

Package ‘PCADSC’

April 19, 2017

Type Package

Title Tools for Principal Component Analysis-Based Data Structure Comparisons

Version 0.8.0

Description A suite of non-parametric, visual tools for assessing differences in data structures for two datasets that contain different observations of the same variables. These tools are all based on Principal Component Analysis (PCA) and thus effectively address differences in the structures of the covariance matrices of the two datasets. The PCASDC tools consist of easy-to-use, intuitive plots that each focus on different aspects of the PCA decompositions. The cumulative eigenvalue (CE) plot describes differences in the variance components (eigenvalues) of the deconstructed covariance matrices. The angle plot presents the information loss when moving from the PCA decomposition of one dataset to the PCA decomposition of the other. The chroma plot describes the loading patterns of the two datasets, thereby presenting the relative weighting and importance of the variables from the original dataset.

Depends R (>= 3.2.2)

License GPL-2

Encoding UTF-8

LazyData true

Imports reshape2, methods, pander, ggplot2, Matrix

RoxygenNote 5.0.1

URL <https://github.com/annepetersen1/PCADSC>

BugReports <https://github.com/annepetersen1/PCADSC/issues>

NeedsCompilation no

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Repository CRAN

Date/Publication 2017-04-19 10:07:43 UTC

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anglePlot	<i>Angle plot</i>
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Description

Produce an angle plot from a full or partial PCADSC object, as obtained from a call to [PCADSC](#). In either case, this PCADSC object must have a non-NULL `angleInfo` slot (see examples). The angle plot compares the eigenvalue- and loading patterns from PCA performed on two datasets that consist of different observations of the same variables.

Usage

```
anglePlot(x)
```

Arguments

`x` A PCADSC or `angleInfo` object, as produced by [PCADSC](#) or [doAngle](#), respectively.

See Also

[PCADSC](#), [doAngle](#)

Examples

```
#load iris data
data(iris)

#Define grouping variable, grouping the observations by whether their species is
#Setosa or not
iris$group <- "setosa"
iris$group[iris$Species != "setosa"] <- "non-setosa"
iris$Species <- NULL

## Not run:
#make a full PCADSC object, splitting the data by "group"
irisPCADSC <- PCADSC(iris, "group")
```

```
#make a partial PCADSC object from iris and fill out angleInfo in the next call
irisPCADSC2 <- PCADSC(iris, "group", doAngle = FALSE)
irisPCADSC2 <- doAngle(irisPCADSC2)

#make an angle plot
anglePlot(irisPCADSC)
anglePlot(irisPCADSC2)

## End(Not run)

#Only do angle information for a faster run-time
irisPCADSC_fast <- PCADSC(iris, "group", doCE = FALSE, doChroma = FALSE)
anglePlot(irisPCADSC_fast)
```

CEPlot

Cumulative eigenvalue plot

Description

Produce a cumulative eigenvalue (CE) plot from a full or partial PCADSC object, as obtained from a call to [PCADSC](#). In either case, this PCADSC object must have a non-NULL `CEInfo` slot (see examples). The CE plot compares the eigenvalues obtained from PCA performed separately and jointly on two datasets that consist of different observations of the same variables.

Usage

```
CEPlot(x, nDraw = NULL)
```

Arguments

x	x A PCADSC or <code>angleInfo</code> object, as produced by PCADSC or doAngle , respectively.
nDraw	A positive integer. The number of simulated cumulative eigenvalue curves that should be added to the plot.

Details

In the x-coordinates, cumulative differences in eigenvalues are shown, while the y-coordinates are the cumulative sum of the joint eigenvalues. The plot is annotated with Kolmogorov-Smirnov and Cramer-von Mises tests evaluated by permutation tests, testing the null hypothesis of no difference in eigenvalues. The plot also features a number of cumulative simulated cumulative eigenvalue curves as dashed lines. Moreover, a shaded area presents pointwise 95 % confidence bands for the cumulative difference, also obtained using the permutation test.

