# Package 'klaR'

# August 28, 2012

Index

10
12 14
15
17
19
20
22
23
25
27
29
31
32
34
36
37
38
39
40
41
42
43
44
45
46
49
51
54
57
58
60
63
63
65
66
67
68
70
, 0
<b>72</b>

b.scal 3

b.scal	Calculation of beta scaling parameters

#### **Description**

Calculates the scaling parameter for betascale.

# Usage

```
b.scal(member, grouping, dis = FALSE, eps = 1e-04)
```

#### **Arguments**

member Membership values of an argmax classification method. Eg. posterior proba-

bilities of lda. Row-wise values must sum up to 1 and must be in the interval

[0,1].

grouping Class vector.

dis Logical, whether to optimize the dispersion parameter in pbeta.

eps Minimum variation of membership values. If variance is smaller than eps, the

values are treated as one point.

#### **Details**

With betascale and b.scal, membership values of an argmax classifier are scaled in such a way, that the mean membership value of those values which are assigned to each class reflect the mean correctness rate of that values. This is done via qbeta and pbeta with the appropriate shape parameters. If dis is TRUE, it is tried that the variation of membership values is optimal for the accuracy relative to the correctness rate. If the variation of the membership values is less than eps, they are treated as one point and shifted towards the correctness rate.

## Value

## A list containing

model Estimated parameters for betascale.

eps Value of eps from the call.
member Scaled membership values.

## Author(s)

Karsten Luebke (<karsten.luebke@fom.de>), Uwe Ligges

#### References

Garczarek, Ursula Maria (2002): Classification rules in standardized partition spaces. Dissertation, University of Dortmund. URL http://hdl.handle.net/2003/2789

4 B3

#### See Also

```
betascale, e.scal
```

#### **Examples**

```
library(MASS)
data(B3)
pB3 <- predict(lda(PHASEN ~ ., data = B3))$posterior
pbB3 <- b.scal(pB3, B3$PHASEN, dis = TRUE)
ucpm(pB3, B3$PHASEN)
ucpm(pbB3$member, B3$PHASEN)</pre>
```

B3

West German Business Cycles 1955-1994

# **Description**

West German Business Cycles 1955-1994

#### Usage

data(B3)

#### **Format**

A data frame with 157 observations on the following 14 variables.

**PHASEN** a factor with levels 1 (upswing), 2 (upper turning points), 3 (downswing), and 4 (lower turning points).

BSP91JW GNP (y)

**CP91JW** Private Consumption (y)

**DEFRATE** Government deficit (percent of GNP)

EWAJW Wage and salary earners (y)

**EXIMRATE** Net exports as (percent of GNP)

**GM1JW** Money supply M1 (y)

**IAU91JW** Investment in equipment (y)

**IB91JW** Investment in construction (y)

**LSTKJW** Unit labor cost (y)

**PBSPJW** GNP price deflator (y)

**PCPJW** Consumer price index (y)

**ZINSK** Short term interest rate (nominal)

ZINSLR Long term interest rate (real)

where (y) stands for "yearly growth rates".

Note that years and corresponding year quarters are given in the row names of the data frame, e.g. "1988,3" for the third quarter in 1988.

benchB3 5

#### **Details**

The West German Business Cycles data (1955-1994) is analyzed by the project *B3* of the SFB475 (Collaborative Research Centre "Reduction of Complexity for Multivariate Data Structures"), supported by the Deutsche Forschungsgemeinschaft.

#### Source

RWI (Rheinisch Westfälisches Institut für Wirtschaftsforschung), Essen, Germany.

#### References

Heilemann, U. and Münch, H.J. (1996): West German Business Cycles 1963-1994: A Multivariate Discriminant Analysis. *CIRET–Conference in Singapore, CIRET–Studien* 50.

#### See Also

For benchmarking on this data see also benchB3

#### **Examples**

```
data(B3)
summary(B3)
```

benchB3

Benchmarking on B3 data

# Description

Evaluates the performance of a classification method on the B3 data.

#### Usage

```
benchB3(method, prior = rep(1/4, 4), sv = "4", scale = FALSE, ...)
```

#### **Arguments**

```
method classification method to use
prior prior probabilities of classes
sv class of the start of a business cycle
scale logical, whether to use scale first
... further arguments passed to method
```

#### **Details**

The performance of classification methods on cyclic data can be measured by a special form of cross-validation: Leave-One-Cycle-Out. That means that a complete cycle is used as test data and the others are used as training data. This is repeated for all complete cycles in the data.

