

Package ‘MCRestimate’

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Title Misclassification error estimation with cross-validation

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Description This package includes a function for combining preprocessing and classification methods to calculate misclassification errors

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Depends R (>= 2.7.2), golubEsets (>= 1.4.6)

Imports e1071 (>= 1.5-12), pamr (>= 1.22), randomForest (>= 3.9-6), RColorBrewer (>= 0.1-3), Biobase (>= 2.5.5), graphics, grDevices, stats, utils

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LazyLoad yes

biocViews Classification

NeedsCompilation no

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class.factor.format *A function for creating a factor from the phenoData slot of an exprSet*

Description

This function creates a factor whose levels represent the different classes for a classification problem. It is derived from the column specified in the argument `class.column`. If the factor has more than two levels, the argument `reference.class` can be used to transform this into a two-class problem: reference class versus the rest.

Usage

```
class.factor.format(x, class.column, reference.class=NULL)
```

Arguments

<code>x</code>	an <code>exprSet</code>
<code>class.column</code>	either a number or a character string specifying the relevant column of the <code>phenoData</code> slot in <code>x</code>
<code>reference.class</code>	character vector. If specified the result will be a factor with only 2 levels: the reference class(es) versus all other

Value

A factor of length `nrow(pData(x))`

Author(s)

Markus Ruschhaupt <mailto:m.ruschhaupt@dkfz.de>

Examples

```
library(golubEsets)
data(Golub_Train)
class.factor.format(Golub_Train[,28:35], "FAB", reference="M1")
```

ClassifierBuild	<i>Building a classifier as a combination of preprocessing and classification method</i>
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Description

builds a classifier as a combination of preprocessing and classification methods

Usage

```
ClassifierBuild(eset,
               class.column,
               reference.class=NULL,
               classification.fun,
               variableSel.fun="identity",
               cluster.fun="identity",
               poss.parameters=list(),
               cross.inner=10,
               rand=123,
               information=TRUE,
               thePreprocessingMethods=c(variableSel.fun,cluster.fun))
```

Arguments

eset	an object of class <code>exprSet</code> or <code>exprSetRG</code>
class.column	a number or a character string which indicated the column of the expression set's phenodata containing the class label
reference.class	a character string with the name of one class - if specified the class will form the first class and all the other classes will form the second class
classification.fun	a character string which names the function that should be used for the classification
variableSel.fun	character string which names the function that should be used for variable selection
cluster.fun	character string which names the function that should be used for clustering the variables
thePreprocessingMethods	vector of character with the names of all preprocessing functions- can be used instead of 'variableSel.fun' and 'cluster.fun' - see details
poss.parameters	a list of possible values for the parameter of the classification method
cross.inner	integer - the number of nearly equal sized parts the train set should be divided into
rand	integer - the random number generator will be put in a reproducible state

`important.variable.names`*Writing tables with variable information*

Description

The information slot of a `MCRestimate` object may contain lists of variable names that are important for each classification. This function produces summary tables of these variables. It is assumed that the first column of each information list contains the variable names if not otherwise specified with the argument `listName`. This is important if someone wants to write a new wrapper for a classification method.

Usage

```
important.variable.names(mcr, file="important_variables", listName=NULL, writeFile=TRUE, ...)
```

Arguments

<code>mcr</code>	an object of class <code>MCRestimate</code>
<code>file</code>	a character string specifies the name of the output files
<code>listName</code>	a character string specifying the variable names vector in the information list
<code>writeFile</code>	Should the files be written?
<code>...</code>	Further arguments that are passed on to <code>plot.default</code>

Value

The function is called for its side effect, writing two tables with variable information.

Author(s)

Markus Ruschhaupt <mailto:m.ruschhaupt@dkfz.de>

Examples

```
library(golubEsets)
data(Golub_Train)

class.column <- "ALL.AML"
list.of.poss.parameter <- list(var.numbers = c(250,1000))
Preprocessingfunctions <- c("identity")
list.of.poss.parameter <- list(threshold = 6)
class.function <- "PAM.wrap"
plot.label <- "Samples"

cross.outer <- 10
cross.repeat <- 7
```

```
cross.inner <- 5

PAM.estimate <- MCReestimate(Golub_Train,
  class.column,
  classification.fun = class.function,
  thePreprocessingMethods = Preprocessingfunctions,
  poss.parameters = list.of.poss.parameter,
  cross.outer = cross.outer,
  cross.inner = cross.inner,
  cross.repeat = cross.repeat,
  plot.label = plot.label)

important.variable.names(PAM.estimate)
```

intersectList*A function for creating a all possible intersects for a list of sets.*

Description

The list contains several sets. The function calculates all possible intersections.

