)
```

```

X = rmvnorm(500, rep(0, 2), diag(rep(0.1,2)))
icsX <- ics2(X)
icsOutlierJB <- ics.outlier(icsX, test = "jarque", level.dist = 0.01,
level.test = 0.01, mDist = 100, ncores = 1)
summary(icsOutlierJB)
plot(icsOutlierJB)
rm(.Random.seed)

# Example of no outlier
set.seed(123)
X = matrix(rweibull(1000, 4, 4), 500, 2)
X = apply(X,2, function(x){ifelse(x<5 & x>2, x, runif(sum(!(x<5 & x>2)), 5, 5.5))})
icsX <- ics2(X)
icsOutlierAG <- ics.outlier(icsX, test = "anscombe", level.dist = 0.01,
level.test = 0.05, mDist = 100, ncores = 1)
summary(icsOutlierAG)
plot(icsOutlierAG)
rm(.Random.seed)

```

icsOut-class

Class *icsOut*

Description

A S4 class to store results from performing outlier detection in an ICS context.

Objects from the Class

Objects can be created by calls of the form `new("icsOut", ...)`. But usually objects are created by the function `ics.outlier`.

Slots

outliers: Object of class "integer". A vector containing ones for outliers and zeros for non outliers.

ics.distances: Object of class "numeric". Vector giving the squared ICS distances of the observations from the invariant coordinates centered with the location estimate specified in S1.

ics.dist.cutoff: Object of class "numeric". The cut-off for the distances to decide if an observation is outlying or not.

level.dist: Object of class "numeric". The level for deciding upon the cut-off value for the ICS distances.

level.test: Object of class "numeric". The initial level for selecting the invariant coordinates.

method: Object of class "character". Name of the method used to decide upon the number of ICS components.

index: Object of class "numeric". Vector giving the indices of the ICS components selected.

test: Object of class "character". The name of the normality test as specified in the function call.

criterion: Object of class "numeric". Vector giving the marginal levels for the components selection.

adjust: Object of class "logical". Whether the initial level used to decide upon the number of components has been adjusted for multiple testing or not.

type: Object of class "character". Currently always the string "smallprop".

mDist: Object of class "integer". Number of simulations performed to decide upon the cut-off for the ICS distances.

mEig: Object of class "integer". Number of simulations performed for selecting the ICS components based on simulations.

S1name: Object of class "character". Name of S1 in the original ics2 object.

S2name: Object of class "character". Name of S2 in the original ics2 object.

Methods

For this class the following generic functions are available: [print.icsOut](#), [summary.icsOut](#) and [plot.ics](#)

Note

In case no extractor function for the slots exists, the component can be extracted the usual way using '@'. This S4 class is created by [ics.outlier](#) that reached the end of its lifecycle, please use [ICS_outlier](#) instead for which an object of class S3 is returned. In future versions, [ics.outlier](#) will be deprecated and eventually removed.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

See Also

[ics.outlier](#)

ics_distances

Squared ICS Distances for Invariant Coordinates

Description

Squared ICS Distances for Invariant Coordinates

Usage

```
ics_distances(object, index = NULL)
```

Arguments

object	object of class "ICS" where both S1 and S2 are specified as functions.
index	vector of integers indicating the indices of the components to select.

Details

For outlier detection, the squared ICS distances can be used as a measure of outlierness. Denote as Z the invariant coordinates centered with the location estimate specified in S1 (for details see [ICS\(\)](#)). Let Z_k be the k components of Z selected by index, then the ICS distance of the observation i is defined as:

$$ICSD^2(x_i, k) = ||Z_k||^2.$$

Note that if all components are selected, the ICS distances are equivalent to the Mahalanobis distances computed with respect of the first scatter and associated location specified in S1.

Value

A numeric vector containing the squared ICS distances.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

References

Archimbaud, A., Nordhausen, K. and Ruiz-Gazen, A. (2018), ICS for multivariate outlier detection with application to quality control. Computational Statistics & Data Analysis, 128:184-199. ISSN 0167-9473. doi:[10.1016/j.csda.2018.06.011](https://doi.org/10.1016/j.csda.2018.06.011).

See Also

[ICS\(\)](#), [mahalanobis\(\)](#)

Examples