6 betascale

# Value

A list with elements

MODEL list with the model returned by method of the training data

error vector of test error rates in cycles

11co.error leave-one-cycle-out error rate

# Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

#### See Also

**B3** 

#### **Examples**

```
perLDA <- benchB3("lda")
## Not run:
## due to parameter optimization rda takes a while
perRDA <- benchB3("rda")
library(rpart)
## rpart will not work with prior argument:
perRpart <- benchB3("rpart", prior = NULL)
## End(Not run)</pre>
```

betascale

Scale membership values according to a beta scaling

# Description

Performs the scaling for beta scaling learned by b. scal.

# Usage

```
betascale(betaobj, member)
```

# **Arguments**

betaobj A model learned by b.scal.

member Membership values to be scaled.

#### **Details**

```
See b.scal.
```

calc.trans 7

# Value

A matrix with the scaled membership values.

#### See Also

```
b.scal, e.scal
```

# **Examples**

```
library(MASS)
data(B3)
pB3 <- predict(lda(PHASEN ~ ., data = B3))$posterior
pbB3 <- b.scal(pB3, B3$PHASEN)
betascale(pbB3)</pre>
```

calc.trans

Calculation of transition probabilities

# **Description**

Function to estimate the probabilities of a time series to stay or change the state.

# Usage

```
calc.trans(x)
```

# Arguments

v

(factor) vector of states

#### **Details**

To estimate the transition probabilities the empirical frequencies are counted.

# Value

The transition probabilities matrix. x[i,j] is the probability to change from state i to state j.

# Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

```
data(B3)
calc.trans(B3$PHASEN)
```

8 classscatter

centerlines

Lines from classborders to the center

# Description

Function which constructs the lines from the borders between two classes to the center. To be used in connection with triplot and quadplot.

# Usage

```
centerlines(n)
```

# **Arguments**

n

number of classes. Meaningful are 3 or 4.

# Value

a matrix with n-columns.

# Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

# See Also

```
triplot, quadplot
```

# **Examples**

```
centerlines(3)
centerlines(4)
```

classscatter

Classification scatterplot matrix

# **Description**

Function to plot a scatterplot matrix with a classification result.

# Usage

corclust 9

### **Arguments**

formula	formula of the form groups $\sim x1 + x2 + \ldots$ That is, the response is the grouping factor and the right hand side specifies the (non-factor) discriminators.
data	Data frame from which variables specified in formula are preferentially to be taken.
method	character, name of classification function (e.g. "lda").
col.correct	color to use for correct classified objects.
col.wrong	color to use for missclassified objects.
gs	group symbol (plot character), must have the same length as the data. If NULL, as.character(groups) is the default.
• • •	further arguments passed to the underlying classification method or plot functions.

#### Value

The actual error rate.

# Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

# See Also

plot

# **Examples**

corclust

Function to identify groups of highly correlated variables for removing correlated features from the data for further analysis.

# Description

A hierarchical clustering of variables using hclust is performed using 1 - the absolute correlation as a distance measure between tow variables.

# Usage

```
corclust(x, cl = NULL, mincor = NULL, prnt = FALSE, method = "complete")
```

10 corclust

#### **Arguments**

X	Either a data frame or a matrix consisting of numerical attributes.
cl	Optional vector of ty factor indicating class levels, if class specific correlations should to be considered.
mincor	Optional vector of degrees of correlation within a cluster of variables that will be indicated in the plot by a line.
prnt	Logical indicating whether the matrix of distances should be printed.
method	Linkage to be used for clustering. Default is complete linkage.

#### **Details**

The main output consists in the tree visualization of the clustered variables. Each cluster consists of a set of correlated variables according to the chosen clustering criterion. The default criterion is 'complete'. This choice is meaningful as it represents the *minimum absolute correlation* between all variables of a cluster.\ Further proceeding would consist in chosing one variable of each cluster to obtain a subset of rather uncorrelated variables for further analysis.\ If an additional class vector cl is given to the function for any two variables their minimum correlation over all classes is used.