Usage

```
intersectList(x)
```

Arguments

x a list

Value

A list containing all possible intersections.

Author(s)

Markus Ruschhaupt <mailto:m.ruschhaupt@dkfz.de>

Examples

```
a <- list (x=1:5,y=3:4,z=c(1,3,3))
intersectList(a)
```

`MCRconfusion`*Summary tables for MCRestimate objects*

Description

`MCRwrongsamples` returns a matrix with all the samples that have a higher frequency of being predicted as a member of a wrong class than of the correct class for at least one classification method. `MCRconfusion` summarizes the result of the vote matrices

Usage

```
MCRwrongsamples(x,  
  col.names=names(x),  
  rownames.from.object=TRUE,  
  subgroup=NULL,  
  freq=FALSE)
```

```
MCRconfusion(x,  
  col.names=names(x),  
  row.names=NULL)
```

Arguments

<code>x</code>	List of objects of S3 class <code>MCRestimate</code>
<code>col.names</code>	Vector of strings used for column names. The length must match the number of objects in <code>x</code>
<code>rownames.from.object</code>	Logical. If <code>TRUE</code> then the sample names of the <code>MCRestimate</code> object in <code>x</code> are used as row names
<code>subgroup</code>	Logical. If <code>TRUE</code> then only the samples which belongs to the specified group are listed in the table
<code>freq</code>	Logical. If <code>TRUE</code> then the frequency with which each sample in the table has been misclassified will be printed.
<code>row.names</code>	Vector of strings used for row names. If not specified the names of the groups are used

Value

`MCRwrongsamples` returns a matrix and `MCRconfusion` returns a confusion matrix.

Author(s)

Markus Ruschhaupt <mailto:m.ruschhaupt@dkfz.de>

See Also[MCRestimate](#)**Examples**

```

library(golubEsets)
data(Golub_Train)
exSet <- Golub_Train[1:500,]
result1 <- MCRestimate(exSet,"ALL.AML",classification.fun="RF.wrap",cross.outer=3,cross.repeat=2)
result2 <- MCRestimate(exSet,"ALL.AML",classification.fun="PAM.wrap",poss.parameters=list(threshold=c(0.5,1)),
MCRwrongsamples(list(result1,result2),subgroup="AML",col.names=c("Random Forest","PAM"))
MCRconfusion(list(result1,result2),col.names=c("Random Forest","PAM"))

```

MCRestimate

*Estimation of misclassification error by cross-validation***Description**

Several repetitions of a cross-validation are performed to get 'votes' how stable a method is against different partitions into training and test set

Usage

```

MCRestimate(eset,
            class.column,
            reference.class=NULL,
            classification.fun,
            variableSel.fun="identity",
            cluster.fun="identity",
            poss.parameters=list(),
            cross.outer=10,
            cross.repeat=3,
            cross.inner=cross.outer,
            plot.label=NULL,
            rand=123,
            stratify=FALSE,
            information=TRUE,
            block.column=NULL,
            thePreprocessingMethods=c(variableSel.fun,cluster.fun))

```

Arguments

eset	an object of class ExpressionSet
class.column	a number or a character string which indicates the column of the expression set's phenodata containing the class label