```
Z <- rmvnorm(1000, rep(0, 6))
Z[1:20, 1] <- Z[1:20, 1] + 5
A <- matrix(rnorm(36), ncol = 6)
X <- tcrossprod(Z, A)

pairs(X)
icsX <- ICS(X, center = TRUE)

icsX.dist.all <- ics_distances(icsX, index = 1:6)
maha <- mahalanobis(X, center = colMeans(X), cov = cov(X))
# in this case the distances should be the same
plot(icsX.dist.all, maha)
all.equal(icsX.dist.all, maha)

icsX.dist.first <- ics_distances(icsX, index = 1)
plot(icsX.dist.first)
```

Description

In a multivariate framework outlier(s) are detected using ICS. The function performs `ICS()` and decides automatically about the number of invariant components to use to search for the outliers and the number of outliers detected on these components. Currently the function is restricted to the case of searching outliers only on the first components.

Usage

```
ICS_outlier(
  X,
  S1 = ICS_cov,
  S2 = ICS_cov4,
  S1_args = list(),
  S2_args = list(),
  ICS_algorithm = c("whiten", "standard", "QR"),
  method = "norm_test",
  test = "agostino.test",
  n_eig = 10000,
  level_test = 0.05,
  adjust = TRUE,
  level_dist = 0.025,
  n_dist = 10000,
  type = "smallprop",
  n_cores = NULL,
  iseed = NULL,
  pkg = "ICSOutlier",
  q_type = 7,
  ...
)
```

Arguments

<code>X</code>	a numeric matrix or data frame containing the data to be transformed.
<code>S1</code>	an object of class "ICS_scatter" or a function that contains the location vector and scatter matrix as location and scatter components.
<code>S2</code>	an object of class "ICS_scatter" or a function that contains the location vector and scatter matrix as location and scatter components.
<code>S1_args</code>	a list containing additional arguments for S1.
<code>S2_args</code>	a list containing additional arguments for S2.
<code>ICS_algorithm</code>	a character string specifying with which algorithm the invariant coordinate system is computed. Possible values are "whiten", "standard" or "QR".

method	name of the method used to select the ICS components involved to compute ICS distances. Options are "norm_test" and "simulation". Depending on the method either comp_norm_test or comp_simu_test are used.
test	name of the marginal normality test to use if method = "norm_test". Possibilities are "jarque.test", "anscombe.test", "bonett.test", "agostino.test", "shapiro.test". Default is "agostino.test".
n_eig	number of simulations performed to derive the cut-off values for selecting the ICS components. Only if method = "simulation". See comp_simu_test for details.
level_test	for the comp_norm_test or comp_simu_test functions. The initial level for selecting the invariant coordinates.
adjust	logical. For selecting the invariant coordinates, the level of the test can be adjusted for each component to deal with multiple testing. See comp_norm_test and comp_simu_test for details. Default is TRUE.
level_dist	level for the dist_simu_test function. The (1-level)th quantile used to determine the cut-off value for the ICS distances.
n_dist	number of simulations performed to derive the cut-off value for the ICS distances. See dist_simu_test for details.
type	currently the only option is "smallprop" which means that only the first ICS components can be selected. See comp_norm_test or comp_simu_test for details.
n_cores	number of cores to be used in dist_simu_test and comp_simu_test . If NULL or 1, no parallel computing is used. Otherwise makeCluster with type = "PSOCK" is used.
iseed	If parallel computation is used the seed passed on to clusterSetRNGStream . Default is NULL which means no fixed seed is used.
pkg	When using parallel computing, a character vector listing all the packages which need to be loaded on the different cores via require . Must be at least "ICSOutlier" and must contain the packages needed to compute the scatter matrices.
q_type	specifies the quantile algorithm used in quantile .
...	passed on to other methods.

Details

The ICS method has attractive properties for outlier detection in the case of a small proportion of outliers. As for PCA three steps have to be performed: (i) select the components most useful for the detection, (ii) compute distances as outlierness measures for all observation and finally (iii) label outliers using some cut-off value.

This function performs these three steps automatically:

- For choosing the components of interest two methods are proposed: "norm_test" based on some marginal normality tests (see details in [comp_norm_test](#)) or "simulation" based on a parallel analysis (see details in [comp_simu_test](#)). These two approaches lie on the intrinsic property of ICS in case of a small proportion of outliers with the choice of S1 "more robust" than S2, which ensures to find outliers on the first components. Indeed when using S1 =

ICS_cov and $S2 = ICS_cov4$, the Invariant Coordinates are ordered according to their classical Pearson kurtosis values in decreasing order. The information to find the outliers should be then contained in the first k non-normal directions.

- Then the ICS distances are computed as the Euclidean distances on the selected k centered components Z_k .
- Finally the outliers are identified based on a cut-off derived from simulations. If the distance of an observation exceeds the expectation under the normal model, this observation is labeled as outlier (see details in [dist_simu_test](#)).

As a rule of thumb, the percentage of contamination should be limited to 10% in case of a mixture of gaussian distributions and using the default combination of locations and scatters for ICS.

Value

An object of S3-class 'ICS_Out' which contains:

- outliers: A vector containing ones for outliers and zeros for non outliers.
- ics_distances: A numeric vector containing the squared ICS distances.
- ics_dist_cutoff: The cut-off for the distances to decide if an observation is outlying or not.
- level_dist: The level for deciding upon the cut-off value for the ICS distances.
- level_test: The initial level for selecting the invariant coordinates.
- method: Name of the method used to decide upon the number of ICS components.
- index: Vector giving the indices of the ICS components selected.
- test: The name of the normality test as specified in the function call.
- criterion: Vector giving the marginal levels for the components selection.
- adjust: Whether the initial level used to decide upon the number of components has been adjusted for multiple testing or not.
- type: Currently always the string "smallprop".
- n_dist: Number of simulations performed to decide upon the cut-off for the ICS distances.
- n_eig: Number of simulations performed for selecting the ICS components based on simulations.
- S1_label: Name of S1.
- S2_label : Name of S2.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

References

Archimbaud, A., Nordhausen, K. and Ruiz-Gazen, A. (2018), ICS for multivariate outlier detection with application to quality control. Computational Statistics & Data Analysis, 128:184-199. ISSN 0167-9473. doi:[10.1016/j.csda.2018.06.011](https://doi.org/10.1016/j.csda.2018.06.011).

See Also

[ICS\(\)](#), [comp_norm_test\(\)](#), [comp_simu_test\(\)](#), [dist_simu_test\(\)](#) and [print\(\)](#), [plot\(\)](#), [summary\(\)](#) methods

Examples