#### Value

min.abs.cor	Matrix of distances used for clustering containing 1 - the absolute correlation
	between any two variables.

clustering Result object of the hierarchical clustering.

#### Author(s)

Gero Szepannek

### See Also

See also hclust, for details on the clustering algorithm.

```
data(iris)
classes <- iris$Species
variables <- iris[,1:4]
corclust(variables, classes, mincor = 0.6)</pre>
```

countries 11

countries

Socioeconomic data for the most populous countries.

# Description

Socioeconomic data for the most populous countries.

# Usage

```
data(countries)
```

#### **Format**

A data frame with 42 observations on the following 7 variables.

Country name of the country.

Popul population.

PopDens population density.

**GDPpp** GDP per inhabitant.

LifeEx mean life expectation

InfMor infant mortality

**Illit** illiteracy rate

#### **Source**

```
CIA World Factbook http://www.cia.gov/cia/publications/factbook/
```

# **Examples**

```
data(countries)
summary(countries)
```

dkernel

Estimate density of a given kernel

# **Description**

Given an estimated kernel density this function estimates the density of a new vector.

# Usage

```
dkernel(x, kernel = density(x), interpolate = FALSE, ...)
```

12 drawparti

# Arguments

vector of which the density should be estimated
 be object of class density
 Interpolate or use density of nearest point?
 currently not used.

#### Value

Denstiy of x in kernel.

#### Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

#### See Also

```
density, NaiveBayes
```

#### **Examples**

```
kern <- density(rnorm(50))
x <- seq(-3, 3, len = 100)
y <- dkernel(x, kern)
plot(x, y, type = "1")</pre>
```

drawparti

Plotting the 2-d partitions of classification methods

# **Description**

Plot showing the classification of observations based on classification methods (e.g. 1da, qda) for two variables. Moreover, the classification borders are displayed and the apparent error rates are given in each title.

# Usage

```
drawparti(grouping, x, y, method = "lda", prec = 100, xlab = NULL,
   ylab = NULL, col.correct = "black", col.wrong = "red",
   col.mean = "black", col.contour = "darkgrey",
   gs = as.character(grouping), pch.mean = 19, cex.mean = 1.3,
   print.err = 0.7, legend.err = FALSE, legend.bg = "white",
   imageplot = TRUE, image.colors = cm.colors(nc),
   plot.control = list(), ...)
```

drawparti 13

# Arguments

gr	ouping	factor specifying the class for each observation.
Х		first explanatory vector.
у		second explanatory vector.
me	thod	the method the classification is based on, currently supported are: lda, qda, rpart, naiveBayes, rda, sknn and svmlight.
pr	ec	precision used to draw the classification borders (the higher the more precise; default: 100).
x1	ab	a title for the x axis.
yl.	ab	a title for the y axis.
со	l.correct	color for correct classified objects.
со	l.wrong	color for wrong classified objects.
со	l.mean	color for class means (only for methods 1da and qda).
со	l.contour	color of the contour lines (if imageplot = FALSE).
gs		group symbol (plot character), must have the same length as grouping.
рс	h.mean	plot character for class means (only for methods 1da and qda).
ce	x.mean	character expansion for class means (only for methods 1da and qda).
pr	int.err	character expansion for text specifying the apparent error rate. If print.err = 0, nothing is printed.
le	gend.err	logical; whether to plot the apparent error rate above the plot (if FALSE), or into a legend into the upper right corner of the plot (if TRUE). This argument is ignored, if print.err = 0, i.e. if no error rate is printed.
le	gend.bg	Backgound colour to use for the legend.
im	ageplot	logical; whether to use an image plot or contour lines.
im	age.colors	colors used for the imageplot, if TRUE.
pl	ot.control	A list containing further arguments passed to the underlying plot functions.
		Further arguments passed to the classification method.

# Author(s)

 $Karsten\ Luebke, < karsten.\ luebke @fom.\ de >,\ Uwe\ Ligges,\ Irina\ Czogiel$ 

# See Also

partimat

14 e.scal

e.scal

Function to calculate e- or softmax scaled membership values

#### Description

Calculates the e- or softmax scaled membership values of an argmax based classification rule.

