

# Package ‘MCSim’

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**Type** Package

**Title** Determine the Optimal Number of Clusters

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**Description** Identifies the optimal number of clusters by calculating the similarity between two clustering methods at the same number of clusters using the corrected indices of Rand and Jaccard as described in Albatineh and Niewiadomska-Bugaj (2011). The number of clusters at which the index attain its maximum more frequently is a candidate for being the optimal number of clusters.

**Depends** R (>= 3.1.0)

**Imports** MASS,CircStats,stats,graphics

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**Description**

This package identifies the optimal number of clusters by calculating the similarity between two clustering methods at the same number of clusters using the corrected indices of Rand and Jaccard as described in Albatineh and Niewiadomska-Bugaj (2011). The number of clusters at which the index attain its maximum more frequently is a candidate for being the optimal number of clusters.

**Usage**

```
MCS(data1=data1, nc=nc, method1="method1", method2="method2", index="index",
    print.stats=FALSE, st.data=FALSE, plot.hc=FALSE, circ=FALSE,
    convert=TRUE, plot.data=FALSE)
```

**Arguments**

data1	Numeric data matrix to be clustered.
nc	Maximum number of clusters, similarity will be calculated for $2 \leq nc < n-1$
method1	First clustering method to be used. One of "single", "average", "complete", "ward", "median", "mcquitty", "kmeans")
method2	Second clustering method to be used. One of "single", "average", "complete", "ward", "median", "mcquitty",
index	Similarity index to be used. Either "rand" or "jaccard" index which will be corrected for chance agreement
print.stats	Logical, if "TRUE" the similarity will be outputed for each value between 2 and nc
st.data	Logical, if "TRUE" data will be standadrized. This is for linear (non-circular) data only
plot.hc	Logical, if "TRUE" hierarchical clustering tree (dendrogram) will be produced. This is for linear (non-circular) data only
circ	Logical, if "TRUE" data are circular or measured as angles
convert	Logical, if "TRUE" data will be converted from angular to radians. This is for circular data only
plot.data	Logical, if "TRUE" a circular plot of the data will be produced. This is for circular data only

**Details**

The distance measure used to calculate the distance for linear data is the Euclidean distance. For circular data the distance is calculated using the formula  $d_{ij} = 0.5 * (1 - \cos(A_{ii} - B_{jj}))$ . The correction for Rand index is based on the expectation by Hubert and Arabie (1985). For correcting Jaccard index, see Albatineh & Niewiadomska-Buga (2011).

**Value**

Similarity between the two clustering algorithms at each value of  $nc$  will be calculated, where  $2 \leq nc < n - 1$ , and a plot of the number of clusters vs. the value of either similarity index  $rand$  or  $jaccard$  will be produced.

**Note**

The following packages are needed: "MASS", "CircStats", "stats", "datasets", "graphics"

**Author(s)**

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**References**

Albatineh, A. N., Niewiadomska-Bugaj, M., & Mihalko, D. (2006). On similarity indices and correction for chance agreement. *Journal of Classification*, 23(2), 301-313.

Albatineh, A. N., & Niewiadomska-Bugaj, M. (2011). Correcting Jaccard and other similarity indices for chance agreement in cluster analysis. *Advances in Data Analysis and Classification*, 5(3), 179-200.

Albatineh, A. N., & Niewiadomska-Bugaj, M. (2011). MCS: A method for finding the number of clusters. *Journal of classification*, 28(2), 184-209.

Albatineh, A. N. (2010). Means and variances for a family of similarity indices used in cluster analysis. *Journal of Statistical Planning and Inference*, 140(10), 2828-2838.