reference.class	a character string - the name of one class - if specified, the class will form the first class and all the other classes will form the second class
classification.fun	character string which names the function that should be used for the classification
variableSel.fun	character string which names the function that should be used for the variable selection
cluster.fun	character string which names the function that should be used for the clustering of variables
thePreprocessingMethods	vector of character with the names of all preprocessing functions - can be used instead of 'variableSel.fun' and 'cluster.fun' - see details
poss.parameters	a list of possible values for the parameter of the classification, variable selection, and cluster methods
cross.outer	integer - the number of nearly equal sized parts the sample set should be divided into (outer cross-validation)
cross.repeat	integer - the number of repetitions of the cross-validation procedure
cross.inner	integer - the number of nearly equal sized parts the train set should be divided into (inner cross-validation)
plot.label	name of one column of the phenodata- if specified, the content of this column will form the labels of the x-axis if the 'votematrix' will be plotted with plot.MCRestimate
rand	integer - the random number generator will be put in a reproducible state
stratify	should a stratified version be used for the cross validation?
block.column	a character string which indicates the column of the expression set's phenodata containing the blocking covariate, which sets a constrain on the cross-validation splits: each block is either completely assigned to the test or to the training set
information	information - should classifier specific data be given(depends on the wrapper for the classification method)

Details

The argument 'thePreprocessingMethods' can be used instead of 'variableSel.fun' and 'cluster.fun'. In the first versions of MCRestimate it was only possible to have one variable selection and one cluster functions. Now it is possible to have more than two functions and the ordering is arbitrary, e.g. you can have a variable selection function, then a cluster function and then a second variable selection function.

If MCRestimate is used with an object of class `exprSetRG-class`, the preprocessing steps can use the green and the red channel separately but the classification methods works with green channel - red channel.

Note: 'correct prediction' means that a sample was predicted to be a member of the correct class at least as often as it was predicted to be a member of each other class. So in the two class problem a sample is also 'correct' if it has been predicted correctly half of the time.

Value

an object of class MCRestimate which is a list with fourteen arguments:

votes	a matrix consisting of the different votes for each sample
classes	the class of each sample
table	a 'confusion' table, shows the number of 'correct prediction' for each class
correct.prediction	a logical vector - indicates if a sample was predicted to be a member of the correct class at least as often as it was predicted to be a member of each other class.
correct.class.vote	vector that contains for every sample the vote for it's correct class
parameter	a list consisting of the estimated 'best' parameter for each cross-validation part
class.method	string which names the function used for the classification
thePreprocessingMethods	character string - name of the preprocessing functions that have been used
cross.outer	number of blocks for a the outer cross-validation
cross.repeat	number of outer cross-validation repetitions
cross.inner	number of blocks for a the inner cross-validation
sample.names	names of the sample
information	classifier specific data (if information is TRUE)

Author(s)

Markus Ruschhaupt <mailto:m.ruschhaupt@dkfz.de>, contributions from Andreas Buness and Patrick Warnat

Examples

```
library(golubEsets)
data(Golub_Test)
G2 <- Golub_Test[1:500,]
result <- MCRestimate(G2, "ALL.AML", classification.fun="RF.wrap",
                     cross.outer=4, cross.repeat=3)

result
if (interactive()) {
  x11(width=9, height=4)}
plot(result)
```

MCRestimateMerge *Merging objects of class MCRestimate*

Description

MCRestimateMerge merges objects of S3 class MCRestimate. See vignette MCRestimateBlueprint.Rnw for details.

Usage

```
MCRestimateMerge(MCRestimateList)
```

Arguments

MCRestimateList
list of objects of S3 class MCRestimate

Value

An objects of S3 class MCRestimate

Author(s)

Markus Ruschhaupt <mailto:m.ruschhaupt@dkfz.de>

See Also

[MCRestimate](#)

MCRindError *Individual Error of the outer cross-validations*

Description

MCRindError returns a vector with the individual number of incorrect classified samples for each cross-validation. plotIndGroupVotes plots the individual group votes.

Usage

```
MCRindError(MCRest,
perGroup=FALSE)

plotIndGroupVotes(MCRest,
PvD= 0.5,
dotCol="red",
errCol="black",
```

```
xlab="",  
ylab="# misclassified samples (mean + SD)",  
...)
```

Arguments

MCRE	Object of S3 class MCREstimate
perGroup	returns a vector with the individual number of incorrect classified samples for each group
MCREst	Object of S3 class MCREstimate
PvD	Offset of the text that belongs to a specific point in the plot
dotCol	Color of the dots
errCol	Line color between points
xlab	Label of X-Axis
ylab	Label of Y-Axis
...	Advanced options to the plot command

Value

MCRindError returns a vector of individual errors.

