Package ‘anocva’

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Type Package

Title A Non-Parametric Statistical Test to Compare Clustering Structures

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Description Provides ANOCVA (ANalysis Of Cluster VAriability), a non-parametric statistical test to compare clustering structures with applications in functional magnetic resonance imaging data (fMRI). The ANOCVA allows us to compare the clustering structure of multiple groups simultaneously and also to identify features that contribute to the differential clustering.

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Suggests MASS, igraph

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**Description**

The ANOCVA (ANalysis Of Cluster VAriability) is a non-parametric statistical test to compare clusters with applications in functional magnetic resonance imaging data. The ANOCVA allows us to compare the clustering structure of multiple groups simultaneously and also to identify features that contribute to the differential clustering.

**Usage**

```r
anocva(dataDist, id, replicates = 1000, r = NULL,
       clusteringFunction = NULL, p = 1, maxClust = 20,
       criterion = c("slope", "silhouette"), showElapTime = TRUE)
```

**Arguments**

- **dataDist**: A matrix with multiple matrices of dissimilarites. Given that a subject with N items (e.g. ROIs) has a matrix of dissimilarities of size NxN, the dataDist matrix should contain the dissimilarity matrix of all subjects (n) of all populations, resulting in a three-dimensional (nxNxN) matrix.
- **id**: A list in range 1,2,...,n, where id[i] identifies the population id for the i-th subject.
- **replicates**: The number of bootstrap replicates. The default value is 1000.
- **r**: The optimal number of clusters. If NULL, then it will be estimated by the slope criterion in the interval 2..20.
- **clusteringFunction**: Determines the clustering function that will be used. The default function is 'spectralClustering'. The clustering function is supposed to return the clustering labels.
- **p**: Slope adjust parameter. Only used if r is unknown.
- **maxClust**: The maximum number of clusters to be tried if estimating optimal number of clusters. The default value is 20.
- **criterion**: The criterion that will be used for estimating the number of clusters (if r is unknown). The options are "slope" or "silhouette". If not defined, "slope" will be used.
- **showElapTime**: Determines whether the total processing time should be displayed. The default value is TRUE.

**Details**

The test statistic used is the one proposed by Caetano de Jesus (2017).
Value

ANOCVA p-values

References


Examples

```r
# Install packages if necessary
# install.packages("MASS")
# install.packages("cluster")

library(anocva)
library(MASS)
library(cluster)

set.seed(5000)

# Defines a k-means function that returns cluster labels directly
myKmeans = function(dist, k){
  return(kmeans(dist, k, iter.max = 50, nstart = 5)$cluster)
}

# Number of subjects in each population
nsub = 20
# Number of items in each subject
nitem = 30

# Generate simulated data
data = array(NA, c(nsub*2, nitem*2, 2))
dataDist = array(NA, c(nsub*2, nitem*2, nitem*2))
meanx = 2
delta = 0.5

# Covariance matrix
sigma = matrix(c(0.03, 0, 0, 0.03), 2)
for (i in seq(nsub*2)){
  sub = rbind(mvrnorm(nitem, mu = c(0, 0), Sigma = sigma),
              mvrnorm(nitem, mu = c(meanx,0), Sigma = sigma))
  data[i,] = sub
  # If it’s a sample of population 2.
  if (i > nsub){
    data[i,10,1] = data[i,10,1] + delta
  }
}
# Euclidian distance
dataDist[, ] = as.matrix(dist(data[, ]))

# Population 1 subject
plot(data[5, ], asp = 1, xlab = '', ylab = '', main = 'Population 1 - subject example')

# Population 2 subject
plot(data[35, ], asp = 1, xlab = '', ylab = '', main = 'Population 2 - subject example')

# The first nsub subjects belong to population 1 while the next nsub subjects belong to population 2
id = c(rep(1, nsub), rep(2, nsub))

## Not run:
# ANOCVA call with different clustering function (myKmeans) and inside estimation of
# the number of clusters (r)
res1 = anocva(dataDist, id, replicates=500, r = NULL,
    clusteringFunction = myKmeans,
    p = 1, criterion = "slope")

## End(Not run)

# Estimate the number of clusters previously by using Spectral Clustering and Slope criterion
r = nClustMulti(dataDist, clusteringFunction = spectralClustering, criterion = 'slope')

# Calls ANOCVA statistical test
res = anocva(dataDist, id, replicates=500, r = r,
    clusteringFunction = spectralClustering,
    p = 1, criterion = "slope")

# DeltaS p-value
res$pValueDeltaS

# DeltaSq p-values
res$pValueDeltaSq

# Identifies which items have significant p-values with a significance level of 0.05.
which(res$pValueDeltaSq < 0.05)

# Identifies which items have significant FDR adjusted p-values (q-values)
# with a significance level of 0.05.
qValue = p.adjust(res$pValueDeltaSq, "fdr")
which(qValue < 0.05)

# Check for 0,1 Interval Normalization.
nClust

Description
Verifies if the data is normalized in the range 0,1. If they are not, the normalization is performed and a warning issued.

Usage
checkRange01(data)

Arguments
data A matrix of data

Value
The data matrix normalized in the range 0,1.

Examples
set.seed(2000)
simuData = runif(100, min = 0.5, max=7)
sprintf("The minimum value is %.2f and the maximum is %.2f.", min(simuData), max(simuData))
simuData = checkRange01(simuData)
sprintf("Now the minimum value is %.2f and the maximum is %.2f.", min(simuData), max(simuData))

nClust

Optimal Number of Clusters Estimation

Description
Estimates the optimal number of clusters using either Slope or Silhouette criterion. The optimal number of clusters will be verified in the range 2,..., maxClust.

Usage
nClust(meanDist, p = 1, maxClust = 20, clusteringFunction, criterion = c("slope", "silhouette"))

Arguments
meanDist An NxN matrix that represents the distances between the N items of the sample.
p Slope adjust parameter.
maxClust The maximum number of clusters to be tried. The default value is 20.
clusteringFunction The clustering function to be used.
criterion The criterion that will be used for estimating the number of clusters. The options are "slope" or "silhouette". If not defined, "slope" will be used.
Value
The optimal number of clusters.

References

Examples
# Install packages if necessary
# install.packages("MASS")
# install.packages("cluster")
library(MASS)
library(cluster)
library(anocva)
set.seed(2000)

# Defines a k-means function that returns cluster labels directly
myKmeans = function(dist, k){
  return(kmeans(dist, k, iter.max = 50, nstart = 5)$cluster)
}

# Generate simulated data
nitem = 70
sigma = matrix(c(0.04, 0, 0, 0.04), 2)
simuData = rbind(mvrnorm(nitem, mu = c(0, 0), Sigma = sigma),
  mvrnorm(nitem, mu = c(3,0), Sigma = sigma),
  mvrnorm(nitem, mu = c(2.5,2), Sigma = sigma))
plot(simuData, asp = 1, xlab = '', ylab = '', main = 'Data for clustering')

# Calculate distances and perform {0,1} normalization
distMatrix = as.matrix(dist(simuData))
distMatrix = checkRange01(distMatrix)

# Estimate the optimal number of clusters
r = nClust(meanDist = distMatrix, p = 1, maxClust = 10,
  clusteringFunction = myKmeans, criterion = "silhouette")
sprintf("The optimal number of clusters found was %d.", r)

# K-means Clustering
labels = myKmeans(distMatrix, r)
plot(simuData, col = labels, asp = 1, xlab = '', ylab = '', main = 'K-means clustered data')
**nClustMulti**  

*Multiple Samples Optimal Number of Clusters Estimation*

**Description**

Estimates the optimal number of clusters for multiple samples using either Slope or Silhouette criterion. The optimal number of clusters will be verified in the range 2,..., maxClust. Takes the mean of all samples in order to perform the estimation.

**Usage**