See Also

[PCADSC](#), [doCE](#)

Examples

```

#load iris data
data(iris)

#Define grouping variable, grouping the observations by whether their species is
#Setosa or not
iris$group <- "setosa"
iris$group[iris$Species != "setosa"] <- "non-setosa"
iris$Species <- NULL

## Not run:
#make a PCADSC object, splitting the data by "group"
irisPCADSC <- PCADSC(iris, "group")

#make a partial PCADSC object from iris and fill out CEInfo in the next call
irisPCADSC2 <- PCADSC(iris, "group", doCE = FALSE)
irisPCADSC2 <- doCE(irisPCADSC2)

#make a CE plot
CEPlot(irisPCADSC)
CEPlot(irisPCADSC2)

## End(Not run)

#Only do CE information and use less resamplings for a faster runtime
irisPCADSC_fast <- PCADSC(iris, "group", doAngle = FALSE, doChroma = FALSE,
  B = 1000)
CEPlot(irisPCADSC_fast)

```

chromaPlot

Chroma plot

Description

Produce a chroma plot from a full or partial PCADSC object, as obtained from a call to [PCADSC](#). In either case, this PCADSC object must have a non-NULL chromaInfo slot (see examples). The chroma plot compares the loading patterns from PCA conducted on two datasets consisting of different observations of the same variables.

Usage

```

chromaPlot(x, varLabels = NULL, cvCO = 1, splitLabels = NULL,
  varAnnotation = "cum", useComps = NULL)

```

Arguments

x Either a PCADSC object or a chromaInfo object, as produced by [PCADSC](#) and [doChroma](#).

varLabels	A vector of character string labels for the variables used in <code>pcadscObj</code> . If non-NULL, these labels appear in the plot instead of the variable names.
cvCO	A numeric in the interval $[0, 1]$ where the default, 1, corresponds to no cut-off value. If a value smaller than 1, only the first n components are plotted, where n is the the lowest possible number, such that the cumulative variance contribution of the first n components exceeds <code>cvCO</code> for both datasets. Note that setting <code>covCO</code> will overrule the argument <code>useComps</code> .
splitLabels	Labels for the two categories of the splitting variable used to create the PCADSC object, <code>x</code> , given as a named list (see examples). These labels will appear in the headers of the two PCADSC plots. If NULL (the default), the original levels of the splitting variable are used.
varAnnotation	If "cum" (the default), cummulated explained variance percentages are annotated to the right of the bars for each component. If "raw", the non-cummulated percentages of explained variance are added instead. If NULL, no annotation is added. Note that "cum" is only allowed if <code>useComps</code> is non-NULL.
useComps	A vector of integers with the indexes of the principal component that should be included in the plot.

Details

The plot consists of one display for each of the two datasets. The two displays both consist of a number of vertical bars. Each vertical bar represents a principal component and the width of each colored section (chroma) within the bar corresponds to the normalized PCA loading vector of that component. The bars can be annotated with the (cumulative) variance contributions of the components (see `varAnnotation`).

See Also

[PCADSC](#), [doChroma](#)

Examples

```
#load iris data
data(iris)

#Define grouping variable, grouping the observations by whether their species is
#Setosa or not
iris$group <- "setosa"
iris$group[iris$Species != "setosa"] <- "non-setosa"
iris$Species <- NULL

## Not run:
#make a PCADSC object, splitting the data by "group"
irisPCADSC <- PCADSC(iris, "group")

#make a partial PCADSC object from iris and fill out chromaInfo in the next call
irisPCADSC2 <- PCADSC(iris, "group", doChroma = FALSE)
irisPCADSC2 <- doChroma(irisPCADSC2)
```

```
#make a chroma plot
chromaPlot(irisPCADSC)
chromaPlot(irisPCADSC)

#Change the labels of the splitting variable
chromaPlot(irisPCADSC, splitLabels = list("non-setosa" = "Not Setosa",
    "setosa" = "Setosa"))

#Only plot components 1 and 4 and remove annotated variances
chromaPlot(irisPCADSC, useComps = c(1,4), varAnnotation = "no")

#Only plot the first components responsible for explaining 80 percent variance
chromaPlot(irisPCADSC, cvCO = 0.8)

#Change variable labels
chromaPlot(irisPCADSC, varLabels = c("Sepal length", "Sepal width", "Petal length",
    "Petal width"))

## End(Not run)

#Only do chroma information in order to get a faster runtime:
irisPCADSC_fast <- PCADSC(iris, "group", doCE = FALSE,
    doAngle = FALSE)
chromaPlot(irisPCADSC_fast)
```

doAngle

Compute angle information

Description

Computes the information that is needed in order to make an [anglePlot](#) from a PCADSC or `pcaRes` object. Typically, this function is called on a partial PCADSC object in order to add `angleInfo` (see examples).