Author(s)

Markus Ruschhaupt <mailto:m.ruschhaupt@dkfz.de>

See Also

[MCREstimate](#)

Examples

```
library(golubEsets)  
data(Golub_Train)  
exSet <- Golub_Train[1:500,]  
result1 <- MCREstimate(exSet, "ALL.AML", classification.fun="RF.wrap", cross.outer=3, cross.repeat=3)  
MCRindError(result1)
```

plot.MCRestimate *Plot method for a objects of class MCRestimate*

Description

plot.MCRestimate visualizes a 'vote matrix'. A 'vote matrix' is the result of a classification procedure. For every sample (=row) *i* and every class (=column) *j* the matrix element [*i,j*] is the probability or frequency the classification method predicts sample *i* as a member of class *j*.

Usage

```
## S3 method for class 'MCRestimate'
plot(x,
      class.factor=NULL,
      rownames.from.object=FALSE,
      sample.order=TRUE,
      legend=FALSE,
      mypalette=NULL,
      shading=NULL,
      xlab="Sample ID",
      ylab="Frequency of correct classification",
      cex.axis=1,...)
```

Arguments

<code>x</code>	Object of S3 class MCRestimate or a matrix
<code>class.factor</code>	Factor. Its length must match the number of rows in <code>x</code> and the levels must be the same as the colnames in <code>x</code> . If <code>x</code> is of class MCRestimate this argument will be ignored.
<code>rownames.from.object</code>	Logical. If TRUE then the rownames of the matrix or the sample names of MCRestimate in <code>x</code> are used as labels for the x-axis
<code>sample.order</code>	Logical. If TRUE then the samples are ordered by class membership
<code>legend</code>	Logical. If TRUE then there will be a small legend in the output
<code>mypalette</code>	vector with length equal to the number of classes. The vector specifies the color for the bar representing the classes. If 'NULL' colors chosen by the author are used.
<code>shading</code>	the density of shading lines for the rectangles that indicate the groups, in lines per inch. The default value of 'NULL' means that no shading lines are drawn.
<code>xlab</code>	Character
<code>ylab</code>	Character
<code>cex.axis</code>	numeric
<code>...</code>	Further arguments that are passed on to plot.default

Value

The function is called for its side effect, creating a plot on the active graphics device.

Author(s)

Markus Ruschhaupt <mailto:m.ruschhaupt@dkfz.de>

See Also

[MCReestimate](#)

Examples

```
x <- c(0.5, 0.3, 0.7, 0.3, 0.8, 0.2, 0.3)
mat2 <- cbind(x, 1-x)
fac2 <- factor(c("low", rep("high", 3), rep("low", 3)))
colnames(mat2) <- levels(fac2)

mat3 <- cbind(x/3, 2*x/3, 1-x)
fac3 <- factor(c(rep("high", 3), rep("intermediate", 2), rep("low", 2)))
colnames(mat3) <- levels(fac3)
if (interactive()) {
  x11(width=9, height=9)
  par(mfrow=c(3,1))
  plot.MCReestimate(mat2, fac2)
  plot.MCReestimate(mat2, fac2, sample.order=FALSE)
  plot.MCReestimate(mat3, fac3)
```

PLR

A function which performs penalised logistic regression classification for two groups

Description

A function which performs penalised logistic regression.

Usage

```
PLR(trainmatrix, resultvector, kappa=0, eps=1e-4)
  ## S3 method for class 'PLR'
predict(object,...)
```

Arguments

`resultvector` a vector which contains the labeling of the samples
`trainmatrix` a matrix which includes the data. The rows corresponds to the observations and the columns to the variables.

kappa	value range for penalty parameter. If more than one parameter is specified the one with the lowest AIC will be used.
eps	precision of convergence
object	a fitted PLR model
...	here a data matrix from samples that should be predicted

Value

a list with three arguments

a	Intercept estimate of the linear predictor
b	vector of estimated regression coefficients
factorlevel	levels of grouping variable
aics	vector of AIC values with respect to penalty parameter kappa
trs	vector of effective degrees of freedom with respect to penalty parameter kappa

Author(s)

Axel Benner, Ulrich Mansmann, based on MathLab code by Paul Eilers

Examples

```
library(golubEsets)
data(Golub_Merge)
eSet<-Golub_Merge
X0 <- t(exprs(eSet))
m <- nrow(X0); n <- ncol(X0)
y <- pData(eSet)$ALL.AML
f <- PLR(X0, y, kappa=10^seq(0, 7, 0.5))
if (interactive()) {
  x11(width=9, height=4)
  par(mfrow=c(1,2))
  plot(log10(f$kappas), f$aics, type="l", main="Akaike's Information Criterion", xlab="log kappa", ylab="AIC")
  plot(log10(f$kappas), f$trs, type="l", xlab="log kappa",
        ylab="Dim", main="Effective dimension")
}
```

replace.NA

Replaces in a given numeric matrix NA values per row or per column.