# Usage

```
e.scal(x, k = 1, tc = NULL)
```

# **Arguments**

x matrix of membership values

k parameter for e-scaling (1 for softmax)

tc vector of true classes (required if k has to be optimized)

#### **Details**

For any membership vector  $y \exp(y \cdot k) / \sum \exp(y \cdot k)$  is calculated. If k=1, the classical softmax scaling is used. If the true classes are given, k is optimized so that the apparent error rate is minimized.

#### Value

A list containing elements

sv Scaled values k Optimal k

# Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

#### References

Garczarek, Ursula Maria (2002): Classification rules in standardized partition spaces. Dissertation, University of Dortmund. URL http://hdl.handle.net/2003/2789

```
library(MASS)
data(iris)
ldaobj <- lda(Species ~ ., data = iris)
ldapred <- predict(ldaobj)$posterior
e.scal(ldapred)
e.scal(ldapred, tc = iris$Species)</pre>
```

EDAM 15

EDAM	Computation of an Eight Direction Arranged Map

# Description

Produces an object of class EDAM which is a two dimensional representation of data in a rectangular, equally spaced grid as known from Self-Organizing Maps.

# Usage

```
EDAM(EV0, nzx = 0, iter.max = 10, random = TRUE, standardize = FALSE,
   wghts = 0, classes = 0, sa = TRUE, temp.in = 0.5, temp.fin = 1e-07,
   temp.gamma = 0)
```

# Arguments

EV0	either a symmetric dissimilarity matrix or a matrix of arbitrary dimensions whose n rows correspond to cases and whose k columns correspond to variables.
nzx	an integer specifying the number of vertical bars in the grid. By default, nzx is chosen automatically, so that the grid gets closest do a square. If n is no multiple of nzx, all surplus objects are skipped.
iter.max	an integer giving the maxmimum number of iterations to perform for the same neighborhood size.
random	logical. If TRUE, the initital order is drawn from a uniform distribution.
standardize	logical. If TRUE, the measurements in EV0 are standardized before calculating Euclidean distances. Measurements are standardized for each variable by dividing by the variable's standard deviation. Meaningless if EV0 is a dissimilarity matrix.
wghts	an optional vector of length k giving relative weights of the variables in computing Euclidean distances. Meaningless if EV0 is a dissimilarity matrix.
classes	an optional vector of length n specifying the membership to classes for all objects.
sa	logical. If TRUE, the optimization is obtained by Simulated Annealing.
temp.in	numeric giving the initial temperature, if sa is set to TRUE.
temp.fin	numeric giving the final temperature, if so is set to TRUE. Meaningless if temp. gamma is greater than $0.$
temp.gamma	numeric giving the relative change of the temperature from one iteration to the other, if sa is set to TRUE.

16 EDAM

#### **Details**

The data given by EV0 is visualized by the EDAM-algorithm. This method approximates the best visualization where goodness is measured by S, a transformation of the criterion stress as i.e. known from sammon. The target space of the visualization is restricted to a grid so the problem has a discrete solution space. Originally this restriction was made to make the results comparable to those of Kohonen Self-Organizing Maps. But it turns out that also for reasons of a clear arrangement the representation in a grid can be more favorable than in the hole plane.

During the computation of EDAM 3 values indicating its progress are given online. The first is the number of the actual iteration, the second the maximum number of overall performed iterations. The latter may reduce during computation, since the neighborhood reduces in case of convergence before the last iteration. The last number gives the actual criterion S. The default plot method plot.edam for objects of class EDAM is shardsplot.

#### Value

EDAM returns an object of class EDAM, which is a list containing the following components:

preimages	the re-ordered data; the position of the i-th object is where Z equals i.
Z	a matrix representing the positions of the preimages in the grid by their numbers.
Z.old.terms	a matrix representing the positions of the data in original order in the grid by their numbers.
cl.ord	a vector giving the re-ordered classes. All elements equal 1 if argument classes is undefined.
S	the criterion of the map

# Author(s)

Nils Raabe

#### References

Raabe, N. (2003). Vergleich von Kohonen Self-Organizing-Maps mit einem nichtsimultanen Klassifikationsund Visualisierungsverfahren. Diploma Thesis, Department of Statistics, University of Dortmund. http://www.statistik.tu-dortmund.de/de/content/einrichtungen/lehrstuehle/personen/raabe/Diplomarbeit.pdf.

