Package 'Modalclust'

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Type Package

Title Hierarchical Modal Clustering

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Description Performs Modal Clustering (MAC) including Hierarchical Modal Cluster-
ing (HMAC) along with their parallel implementation (PHMAC) over several proces-
sors. These model-based non-parametric clustering techniques can extract clus-
ters in very high dimensions with arbitrary density shapes. By default clustering is per-
formed over several resolutions and the results are summarised as a hierarchical tree. Associ-
ated plot functions are also provided. There is a package vignette that provides many exam-
ples. This version adheres to CRAN policy of not spanning more than two child processes by de-
fault.

Depends R (>= 2.14.0), mvtnorm, zoo, class

Suggests parallel, MASS

License GPL-2

NeedsCompilation no

Repository CRAN

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choose.cluster	*Choosing the cluster which is closest to a specified point*

Description

Choosing the cluster which is closest to a point specified by user. Works only for two dimensional
data.

Usage

```
choose.cluster(hmacobj,x=NULL,level=NULL,n.cluster=NULL)
```

Arguments

hmacobj	The output of HMAC analysis. An object of class 'hmac'.
x	The user-specified location. Deafult value is NULL in which case user chooses a point using the locator function.
level	The specified level
n.cluster	The specified number of clusters. Either `level` or `n.cluster` needs to be specified

Author(s)

Surajit Ray and Yansong Cheng

References

Li. J, Ray. S, Lindsay. B. G, "A nonparametric statistical approach to clustering via mode identification," Journal of Machine Learning Research , 8(8):1687-1723, 2007.

Lindsay, B.G., Markatou M., Ray, S., Yang, K., Chen, S.C. "Quadratic distances on probabilities: the foundations," The Annals of Statistics Vol. 36, No. 2, page 983–1006, 2008.

See Also

[phmac](#) for front end of using modal clustering and also for parallel implementation of modal clustering.

Examples

```
data(disc2d.hmac)
#disc2d.hmac is the output of phmac(disc2d,npart=1)

choose.cluster(disc2d.hmac,x=c(0,0),level=3)
choose.cluster(disc2d.hmac,x=c(0,0),n.cluster=2)

# Users can choose anypoint they want by clicking the point
# in the plot after the following command.
# choose.cluster(disc2d.hmac,level=3)
```

---

contour.hmac	*Plot clusters with different colors for two dimensional data overlayed on the contours of the original data.*

Description

Plot clusters for two dimensional data with contours of the original data

Usage

```
## S3 method for class 'hmac'
contour(x, n.cluster=NULL,level=NULL,prob=NULL,smoothplot=FALSE,...)
```

Arguments

x	The output of HMAC analysis. An object of class 'hmac'.
level	The specified level
n.cluster	The specified number of clusters. Either `level` or `n.cluster` needs to be specified
prob	The specified level of the contour plot. Default value is NULL, plot all levels of the contour plot. Must be between 0 and 1
smoothplot	Get the smooth scatter plot of the original data set. Default value is FALSE, which does not provide the smooth scatter plot.
...	Further arguments passed to or from other methods.

Author(s)

Surajit Ray and Yansong Cheng

References

Li. J, Ray. S, Lindsay. B. G, "A nonparametric statistical approach to clustering via mode identification," Journal of Machine Learning Research , 8(8):1687-1723, 2007.

Lindsay, B.G., Markatou M., Ray, S., Yang, K., Chen, S.C. "Quadratic distances on probabilities: the foundations," The Annals of Statistics Vol. 36, No. 2, page 983–1006, 2008.

See Also

phmac for front end of using modal clustering and also for parallel implementation of modal clustering. soft.hmac for soft clustering at specified levels. hard.hmac for hard clustering at specified levels. See plot for plotting the whole dendrogram.