Description

Replaces in a given numeric matrix NA values per row or per column.

Usage

```
replace.NA(x, replacement, byRow = TRUE)
```

Arguments

x	numeric input matrix
replacement	numeric vector containing the values which are used for NA replacement. If byRow = TRUE, this vector must contain as many values as matrix X has rows. Else, this vector must contain as many elements as matrix X has columns.
byRow	logical. If TRUE, then NA values in row n are replaced by the value at position n in the vector 'replacement'. Else, NA values are replaced according to their column position.

Value

The numeric input matrix with replaced NA values.

Author(s)

Patrick Warnat <mailto:p.warnat@dkfz-heidelberg.de>

RF.wrap

Wrapper function for different classification methods

Description

Wrapper function for different classification methods used by MCRestimator. These functions are mainly used within the function [MCRestimate](#)

Usage

```
RF.wrap(x,y,...)
PAM.wrap(x,y,threshold,...)
PLR.wrap(x,y,kappa=0,eps=1e-4,...)
SVM.wrap(x,y,gamma = NULL, kernel = "radial", ...)
GPLS.wrap(x,y,...)
```

Arguments

x,y	x is a matrix where each row refers to a sample a each column refers to a gene; y is a factor which includes the class for each sample
threshold	the threshold for PAM
kappa	the penalty parameter for the penalised logistic regression
eps	precision of convergence
gamma	parameter for support vector machines
kernel	parameter for support vector machines
...	Further parameters

Value

Every function return a predict function which can be used to predict the classes for a new data set.

Author(s)

Markus Ruschhaupt <mailto:m.ruschhaupt@dkfz.de>

See Also

[MCReestimate](#)

Examples

```
library(golubEsets)
data(Golub_Train)

class.column <- "ALL.AML"
Preprocessingfunctions <- c("varSel.highest.var")
list.of.poss.parameter <- list(threshold = 6)

Preprocessingfunctions <- c("identity")
class.function <- "PAM.wrap"
plot.label <- "Samples"

cross.outer <- 10
cross.repeat <- 7
cross.inner <- 5

PAM.estimate <- MCReestimate(Golub_Train,
  class.column,
  classification.fun = class.function,
  thePreprocessingMethods = Preprocessingfunctions,
  poss.parameters = list.of.poss.parameter,
  cross.outer = cross.outer, cross.inner = cross.inner,
  cross.repeat = cross.repeat, plot.label = plot.label)
```

select.NA.elements *Selects NA values of a given numeric matrix*

Description

Selects of a given numeric matrix rows or columns containing more NA values than defined by a given threshold.

Usage

```
select.NA.elements(x, NAtreshold, byRow = TRUE)
```

Arguments

x	numeric input matrix
NAthreshold	numeric value between 0 and 1, determining the allowed percentage of NA values per row or column. Rows or columns containing more NA values are selected.
byRow	logical. If TRUE, then rows with more NA values than determined by the argument threshold are selected, else columns.

Value

logical vector containing the row or column selection. If argument byRow = TRUE, then value contains as many values as the input matrix contains rows, else it contains as many values as the input matrix contains columns.

Author(s)

Patrick Warnat <mailto:p.warnat@dkfz-heidelberg.de>

SVM.OVA.wrap

SVM with 'One-Versus-All' multiclass approach

Description

Multiclass approach where k binary SVM classifiers are constructed for a classification problem with k classes: Every classifier is trained to distinguish samples of one class from samples of all other classes. For prediction of the class of a new sample, the sample is classified by all k classifiers, and the class corresponding to the classifier with the maximum decision value is chosen.