#### See Also

```
shardsplot, TopoS
```

```
# Compute an Eight Directions Arranged Map for a random sample
# of the iris data.
data(iris)
set.seed(1234)
iris.sample <- sample(150, 42)</pre>
```

errormatrix 17

```
irisEDAM <- EDAM(iris[iris.sample, 1:4], classes = iris[iris.sample, 5],</pre>
    standardize = TRUE, iter.max = 3)
plot(irisEDAM, vertices = FALSE)
legend(3, 5, col = rainbow(3), legend = levels(iris[,5]), pch = 16)
print(irisEDAM)
# Construct clusters within the phases of the german business data
# and visualize the centroids by EDAM.
data(B3)
phasemat <- lapply(1:4, function(x) B3[B3[,1] == x, 2:14])
subclasses <- lapply(phasemat,</pre>
    function(x) cutree(hclust(dist(x)), k = round(nrow(x) / 4.47)))
centroids <- lapply(1:4,
    function(y) apply(phasemat[[y]], 2,
        function(x) by(x, subclasses[[y]], mean)))
centmat <- matrix(unlist(sapply(centroids, t)), ncol = 13,</pre>
    byrow = TRUE, dimnames = list(NULL, colnames(centroids[[1]])))
centclasses <- unlist(lapply(1:4,</pre>
    function(x) rep(x, unlist(lapply(centroids, nrow))[x])))
B3EDAM <- EDAM(centmat, classes = centclasses, standardize = TRUE,
    iter.max = 6, rand = FALSE)
plot(B3EDAM, standardize = TRUE)
opar <- par(xpd = NA)
legend(4, 5.1, col = rainbow(4), pch = 16, xjust = 0.5, yjust = 0,
    ncol = 2, legend = c("upswing", "upper turning point",
                          "downswing", "lower turning point"))
print(B3EDAM)
par(opar)
```

errormatrix

Tabulation of prediction errors by classes

#### **Description**

Cross-tabulates true and predicted classes with the option to show relative frequencies.

#### Usage

```
errormatrix(true, predicted, relative = FALSE)
```

#### **Arguments**

true Vector of true classes.

predicted Vector of predicted classes.

relative Logical. If TRUE rows are normalized to show relative frequencies (see below).

18 errormatrix

#### **Details**

Given vectors of true and predicted classes, a (symmetric) table of misclassifications is constructed.

Element [i,j] shows the number of objects of class i that were classified as class j; so the main diagonal shows the correct classifications. The last row and column show the corresponding sums of misclassifications, the lower right element is the total sum of misclassifications.

If 'relative' is TRUE, the *rows* are normalized so they show relative frequencies instead. The lower right element now shows the total error rate, and the remaining last row sums up to one, so it shows "where the misclassifications went".

#### Value

A (named) matrix.

#### Note

Concerning the case that 'relative' is TRUE:

If a prior distribution over the classes is given, the misclassification rate that is returned as the lower right element (which is only the fraction of misclassified *data*) is not an estimator for the expected misclassification rate.

In that case you have to multiply the individual error rates for each class (returned in the last column) with the corresponding prior probabilities and sum these up (see example below).

Both error rate estimates are equal, if the fractions of classes in the data are equal to the prior probabilities.

#### Author(s)

Christian Röver, <roever@statistik.tu-dortmund.de>

# See Also

table

```
data(iris)
library(MASS)
x <- lda(Species ~ Sepal.Length + Sepal.Width, data=iris)
y <- predict(x, iris)

# absolute numbers:
errormatrix(iris$Species, y$class)

# relative frequencies:
errormatrix(iris$Species, y$class, relative = TRUE)

# percentages:
round(100 * errormatrix(iris$Species, y$class, relative = TRUE), 0)

# expected error rate in case of class prior:</pre>
```

friedman,data 19

```
indiv.rates <- errormatrix(iris$Species, y$class, relative = TRUE)[1:3, 4]
prior <- c("setosa" = 0.2, "versicolor" = 0.3, "virginica" = 0.5)
total.rate <- t(indiv.rates) %*% prior
total.rate</pre>
```

friedman.data

Friedman's classification benchmark data

# **Description**

Function to generate 3-class classification benchmarking data as introduced by J.H. Friedman (1989)

#### Usage

```
friedman.data(setting = 1, p = 6, samplesize = 40, asmatrix = FALSE)
```

#### **Arguments**

```
setting the problem setting (integer 1,2,...,6).

p number of variables (6, 10, 20 or 40).

samplesize sample size (number of observations, >=6).

asmatrix if TRUE, results are returned as a matrix, otherwise as a data frame (default).
```

#### **Details**

When J.H. Friedman introduced the Regularized Discriminant Analysis (rda) in 1989, he used artificially generated data to test the procedure and to examine its performance in comparison to Linear and Quadratic Discriminant Analysis (see also 1da and qda).