Examples

```
data(disc2d.hmac)
# disc2d.hmac is the output of phmac(disc2d,npart=1)

contour.hmac(disc2d.hmac,level=3,col=gray(0.7))

# Provide contour line at probability density 0.05.
contour(disc2d.hmac,n.cluster=2,prob=0.05)

# Plot using smooth scatter plot.
contour.hmac(disc2d.hmac,n.cluster=2,smoothplot=TRUE)
```

---

cta20   *Two dimensional data in original and log scale*

Description

Two dimensional data in original and log scale and their hierarchical modal clustering. This dataset demonstrates the fact that modal clustering techniques can be used to cluster untransformed data as it does not depend on parametric assumptions. The clustering results, before and after the log transformation both produce nice separation of the three clusters.

Usage

```
data(cta20)
data(cta20.hmac)
data(logcta20)
data(logcta20.hmac)
```

Format

cta20 and logcta20 are two dimensional matrices. cta20.hmac and logcta20.hmac are objects of class hmac obtained from applying phmac on cta20 and logcta20 respectively

Details

The dataset is generated by illumina technology for high throughput genotyping named **GOLDEN GATE**. The data values are actual measurements made by the machine (intensity), after these are normalized (background subtracted etc). The data set is used for making genotype calls by Illumina. The data around X- and Y-axes represents the two homozygous genotypes (e.g. AA and TT), while the cluster along the 45-degree line represents the heterozygous (e.g. AT) genotype. Due to noisy reads, the data points often lie in-between the axes, and cluster detection is used for making automatic genotype calls.

Author(s)

Surajit Ray and Yansong Cheng

Examples

```
data(logcta20)
data(logcta20.hmac)
plot(logcta20)
plot(logcta20.hmac)
plot(logcta20.hmac,level=4)
```

---

disc2d   *Two and three dimensional data representing two half discs*

Description

Two and three dimensional data and their hierarchical modal clustering with 400 observations where the first two dimensions represent the shape of two discs.

Usage

```
data(disc2d)
data(disc2d.hmac)
data(disc3d)
data(disc3d.hmac)
```

Format

disc2d and disc3d are two and three dimensional matrices. disc2d.hmac and disc3d.hmac are objects of class hmac obtained from applying phmac on disc2d and disc3d respectively

Details

Two dimensional data with 400 observations representing the shape of two half discs.

Author(s)

Surajit Ray and Yansong Cheng

References

Li. J, Ray. S, Lindsay. B. G, "A nonparametric statistical approach to clustering via mode identification," Journal of Machine Learning Research , 8(8):1687-1723, 2007.

Lindsay, B.G., Markatou M., Ray, S., Yang, K., Chen, S.C. "Quadratic distances on probabilities: the foundations," The Annals of Statistics Vol. 36, No. 2, page 983–1006, 2008.

Examples

```
data(disc2d)
plot(disc2d)
data(disc2d.hmac)
summary.hmac(disc2d.hmac)
hard.hmac(disc2d.hmac,n.clust=2)
```

---

findmid   *Find the mid point of memberships of each cluster*

Description

Find the mid point of memberships of each cluster. Sub function of [`plot.hmac`](#).

Usage

```
findmid(x,memb)
```

Arguments

x	Input data
memb	Membership of each observation

Author(s)

Surajit Ray and Yansong Cheng

See Also

[`plot`](#) for plotting the dendrogram

---

hard.hmac   *Plot clusters with different colors.*

Description

Plot clusters with colors obtained from hard density. Plot one dimensional data with density plot.
Plot two dimensional data with scatter plot. Pairwise scatter plot will be provided for data with
more than two dimensions.

Usage

```
hard.hmac(hmacobj,level=NULL, n.cluster=NULL,plot=TRUE,colors=1:6,...)
```

Arguments

hmacobj	The output of HMAC analysis. An object of class 'hmac'.
level	The specified level of HMAC output
n.cluster	The specified number of clusters. If neither level nor n.cluster is specified, hard clustering output is shown for each level.
plot	Get the plot of the clusters with different colors. Default value is TRUE, draws a plot on the current graphics device; plot=FALSE indicates do not get the plot and returns the membership of data.
colors	Colors used to represent different clusters.
...	Further graphical parameters

Value

Returns the membership of each observation of the specified level if plot=FALSE

Author(s)

Surajit Ray and Yansong Cheng

References

Li. J, Ray. S, Lindsay. B. G, "A nonparametric statistical approach to clustering via mode identification," Journal of Machine Learning Research , 8(8):1687-1723, 2007.