Usage

```
SVM.OVA.wrap(x,y,gamma = NULL, kernel = "radial", ...)
```

Arguments

x,y	x is a matrix where each row refers to a sample and each column refers to a gene; y is a factor which includes the class for each sample
gamma	parameter for support vector machines
kernel	parameter for support vector machines
...	Further parameters

Value

A predict function which can be used to predict the classes for a new data set.

Author(s)

Patrick Warnat <mailto:p.warnat@dkfz-heidelberg.de>

See Also

[MCReestimate](#)

Examples

```
## Not run:
library(golubEsets)
data(Golub_Train)

class.column <- "ALL.AML"
Preprocessingfunctions <- c("varSel.highest.var")
list.of.poss.parameter <- list(var.numbers = c(250,1000))

Preprocessingfunctions <- c("identity")
class.function <- "SVM.OVA.wrap"
list.of.poss.parameter <- list(gamma = 6)
plot.label <- "Samples"

cross.outer <- 10
cross.repeat <- 20
cross.inner <- 5

SVM.estimate <- MCReestimate(Golub_Train,
  class.column,
  classification.fun = class.function,
  thePreprocessingMethods = Preprocessingfunctions,
  poss.parameters = list.of.poss.parameter,
  cross.outer = cross.outer, cross.inner = cross.inner,
  cross.repeat = cross.repeat, plot.label = plot.label)

## End(Not run)
```

varSel.highest.var *Variable selection and cluster functions*

Description

Different functions for a variable selection and clustering methods. These functions are mainly used for the function [MCReestimate](#)

Usage

```
identity(sample.gene.matrix,classfactor,...)
varSel.highest.t.stat(sample.gene.matrix,classfactor,theParameter=NULL,var.numbers=500,...)

varSel.highest.var(sample.gene.matrix,classfactor,theParameter=NULL,var.numbers=2000,...)

varSel.AUC(sample.gene.matrix, classfactor, theParameter=NULL,var.numbers=200,...)
cluster.kmeans.mean(sample.gene.matrix,classfactor,theParameter=NULL,number.clusters=500,...)

varSel.removeManyNA(sample.gene.matrix,classfactor, theParameter=NULL, NAthreshold=0.25,...)
varSel.impute.NA(sample.gene.matrix ,classfactor,theParameter=NULL,...)
```

Arguments

<code>sample.gene.matrix</code>	a matrix in which the rows corresponds to genes and the columns corresponds to samples
<code>classfactor</code>	a factor containing the values that should be predicted
<code>theParameter</code>	Parameter that depends on the function. For 'cluster.kmeans.mean' either NULL or an output of the function kmeans. If it is NULL then kmeans will be used to form clusters of the genes. Otherwise the already existing clusters will be used. In both ways there will be a calculation of the metagene intensities afterwards. For the other functions either NULL or a logical vector which indicates for every gene if it should be left out from further analysis or not
<code>number.clusters</code>	parameter which specifies the number of clusters
<code>var.numbers</code>	some methods needs an argument which specifies how many variables should be taken
<code>NAthreshold</code>	integer- if the percentage of the NA is higher than this threshold the variable will be deleted
<code>...</code>	Further parameters

Details

`metagene.kmeans.mean` performs a kmeans clustering with a number of clusters specified by 'number clusters' and takes the mean of each cluster. `varSel.highest.var` selects a number (specified by 'var.numbers') of variables with the highest variance. `varSel.AUC` chooses the most discriminating variables due to the AUC criterium (the library ROC is required).

Value

Every function returns a list consisting of two arguments:

<code>matrix</code>	the result matrix of the variable reduction or the clustering
<code>parameter</code>	The parameter which are used to reproduce the algorithm, i.e. a vector which indicates for every gene if it will be left out from further analysis or not if a gene reduction is performed or the output of the function kmeans for the clustering algorithm.

Author(s)

Markus Ruschhaupt <mailto:m.ruschhaupt@dkfz.de>

See Also

[MCReestimate](#)

Examples

```
m <- matrix(c(rnorm(10,2,0.5),rnorm(10,4,0.5),rnorm(10,7,0.5),rnorm(10,2,0.5),rnorm(10,4,0.5),rnorm(10,2,0.5)),
cluster.kmeans.mean(m ,number.clusters=3)
```

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