6 different settings were considered to demonstrate potential strengths and weaknesses of the new method:

- 1. equal spherical covariance matrices,
- 2. unequal spherical covariance matrices,
- 3. equal, highly ellipsoidal covariance matrices with mean differences in low-variance subspace,
- 4. equal, highly ellipsoidal covariance matrices with mean differences in high-variance subspace,
- 5. unequal, highly ellipsoidal covariance matrices with zero mean differences and
- 6. unequal, highly ellipsoidal covariance matrices with nonzero mean differences.

For each of the 6 settings data was generated with 6, 10, 20 and 40 variables.

Classification performance was then measured by repeatedly creating training-datasets of 40 observations and estimating the misclassification rates by test sets of 100 observations.

The number of classes is always 3, class labels are assigned randomly (with equal probabilities) to observations, so the contributions of classes to the data differs from dataset to dataset. To make sure covariances can be estimated at all, there are always at least two observations from each class in a dataset.

20 greedy.wilks

#### Value

Depending on asmatrix either a data frame or a matrix with samplesize rows and p+1 columns, the first column containing the class labels, the remaining columns being the variables.

#### Author(s)

Christian Röver, <roever@statistik.tu-dortmund.de>

#### References

Friedman, J.H. (1989): Regularized Discriminant Analysis. In: *Journal of the American Statistical Association* 84, 165-175.

# See Also

rda

# **Examples**

```
# Reproduce the 1st setting with 6 variables.
# Error rate should be somewhat near 9 percent.
training <- friedman.data(1, 6, 40)
x <- rda(class ~ ., data = training, gamma = 0.74, lambda = 0.77)
test <- friedman.data(1, 6, 100)
y <- predict(x, test[,-1])
errormatrix(test[,1], y$class)</pre>
```

greedy.wilks

Stepwise forward variable selection for classification

# Description

Performs a stepwise forward variable/model selection using the Wilk's Lambda criterion.

#### Usage

```
greedy.wilks(X, ...)
## Default S3 method:
greedy.wilks(X, grouping, niveau = 0.2, ...)
## S3 method for class 'formula'
greedy.wilks(formula, data = NULL, ...)
```

greedy.wilks 21

#### **Arguments**

X	matrix or data frame (rows=cases, columns=variables)
grouping	class indicator vector

formula of the form 'groups  $\sim x1 + x2 + ...$ '

data frame (or matrix) containing the explanatory variables

niveau level for the approximate F-test decision

... further arguments to be passed to the default method, e.g. niveau

#### **Details**

A stepwise forward variable selection is performed. The initial model is defined by starting with the variable which separates the groups most. The model is then extended by including further variables depending on the Wilk's lambda criterion: Select the one which minimizes the Wilk's lambda of the model including the variable if its p-value still shows statistical significance.

#### Value

A list of two components, a formula of the form 'response ~ list + of + selected + variables', and a data.frame results containing the following variables:

vars the names of the variables in the final model in the order of selection.

Wilks.lambda the appropriate Wilks' lambda for the selected variables.

F.statistics.overall

the approximated F-statistic for the so far selected model.

p.value.overall

the appropriate p-value of the F-statistic.

F.statistics.diff

the approximated F-statistic of the partial Wilks's lambda (for comparing the model including the new variable with the model not including it).

p.value.diff the appropriate p-value of the F-statistic of the partial Wilk's lambda.

# Author(s)

Andrea Preusser, Karsten Luebke (<karsten.luebke@fom.de>)

# References

Mardia, K. V., Kent, J. T. and Bibby, J. M. (1979), *Multivariate analysis*, Academic Press (New York; London)

# See Also

```
stepclass, manova
```

hmm.sop

#### **Examples**

```
data(B3)
gw_obj <- greedy.wilks(PHASEN ~ ., data = B3, niveau = 0.1)
gw_obj
## now you can say stuff like
## lda(gw_obj$formula, data = B3)</pre>
```

hmm.sop

Calculation of HMM Sum of Path

# **Description**

A Hidden Markov Model for the classification of states in a time series. Based on the transition probabilities and the so called emission probabilities (p(class|x)) the 'prior probabilities' of states (classes) in time period t given all past information in time period t are calculated.