```
# ReliabilityData example: the observations 414 and 512 are suspected to be outliers
library(REPPlab)
data(ReliabilityData)
# For demo purpose only small mDist value, but as extreme quantiles
# are of interest mDist should be much larger. Also number of cores used
# should be larger if available
icsOutlierDA <- ICS_outlier(ReliabilityData, S1 = ICS_tM, S2 = ICS_cov,
  level_dist = 0.01, n_dist = 50, n_cores = 1)
icsOutlierDA
summary(icsOutlierDA)
plot(icsOutlierDA)

## Not run:
# For using several cores and for using a scatter function from a different package
# Using the parallel package to detect automatically the number of cores
library(parallel)
# ICS with MCD estimates and the usual estimates
# Need to create a wrapper for the CovMcd function to return first the location estimate
# and the scatter estimate secondly.
data(HTP)
library(ICSClust)
# For demo purpose only small m value, should select the first seven components
icsOutlier <- ICS_outlier(HTP, S1 = ICS_mcd_rwt, S2 = ICS_cov,
  S1_args = list(location = TRUE, alpha = 0.75),
  n_eig = 50, level_test = 0.05, adjust = TRUE,
  level_dist = 0.025, n_dist = 50,
  n_cores = detectCores()-1, iseed = 123,
  pkg = c("ICSOutlier", "ICSClust"))
icsOutlier

## End(Not run)

# Example of no direction and hence also no outlier
set.seed(123)
X = rmvnorm(500, rep(0, 2), diag(rep(0.1,2)))
icsOutlierJB <- ICS_outlier(X, test = "jarque.test", level_dist = 0.01,
  level_test = 0.01, n_dist = 100, n_cores = 1)
summary(icsOutlierJB)
plot(icsOutlierJB)
rm(.Random.seed)

# Example of no outlier
set.seed(123)
X = matrix(rweibull(1000, 4, 4), 500, 2)
X = apply(X,2, function(x){ifelse(x<5 & x>2, x, runif(sum(!(x<5 & x>2)), 5, 5.5))})
icsOutlierAG <- ICS_outlier(X, test = "anscombe.test", level_dist = 0.01,
```

```

                                level_test = 0.05, n_dist = 100, n_cores = 1)
summary(icsOutlierAG)
plot(icsOutlierAG)
rm(.Random.seed)

```

plot.icsOut

Distances Plot for an icsOut Object

Description

Distances plot for an icsOut object visualizing the separation of the outliers from the good data points.

Usage

