

Package ‘HotellingEllipse’

May 18, 2021

Title Hotelling T-Square and Confidence Ellipse

Version 0.1.1

Description Functions to compute the semi-axes lengths and coordinate points of Hotelling ellipse. Bro and Smilde (2014) <DOI:10.1039/c3ay41907j>. Brerton (2016) <DOI:10.1002/cem.2763>.

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Encoding UTF-8

LazyData true

RoxygenNote 7.1.1

URL <https://github.com/ChristianGoueguel/HotellingEllipse>

BugReports <https://github.com/ChristianGoueguel/HotellingEllipse/issues>

Imports dplyr, FactoMineR, ggforce, ggplot2, lifecycle, magrittr, purrr, stats, tibble

Depends R (>= 2.10)

Suggests rmarkdown, knitr, markdown, testthat (>= 3.0.0), spelling

VignetteBuilder knitr

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Language en-US

NeedsCompilation no

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ellipseCoord	<i>Coordinate Points Of Hotelling Ellipse</i>
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Description

Get the x and y coordinates of Hotelling ellipse.

Usage

```
ellipseCoord(data, pcx = 1, pcy = 2, conf.limit = 0.95, pts = 200)
```

Arguments

data	a data frame or tibble of PCA/PLS scores
pcx	an integer specifying which component is on the x-axis (by default 1)
pcy	an integer specifying which component is on the y-axis (by default 2)
conf.limit	an integer specifying the confidence level (by default 0.95)
pts	an integer indicating the number of points of Hotelling ellipse (by default 200)

Value

a data frame with x and y coordinates

Author(s)

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Examples

```
## Principal components analysis (PCA)
library(dplyr)
set.seed(123)
pca_mod <- specData %>%
  dplyr::select(where(is.numeric)) %>%
  FactoMineR::PCA(scale.unit = FALSE, graph = FALSE)

## Extract PCA scores
pca_scores <- pca_mod %>%
  purrr::pluck("ind", "coord") %>%
  tibble::as_tibble()

## Get Hotelling ellipse coordinate points
library(HotellingEllipse)
xy_coord <- ellipseCoord(data = pca_scores, pcx = 1, pcy = 2, conf.limit = 0.95, pts = 200)
```

`ellipseParam`*Lengths Of The Semi-Axes Of Hotelling Ellipse*

Description

Compute the lengths of the semi-axes of Hotelling ellipse.

Usage

```
ellipseParam(data, k = 2, pcx = 1, pcy = 2)
```

Arguments

<code>data</code>	a data frame or tibble of PCA/PLS scores
<code>k</code>	number of components (by default 2)
<code>pcx</code>	an integer specifying which component is on the x-axis (by default 1)
<code>pcy</code>	an integer specifying which component is on the y-axis (by default 2)

Value

Returns a list including: (1) `Tsquare`, a data frame containing Hotelling T2-value. (2) `Ellipse`, a data frame containing the lengths of the semi-minor and semi-major axes. (3) `cutoff.99pct`, an integer indicating the T-square cutoff at 99% confidence level. (4) `cutoff.95pct`, an integer indicating the T-square cutoff at 95% confidence level.

Author(s)

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Examples

```
## Principal components analysis (PCA)
library(dplyr)
set.seed(123)
pca_mod <- specData %>%
  dplyr::select(where(is.numeric)) %>%
  FactoMineR::PCA(scale.unit = FALSE, graph = FALSE)

## Extract PCA scores
pca_scores <- pca_mod %>%
  purrr::pluck("ind", "coord") %>%
  tibble::as_tibble()

## Get Hotelling T2-value and the lengths of the ellipse semi-axes
library(HotellingEllipse)
T2 <- ellipseParam(data = pca_scores, k = 2, pcx = 1, pcy = 2)
```

specData	<i>Laser-induced breakdown spectroscopy (LIBS) spectra of 171 soil samples</i>
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Description

A dataset containing the emission spectra of 171 soils measured in laboratory.

Usage

specData

Format

A data frame with 171 rows and 6670 variables (wavelengths).

Source

doi: [10.1039/C9JA00090A](https://doi.org/10.1039/C9JA00090A)

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