#### **Usage**

```
hmm.sop(sv, trans.matrix, prob.matrix)
```

# **Arguments**

```
sv state at time 0 trans.matrix matrix of transition probabilities prob.matrix matrix of p(class|x)
```

# Value

Returns the 'prior probablilities' of states.

#### Author(s)

Daniel Fischer, Reinald Oetsch

# References

Garczarek, Ursula Maria (2002): Classification rules in standardized partition spaces. Dissertation, University of Dortmund. URL http://hdl.handle.net/2003/2789

#### See Also

```
calc.trans
```

kmodes 23

### **Examples**

```
library(MASS)
data(B3)
trans.matrix <- calc.trans(B3$PHASEN)

# Calculate posterior prob. for the classes via lda
prob.matrix <- predict(lda(PHASEN ~ ., data = B3))$post
errormatrix(B3$PHASEN, apply(prob.matrix, 1, which.max))
prior.prob <- hmm.sop("2", trans.matrix, prob.matrix)
errormatrix(B3$PHASEN, apply(prior.prob, 1, which.max))</pre>
```

kmodes

K-Modes Clustering

# **Description**

Perform k-modes clustering on categorical data.

#### Usage

```
kmodes(data, modes, iter.max = 10, weighted = FALSE)
```

# Arguments

data	A matrix or data frame of categorical data. Objects have to be in rows, variables in columns.
modes	Either the number of modes or a set of initial (distinct) cluster modes. If a number, a random set of (distinct) rows in data is chosen as the initial modes.
iter.max	The maximum number of iterations allowed.
weighted	Whether usual simple-matching distance between objects is used, or a weighted version of this distance.

#### **Details**

The k-modes algorithm (Huang, 1997) an extension of the k-means algorithm by MacQueen (1967).

The data given by data is clustered by the k-modes method (Huang, 1997) which aims to partition the objects into k groups such that the distance from objects to the assigned cluster modes is minimized.

By default simple-matching distance is used to determine the dissimilarity of two objects. It is computed by counting the number of mismatches in all variables. Alternative this distance is weighted by the frequencies of the categories in data (see Huang, 1997, for details).

If an initial matrix of modes is supplied, it is possible that no object will be closest to one or more modes. In this case less cluster than supplied modes will be returned and a warning is given.

24 kmodes

#### Value

An object of class "kmodes" which is a list with components:

cluster A vector of integers indicating the cluster to which each object is allocated.

size The number of objects in each cluster.

modes A matrix of cluster modes.

withindiff The within-cluster simple-matching distance for each cluster.

iterations The number of iterations the algorithm has run.

weighted Whether weighted distances were used or not.

# Author(s)

Christian Neumann, <christian2.neumann@tu-dortmund.de>

#### References

Huang, Z. (1997) A Fast Clustering Algorithm to Cluster Very Large Categorical Data Sets in Data Mining. in *KDD: Techniques and Applications* (H. Lu, H. Motoda and H. Luu, Eds.), pp. 21-34, World Scientific, Singapore.

MacQueen, J. (1967) Some methods for classification and analysis of multivariate observations. In *Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability*, eds L. M. Le Cam & J. Neyman, 1, pp. 281-297. Berkeley, CA: University of California Press.

locida 25

loclda

Localized Linear Discriminant Analysis (LocLDA)

# Description

A localized version of Linear Discriminant Analysis.

# Usage

# **Arguments**

formula	Formula of the form 'groups $\sim x1 + x2 +$ '.	
data	Data frame from which variables specified in formula are to be taken.	
Х	Matrix or data frame containing the explanatory variables (required, if formula is not given).	
grouping	(required if no formula principal argument is given.) A factor specifying the class for each observation.	
weight.func	Function used to compute local weights. Must be finite over the interval [0,1]. See Details below.	
k	Number of nearest neighbours used to construct localized classification rules. See Details below.	
weighted.apriori		
	Logical: if TRUE, class prior probabilities are computed using local weights (see Details below). If FALSE, equal priors for all classes actually occurring in the train data are used.	
subset	An index vector specifying the cases to be used in the training sample.	
na.action	A function to specify the action to be taken if NAs are found. The default action is for the procedure to fail. An alternative is na.omit which leads to rejection of cases with missing values on any required variable.	
	Further arguments to be passed to loclda.default.	