Usage

```
doAngle(x)
```

Arguments

x Either a PCADSC or a `pcaRes` object.

See Also

[anglePlot](#), [PCADSC](#)

Examples

```

#load iris data
data(iris)

#Define grouping variable, grouping the observations by whether their species is
#Setosa or not
iris$group <- "setosa"
iris$group[iris$Species != "setosa"] <- "non-setosa"
iris$Species <- NULL

## Not run:
#make a partial PCADSC object, splitting the data by "group"
irisPCADSC <- PCADSC(iris, "group", doAngle = FALSE)

#No angleInfo available
irisPCADSC$angleInfo

#Add and show angleInfo
irisPCADSC <- doAngle(irisPCADSC)
irisPCADSC$angleInfo

## End(Not run)

#Make a partial PCADSC object and only add angle information for a
#faster runtime
irisPCADSC_fast <- PCADSC(iris, "group", doAngle = FALSE,
  doChroma = FALSE, doCE = FALSE)
irisPCADSC_fast <- doAngle(irisPCADSC_fast)
irisPCADSC_fast$angleInfo

```

doCE

*Compute cumulative eigenvalue information***Description**

Computes the information that is needed in order to make a [CEPlot](#) from a PCADSC or pcaRes object. Typically, this function is called on a partial PCADSC object in order to add CEInfo (see examples).

Usage

```
doCE(x, ...)
```

Arguments

x	Either a PCADSC or a pcaRes object.
...	If doCE is called on a pcaRes object, the full dataset must also be supplied (as data), as well as the number of resampling steps (B).

See Also

[CEPlot](#), [PCADSC](#)

Examples

```
#load iris data
data(iris)

#Define grouping variable, grouping the observations by whether their species is
#Setosa or not
iris$group <- "setosa"
iris$group[iris$Species != "setosa"] <- "non-setosa"
iris$Species <- NULL

## Not run:
#make a partial PCADSC object, splitting the data by "group"
irisPCADSC <- PCADSC(iris, "group", doCE = FALSE)

#No CEInfo available
irisPCADSC$CEInfo

#Add and show CEInfo
irisPCADSC <- doCE(irisPCADSC)
irisPCADSC$CEInfo

## End(Not run)

#Make a partial PCADSC object and only add CE information with no
#bootstrapping (and thus no test)
irisPCADSC_fast <- PCADSC(iris, "group", doAngle = FALSE,
  doChroma = FALSE, doCE = FALSE)
irisPCADSC_fast <- doCE(irisPCADSC_fast, B = 100)
irisPCADSC_fast$CEInfo
```

doChroma

Compute chroma information

Description

Computes the information that is needed in order to make a [chromaPlot](#) from a PCADSC or `pcaRes` object. Typically, this function is called on a partial PCADSC object in order to add `chromaInfo` (see examples).

Usage

```
doChroma(x)
```


Arguments

x Either a PCADSC or a `pcaRes` object.

See Also

[chromaPlot](#), [PCADSC](#)

Examples

```
#load iris data
data(iris)

#Define grouping variable, grouping the observations by whether their species is
#Setosa or not
iris$group <- "setosa"
iris$group[iris$Species != "setosa"] <- "non-setosa"
iris$Species <- NULL

## Not run:
#make a partial PCADSC object, splitting the data by "group"
irisPCADSC <- PCADSC(iris, "group", doChroma = FALSE)

#No chromaInfo available
irisPCADSC$chromaInfo

#Add and show chromaInfo
irisPCADSC <- doChroma(irisPCADSC)
irisPCADSC$chromaInfo

## End(Not run)

#Make a partial PCADSC object and only add chroma information for a
#faster runtime
irisPCADSC_fast <- PCADSC(iris, "group", doAngle = FALSE,
  doChroma = FALSE, doCE = FALSE)
irisPCADSC_fast <- doChroma(irisPCADSC_fast)
irisPCADSC_fast$chromaInfo
```