Lindsay, B.G., Markatou M., Ray, S., Yang, K., Chen, S.C. "Quadratic distances on probabilities: the foundations," The Annals of Statistics Vol. 36, No. 2, page 983–1006, 2008.

See Also

phmac for front end of using modal clustering and also for parallel implementation of modal clustering soft.hmac for soft clustering at specified levels. See plot.hmac.

Examples

```
data(disc2d.hmac)
#disc2d.hmac is the output of phmac(disc2d,npart=1)

hard.hmac(disc2d.hmac,level=3)

#returns the membership of each observation
disc2d.2clus=hard.hmac(hmacobj=disc2d.hmac,n.cluster=2,plot=FALSE)
table(disc2d.2clus)

#hard.hmac(disc2d.hmac)

iris.hmac=phmac(iris[,-5])
# For more than two dimensions it produces the pairs plot
hard.hmac(iris.hmac,n.cluster=2)
```

---

hmac   *Perform Modal Clustering in serial mode only*

Description

Performs Modal Cluster with specified smoothing paramters. Used as a sub function of [phmac](#).

Usage

```
hmac(dat,Sigmas,G=NULL,member=NULL)
```

Arguments

dat	Matrix of data points
Sigmas	Specified smoothing levels
G	Specified values of modes. A matrix with number of rows equal to the number of modes and number of columns equal to the dimension of the data. Defualt value is NULL
member	Membership of the observations to the modes given in G. Default value is NULL

Value

data	Same as the input dat.
n.cluster	Number of clusters at each level.
level	Levels corresponding to each smoothing parameter.
Sigmas	Same as input sigmas.
mode	List of modes at each distinct levels.
membership	List of memmbership to modes at each distinct levels.

Author(s)

Surajit Ray and Yansong Cheng

References

Li. J, Ray. S, Lindsay. B. G, "A nonparametric statistical approach to clustering via mode identification," Journal of Machine Learning Research , 8(8):1687-1723, 2007.

Lindsay, B.G., Markatou M., Ray, S., Yang, K., Chen, S.C. "Quadratic distances on probabilities: the foundations," The Annals of Statistics Vol. 36, No. 2, page 983–1006, 2008.

See Also

[phmac](#) for front end of using modal clustering and also for parallel implementation of modal clustering.

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khat.inv	*Calculate the smoothing paramters for implementation of Modal Clustering.*

Description

these set of functions are based on the concept of pseudo degrees of freedom (Lindsay et al 2008) and are used to calculate the Sigmas that are used for the 'hmac' function

Usage

```
khat.inv(p,len=10)
sdofnorm(h,p)
khat(dof,p)
```

Arguments

len	Number of smoothing parameters.
h	Smoothing parameter
p	Number of column of data
dof	Degrees of freedom

Author(s)

Surajit Ray

References

Lindsay, B.G., Markatou M., Ray, S., Yang, K., Chen, S.C. "Quadratic distances on probabilities: the foundations," The Annals of Statistics Vol. 36, No. 2, page 983–1006, 2008.

See Also

[phmac](#) for front end of using HMAC and also for parallel implementation of modal clustering.

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mydmvnorm	*Calculate Density of Multivariate Normal for diagonal covariance*

Description

Faster calculation of density of multivariate normal with diagonal covariance matrix

Usage

```
mydmvnorm(x, mean, sigmasq)
```

Arguments

x	The input data
mean	The vector of mean values
sigmasq	The variance of each dimension. Assume the variance are the same for all dimensions.

Author(s)

Surajit Ray and Yansong Cheng

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oned   *One dimensional data with two main clusters*

Description

A one dimensional data and its hierarchical modal clustering with 2 main clusters

Usage

```
data(oned)
data(oned.hmac)
```

Format

oned is a one dimensional data with 2 main clusters and several subclusters. oned.hmac is an object of class 'hmac' obtained from applying phmac on disc2d and disc3d respectively

Author(s)

Surajit Ray and Yansong Cheng

References

Li. J, Ray. S, Lindsay. B. G, "A nonparametric statistical approach to clustering via mode identification," Journal of Machine Learning Research , 8(8):1687-1723, 2007.