```

## S4 method for signature 'icsOut,missing'
plot(x, pch.out = 16, pch.good = 4, col.out = 1, col.good = grey(0.5),
     col.cut = 1, lwd.cut = 1, lty.cut = 1, xlab = "Observation Number",
     ylab = "ICS distances", ...)

```

Arguments

x	object of class icsOut.
pch.out	plotting symbol for the outliers.
pch.good	plotting symbol for the ‘good’ data points.
col.out	color for the outliers.
col.good	color for the ‘good’ data points.
col.cut	color for cut-off line.
lwd.cut	lwd value for cut-off line.
lty.cut	lty value for cut-off line.
xlab	default x-axis label.
ylab	default y-axis label.
...	other arguments for plot

Details

For the figure the IC distances are plotted versus their index. The cut-off value for distances is given as a horizontal line and all observations above the line are considered as outliers.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

See Also

[icsOut-class](#) and [ics.outlier](#)

Examples

```

Z <- rmvnorm(1000, rep(0, 6))
Z[1:20, 1] <- Z[1:20, 1] + 10
A <- matrix(rnorm(36), ncol = 6)
X <- tcrossprod(Z, A)
icsX <- ics2(X)
# For demonstration purposes mDist is small, should be larger for real data analysis
icsXoutliers <- ics.outlier(icsX, mDist = 500)
plot(icsXoutliers, col.out = 2)

```

plot.ICS_Out

*Distances Plot for an 'ICS_Out' Object***Description**

Distances plot for an 'ICS_Out' object visualizing the separation of the outliers from the good data points.

Usage

```

## S3 method for class 'ICS_Out'
plot(
  x,
  pch.out = 16,
  pch.good = 4,
  col.out = 1,
  col.good = grey(0.5),
  col.cut = 1,
  lwd.cut = 1,
  lty.cut = 1,
  xlab = "Observation Number",
  ylab = "ICS distances",
  ...
)

```

Arguments

x	object of class "ICS_Out".
pch.out	plotting symbol for the outliers.
pch.good	plotting symbol for the 'good' data points.
col.out	color for the outliers.
col.good	color for the 'good' data points.
col.cut	color for cut-off line.
lwd.cut	lwd value for cut-off line.
lty.cut	lty value for cut-off line.

xlab	default x-axis label.
ylab	default y-axis label.
...	other arguments for plot

Details

For the figure the IC distances are plotted versus their index. The cut-off value for distances is given as a horizontal line and all observations above the line are considered as outliers.

Value

A plot is displayed.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

print.icsOut	<i>Vector of Outlier Indicators</i>
--------------	-------------------------------------

Description

Short statement about how many components are selected for the outlier detection and how many outliers are detected.

Usage

```
## S4 method for signature 'icsOut'
show(object)
```

Arguments

object	object of class icsOut.
--------	-------------------------

Author(s)

Aurore Archimbaud and Klaus Nordhausen

See Also

[icsOut-class](#) and [ics.outlier](#)

print.ICS_Out	<i>Vector of Outlier Indicators</i>
---------------	-------------------------------------

Description

Short statement about how many components are selected for the outlier detection and how many outliers are detected.

Usage

```
## S3 method for class 'ICS_Out'
print(x, ...)
```

Arguments

x	object object of class "ICS_Out".
...	additional arguments, not used.

Value

The supplied object of class "ICS_Out_summary" is returned invisibly.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

summary.icsOut	<i>Summarize a icsOut object</i>
----------------	----------------------------------

Description

Summarizes and prints an icsOut object in an informative way.

Usage

```
## S4 method for signature 'icsOut'
summary(object, digits = 4)
```

Arguments

object	object of class icsOut.
digits	number of digits for the numeric output.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

See Also

[icsOut-class](#) and [ics.outlier](#)

summary.ICS_Out	<i>Summary of an 'ICS_Out' Object Summarizes an 'ICS_Out' object in an informative way.</i>
-----------------	---

Description

Summary of an 'ICS_Out' Object

Summarizes an 'ICS_Out' object in an informative way.

Usage

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

Arguments

object	object object of class "ICS_Out".
...	additional arguments passed to summary()

Value

An object of class "ICS_Out_summary" with the following components:

- comps: Vector giving the indices of the ICS components selected.
- method: Name of the method used to decide upon the number of ICS components.
- test: the name of the normality test as specified in the function call.
- S1_label: Name of S1.
- S2_label: Name of S2.
- level_test: The level for deciding upon the cut-off value for the ICS distances.
- level_dist: The initial level for selecting the invariant coordinates.
- nb_outliers: the number of observations identified as outliers.

Author(s)

Aurore Archimbaud and Klaus Nordhausen

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