**Examples**

```
library("MASS")
library("CircStats")
library("stats")
library("datasets")
library("graphics")
##### Simulated data from four bivariate normal distributions
set.seed(12345)
clust1<- mvrnorm(100,mu=c(5,5),Sigma=matrix(c(1,0.5,0.5,1),ncol=2))
clust2<- mvrnorm(100,mu=c(5,20),Sigma=matrix(c(1,0.5,0.5,1),ncol=2))
clust3<- mvrnorm(100,mu=c(20,5),Sigma=matrix(c(1,0.5,0.5,1),ncol=2))
clust4<- mvrnorm(100,mu=c(20,20),Sigma=matrix(c(1,0.5,0.5,1),ncol=2))
simdat<- rbind(clust1,clust2,clust3,clust4)

MCS(data1=simdat, nc=10, method1="single", method2="ward.D2", index="rand", print.stats=TRUE,
st.data=FALSE, plot.hc=FALSE)

MCS(data1=simdat, nc=10, method1="kmeans", method2="single", index="rand", print.stats=TRUE,
st.data=FALSE, plot.hc=FALSE)
#####
## Data from three bivariate normal distributions (elongated clusters)
set.seed(1965)
clust1<- mvrnorm(100,mu=c(5,5),Sigma=matrix(c(1,0.9,0.9,1),ncol=2))
clust2<- mvrnorm(100,mu=c(5,20),Sigma=matrix(c(1,0.9,0.9,1),ncol=2))
```

```

clust3<- mvrnorm(100,mu=c(20,5),Sigma=matrix(c(1,0.9,0.9,1),ncol=2))
simdat<- rbind(clust1,clust2,clust3)

MCS(data1=simdat, nc=10, method1="complete", method2="average", index="rand", print.stats=TRUE,
st.data=FALSE, plot.hc=FALSE)

MCS(data1=simdat, nc=10, method1="median", method2="kmeans", index="rand", print.stats=TRUE,
st.data=FALSE, plot.hc=FALSE)
#####
## Old Faithful Geyser Data Example #####
library("datasets")
data1<- as.matrix(faithful,nrows=272,ncol=2,byrows=TRUE)

MCS(data1=data1, nc=10, method1="average", method2="ward.D2", index="rand", print.stats=TRUE,
st.data=FALSE, plot.hc=FALSE)

MCS(data1=data1, nc=10, method1="average", method2="kmeans", index="jaccard", print.stats=TRUE,
st.data=FALSE, plot.hc=FALSE)
### Simulated Circular data from five von Mises distributions ###
set.seed(1945)
clust1<- as.vector(rvm(50,5,15))
clust2<- as.vector(rvm(50,10,15))
clust3<- as.vector(rvm(50,15,15))
clust4<- as.vector(rvm(50,20,15))
clust5<- as.vector(rvm(50,25,15))
data1<- rbind(clust1,clust2,clust3,clust4,clust5)
MCS(data1=data1, nc=10, method1="kmeans", method2="complete", index="rand", print.stats=TRUE,
circ=TRUE, convert=FALSE, plot.data=FALSE)
### Turtles Data Example
turtles<- c(8,9,13,13,14,18,22,27,30,34,
38,38,40,44,45,47,48,48,48,48,50,53,56,
57,58,58,61,63,64,64,64,65,65,68,70,73,
78,78,78,83,83,88,88,88,90,92,92,93,95,
96,98,100,103,106,113,118,138,153,153,
155,204,215,223,226,237,238,243,244,250,
251,257,268,285,319,343,350)

MCS(data1=turtles, nc=10, method1="single", method2="ward.D2", index="rand", print.stats=TRUE,
circ=TRUE, convert=TRUE, plot.data=FALSE)

MCS(data1=turtles, nc=10, method1="ward.D2", method2="kmeans", index="jaccard", print.stats=TRUE,
circ=TRUE, convert=TRUE, plot.data=FALSE)
##### Wind data example ##
wind<- c(67,87,101,101,101,103,131,140,140,142,144,149,182,
199,206,251,253,278,279,287,290,295,299,301,301,307,308,308,
309,310,312,316,319,319,325,325,326,331,344,15)

MCS(data1=wind, nc=10, method1="ward.D2", method2="median", index="jaccard", print.stats=TRUE,
circ=TRUE, convert=TRUE, plot.data=FALSE)

MCS(data1=wind, nc=10, method1="complete", method2="average", index="jaccard", print.stats=TRUE,
circ=TRUE, convert=TRUE, plot.data=FALSE)

```

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