```r
nClustMulti(dataDist, p = 1, maxClust = 20, clusteringFunction, criterion = c("slope", "silhouette"))
```

**Arguments**

- `dataDist`: An matrix with n subjects. Each subject has the size of NxN and represents the distances between the elements of the sample.
- `p`: Slope adjust parameter.
- `maxClust`: The maximum number of clusters to be tried.
- `clusteringFunction`: The clustering function to be used.
- `criterion`: The criterion that will be used for estimating the number of clusters. The options are "slope" or "silhouette". If not defined, "slope" will be used.

**Value**

The optimal number of clusters.

**References**


**Examples**

```r
# Install packages if necessary
# install.packages("MASS")
# install.packages("cluster")

library(anocva)
library(MASS)
library(cluster)

set.seed(5000)
```
# A k-means function that returns cluster labels directly.
myKmeans = function(dist, k){
  return(kmeans(dist, k, iter.max = 50, nstart = 5)$cluster)
}

# Number of subjects in each population
nsub = 25
# Number of items in each subject
nitem = 60

# Generate simulated data
data = array(NA, c(nsub, nitem*2, 2))
data.dist = array(NA, c(nsub, nitem*2, nitem*2))
meanx = 2
delta = 0.5

# Covariance matrix
sigma = matrix(c(0.03, 0, 0, 0.03), 2)
for (i in seq(nsub)){
  sub = rbind(mvrnorm(nitem, mu = c(0, 0), Sigma = sigma ),
           mvrnorm(nitem, mu = c(meanx,0), Sigma = sigma))
data[i,,] = sub
data.dist[i,,] = as.matrix(dist(data[i,,]))
}

# Estimate the optimal number of clusters
r = nClustMulti(dataDist = data.dist, p = 1, maxClust = 20,
                 clusteringFunction = myKmeans, criterion = "slope")
sprintf("The optimal number of clusters found was %d.", r)

---

spectralClustering  Spectral clustering

Description


Usage

spectralClustering(W, k)

Arguments

W       NxN similarity matrix
k       Number of clusters
Value

Cluster labels

References


Examples

```r
# Install igraph if necessary
# install.packages('igraph')
# install.packages('cluster')

library(anocva)

set.seed(2000)

if (requireNamespace("igraph", quietly = TRUE)) {
  # Create a tree graph
  treeGraph = igraph::make_tree(80, children = 4, mode = "undirected")

  # Visualize the tree graph
  plot(treeGraph, vertex.size = 10, vertex.label = NA)

  # Get the adjacency matrix of the tree graph
  adj = as.matrix(igraph::get.adjacency(treeGraph))

  # Cluster the tree graph into four clusters
  cluster = spectralClustering(adj, 4)

  # See the result clustering
  plot(treeGraph, vertex.size=10, vertex.color = cluster, vertex.label = NA)
}
```
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