PCADSC

Compute the elements used for PCADSC

Description

Principal Component Analysis-based Data Structure Comparison tools that prepare a dataset for various diagnostic plots for comparing data structures. More specifically, PCADSC performs PCA on two subsets of a dataset in order to compare the structures of these datasets, e.g. to assess whether they can be analyzed pooled or not. The results of the PCAs are then manipulated in various ways and stored for easy plotting using the three PCADSC plotting tools, the [CEPlot](#), the [anglePlot](#) and the [chromaPlot](#).

Usage

```
PCADSC(data, splitBy, vars = NULL, doCE = TRUE, doAngle = TRUE,
        doChroma = TRUE, B = 10000)
```

Arguments

<code>data</code>	A dataset, either a <code>data.frame</code> or a <code>matrix</code> with variables in columns and observations in rows. Note that <code>tibbles</code> and <code>data.tables</code> are accepted as input, but they are instantly converted to <code>data.frames</code> . Future releases might include specific implementation for these data representations.
<code>splitBy</code>	The name of a grouping variable with two levels defining the two groups within the dataset whose data structures we wish to compare.
<code>vars</code>	The variable names in <code>data</code> to include in the PCADSC. If <code>NULL</code> (the default), all variables except for <code>splitBy</code> are used.
<code>doCE</code>	Logical. Should the cumulative eigenvalue plot information be computed?
<code>doAngle</code>	Logical. Should the angle plot information be computed?
<code>doChroma</code>	Logical. Should the chroma plot information be computed?
<code>B</code>	A positive integer. The number of resampling steps performed in the cumulative eigenvalue step, if relevant.

Details

PCADSC presents a suite of non-parametric, visual tools for comparing the structures of two subsets of a dataset. These tools are all based on PCA (principal component analysis) and thus they can be interpreted as comparisons of the covariance matrices of the two (sub)datasets. PCADSC performs PCA using singular value decomposition for increased numerical precision. Before performing PCA on the full dataset and the two subsets, all variables within each such dataset are standardized.

Value

An object of class `PCADSC`, which is a named list with the following entries:

pcaRes The results of the PCAs performed on the first subset, the second subset and the full subset and also information about the data splitting.

CEInfo The information needed for making a cumulative eigenvalue plot (see [CEPlot](#)).

angleInfo The information needed for making an angle plot (see [anglePlot](#)).

chromaInfo The information needed for making a chroma plot (see [chromaPlot](#)).

data The original (full) dataset.

splitBy The name of the variable that splits the dataset in two.

vars The names of the variables in the dataset that should be used for PCA.

B The number of resamplings performed for the `CEInfo`.

See Also

[doCE](#), [doAngle](#), [doChroma](#), [CEPlot](#), [anglePlot](#), [chromaPlot](#)

Examples

```
#load iris data
data(iris)

#Define grouping variable, grouping the observations by whether their species is
#Setosa or not
iris$group <- "setosa"
iris$group[iris$Species != "setosa"] <- "non-setosa"
iris$Species <- NULL

## Not run:
#Make a full PCADSC object, splitting the data by "group"
irisPCADSC <- PCADSC(iris, "group")

#The three plotting functions can now be called on irisPCADSC:
CEPlot(irisPCADSC)
anglePlot(irisPCADSC)
chromaPlot(irisPCADSC)

#Make a partial PCADSC object with no angle plot information and add
#angle plot information afterwards:
irisPCADSC2 <- PCADSC(iris, "group", doAngle = FALSE)
irisPCADSC2 <- doAngle(irisPCADSC)

## End(Not run)

#Make a partial PCADSC object with no plotting (angle/CE/chroma)
#information:
irisPCADSC_minimal <- PCADSC(iris, "group", doAngle = FALSE,
  doCE = FALSE, doChroma = FALSE)
```

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