Lindsay, B.G., Markatou M., Ray, S., Yang, K., Chen, S.C. "Quadratic distances on probabilities: the foundations," The Annals of Statistics Vol. 36, No. 2, page 983–1006, 2008.

Examples

```
data(oned)
hist(oned,col="lavender",n=15)
data(oned.hmac)
plot(oned.hmac)
plot(oned.hmac,n.clust=2)
```

---

phmac	*Main function for performing Modal Clusters either parallel or serial mode.*

Description

Performing Modal Clustering

Usage

```
phmac(dat, length = 10, npart = 1, parallel = TRUE, sigmaselect = NULL,
G= NULL)
modalclust(dat, length = 10, npart = 1, parallel = TRUE, sigmaselect = NULL,
G= NULL)
```

Arguments

dat	Matrix of data points
length	number of smoothing levels. Default is 10
sigmaselect	Specified Smoothing levels. Default NULL will calculate the Sigma levels using concept of spectral degrees of freedom given in Lindsay et al (2008)
npart	Number of random partitions when using parallel computing. If using several processors of a machine one option is to choose the number of partitions equal to the number of processors
parallel	If TRUE uses parallel comptation using npart processors. Requires the package multicore to perform parallel computing
G	Specified values of modes. A matrix with number or rows equal to the number of modes and number of columns equal to the dimension of the data. Defualt value is NULL

Value

data	Same as the input Data
n.cluster	Number of clusters at each level.
level	Levels corresponding to each smoothing parameter.
sigmas	Same as input sigmaselect if provided or dynamically calculated smoothing levels based on Spectral Degrees of Freedom criterion. Uses the function khat.inv
mode	List of modes at each distinct levels.
membership	List of memmbership to modes at each distinct levels.

Author(s)

Surajit Ray and Yansong Cheng

References

Li. J, Ray. S, Lindsay. B. G, "A nonparametric statistical approach to clustering via mode identification," Journal of Machine Learning Research , 8(8):1687-1723, 2007.

Lindsay, B.G., Markatou M., Ray, S., Yang, K., Chen, S.C. "Quadratic distances on probabilities: the foundations," The Annals of Statistics Vol. 36, No. 2, page 983–1006, 2008.

See Also

`soft.hmac` for soft clustering at specified levels. `hard.hmac` for hard clustering at specified levels. See `plot.hmac`.

Examples

```
data(disc2d)
## Not run: disc2d.hmac=phmac(disc2d,npart=1)

plot.hmac(disc2d.hmac,level=2)


## For parallel implementation
## Not run: disc2d.hmac.parallel=phmac(disc2d,npart=2,parallel=TRUE)

soft.hmac(disc2d.hmac,level=2)
soft.hmac(disc2d.hmac,n.cluster=3)

hard.hmac(disc2d.hmac,n.cluster=3)
```

---

plot.hmac   *Plots of heierarchical tree for a 'hmac' object*

Description

Plots the dendrogram of the entire heierarchical tree for a 'hmac' object starting from any specified smoothing level.

Usage

```
## S3 method for class 'hmac'
plot(x,mycol=1:6,level=1,n.cluster=NULL,userclus=NULL,sep=.1,...)
```

Arguments

x	The output of HMAC analysis. An object of class 'hmac'.
mycol	Colors used to represent different clusters.
level	The specified level that dendrogram starts. Default value is 1.
n.cluster	The specified number of clusters. If neither `level` nor `n.cluster` is specified, the full tree is plotted.

userclus	If user provides membership, the tree colors the node according to this membership and the tree can be used for validation.
sep	It provides the distance between the lowest layer of nodes of the clusters.
...	further arguments passed to or from other methods.

Author(s)

Surajit Ray and Yansong Cheng

References

Li. J, Ray. S, Lindsay. B. G, "A nonparametric statistical approach to clustering via mode identification," Journal of Machine Learning Research , 8(8):1687-1723, 2007.

Lindsay, B.G., Markatou M., Ray, S., Yang, K., Chen, S.C. "Quadratic distances on probabilities: the foundations," The Annals of Statistics Vol. 36, No. 2, page 983–1006, 2008.

See Also

phmac for front end of using modal clustering and also for parallel implementation of modal clustering. hard.hmac for hard clustering at specified levels. soft.hmac for soft clustering at specified levels.

Examples

```
data(disc2d.hmac)
# disc2d.hmac is the output of phmac(disc2d,npart=1)
plot(disc2d.hmac)

set.seed(20)
mix4=data.frame(rbind(rmvnorm(20,rep(0,4)), rmvnorm(20,rep(2,4)),
                rmvnorm(20,rep(10,4)),rmvnorm(20,rep(13,4))))
mix4.hmac=phmac(mix4,npart=1)
plot(mix4.hmac,col=1:6)

# Verifying with user provided groups
plot(mix4.hmac,userclus=rep(c(1,2,3,4),each=20),col=1:6)
```

---

soft.hmac	*Plot soft clusters from Modal Clustering output*

Description

Plot clusters for two dimensional data with colors representing the posterior probability of belonging to clusters. Additionally boundary points between the clusters, with specified thresholds are also

Usage

```
soft.hmac(hmacobj,n.cluster=NULL,level=NULL,boundlevel=0.4,plot=TRUE)
```

Arguments

`hmacobj`	The output of HMAC analysis. An object of class 'hmac'.
`level`	The specified level of HMAC output
`n.cluster`	The specified number of clusters. If neither `level` nor `n.cluster` is specified, soft clustering output is shown for each level.
`boundlevel`	Posterior probability threshold. Points having posterior probability below `boundlevel` are assigned as boundary points and colored in gray. Default value is 0.4.
`plot`	Get the two dimensional plot of the clusters with different colors. Default value is TRUE, which returns the two dimensional plot on the current graphics device; plot=FALSE returns the posterior probability of each observation.

Value

Returns the list that contains the posterior probability of each observation and boundary points at specified level if plot=FALSE

Author(s)

Surajit Ray and Yansong Cheng

References

Li. J, Ray. S, Lindsay. B. G, "A nonparametric statistical approach to clustering via mode identification," Journal of Machine Learning Research , 8(8):1687-1723, 2007.

Lindsay, B.G., Markatou M., Ray, S., Yang, K., Chen, S.C. "Quadratic distances on probabilities: the foundations," The Annals of Statistics Vol. 36, No. 2, page 983–1006, 2008.

See Also

phmac for front end of using modal clustering and also for parallel implementation of modal clustering hard.hmac for hard clustering at specified levels.

Examples

```
data(logcta20.hmac)
#logcta20.hmac is the output of phmac(logcta20,npart=1)

soft.hmac(logcta20.hmac,n.cluster=3)

#return the posterior probability of each observation and boundary points.
postprob=soft.hmac(hmacobj=logcta20.hmac,n.cluster=3,plot=FALSE)
```

---

summary   *Summary of HMAC output*

Description

Gives the summary of output of a 'hmac' object.

Usage

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

Arguments

object	The output of HMAC analysis. An object of class 'hmac'.
...	further arguments passed to or from other methods.

Author(s)

Surajit Ray and Yansong Cheng

References

Li. J, Ray. S, Lindsay. B. G, "A nonparametric statistical approach to clustering via mode identification," Journal of Machine Learning Research , 8(8):1687-1723, 2007.

Lindsay, B.G., Markatou M., Ray, S., Yang, K., Chen, S.C. "Quadratic distances on probabilities: the foundations," The Annals of Statistics Vol. 36, No. 2, page 983–1006, 2008.

See Also

[phmac](#) for front end of using modal clustering and also for parallel implementation of modal clustering.

Examples

```
data(disc2d.hmac)
summary(disc2d.hmac)
```

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