26 locIda

#### **Details**

This is an approach to apply the concept of localization described by Tutz and Binder (2005) to Linear Discriminant Analysis. The function loclda generates an object of class loclda (see Value below). As localization makes it necessary to build an individual decision rule for each test observation, this rule construction has to be handled by predict.loclda. For convenience, the rule building procedure is still described here.

To classify a test observation  $x_s$ , only the k nearest neighbours of  $x_s$  within the train data are used. Each of these k train observations  $x_i$ , i = 1, ..., k, is assigned a weight  $w_i$  according to

$$w_i = K\left(\frac{||x_i - x_s||}{d_k}\right), i = 1, \dots, k$$

where K is the weighting function given by weight.func,  $||x_i - x_s||$  is the euclidian distance of  $x_i$  and  $x_s$  and  $d_k$  is the euclidian distance of  $x_s$  to its k-th nearest neighbour. With these weights for each class  $A_g, g = 1, \ldots, G$ , its weighted empirical mean  $\hat{\mu}_g$  and weighted empirical covariance matrix are computed. The estimated pooled (weighted) covariance matrix  $\hat{\Sigma}$  is then calculated from the individual weighted empirical class covariance matrices. If weighted apriori is TRUE (the default), prior class probabilities are estimated according to:

$$prior_g := \frac{\sum_{i=1}^{k} (w_i \cdot I(x_i \in A_g))}{\sum_{i=1}^{k} (w_i)}$$

where I is the indicator function. If FALSE, equal priors for all classes are used. In analogy to Linear Discriminant Analysis, the decision rule for  $x_s$  is

$$\hat{A} := argmax_{q \in 1, \dots, G}(posterior_q)$$

where

$$posterior_g := prior_g \cdot \exp\left((-\frac{1}{2})t(x_s - \hat{\mu}_g)\hat{\Sigma}^{-1}(x_s - \hat{\mu}_g)\right)$$

If  $posterior_g < 10^{(-150)} \forall g \in \{1, \dots, G\}$ ,  $posterior_g$  is set to  $\frac{1}{G}$  for all  $g \in 1, \dots, G$  and the test observation  $x_s$  is simply assigned to the class whose weighted mean has the lowest euclidian distance to  $x_s$ .

#### Value

A list of class loclda containing the following components:

call The (matched) function call.

learn Matrix containing the values of the explanatory variables for all train observa-

tions.

grouping Factor specifying the class for each train observation.

weight.func Value of the argument weight.func.

k Value of the argument k.

weighted.apriori

Value of the argument weighted.apriori.

locpvs 27

#### Author(s)

Marc Zentgraf (<marc-zentgraf@gmx.de>) and Karsten Luebke (<karsten.luebke@fom.de>)

#### References

Tutz, G. and Binder, H. (2005): Localized classification. Statistics and Computing 15, 155-166.

#### See Also

```
predict.loclda,lda
```

# **Examples**

```
benchB3("lda")$11co.error
benchB3("loclda")$11co.error
```

locpvs

Pairwise variable selection for classification in local models

#### **Description**

Performs pairwise variable selection on subclasses.

#### Usage

```
locpvs(x, subclasses, subclass.labels, prior=NULL, method="lda",
    vs.method = c("ks.test", "stepclass", "greedy.wilks"),
    niveau=0.05, fold=10, impr=0.1, direct="backward", out=FALSE, ...)
```

# **Arguments**

x matrix or data frame containing the explanatory variables. x must consist of

numerical data only.

subclasses vector indicating the subclasses (a factor)

subclass.labels

must be a matrix with 2 coloumns, where the first coloumn specifies the subclass

and the second coloumn the according upper class

prior probabilites for the classes. If not specified the prior probabilities will

be set according to proportion in "subclasses". If specified the order of prior

probabilities must be the same as in "subclasses".

method character, name of classification function (e.g. "lda" (default)).

vs.method character, name of variable selection method. Must be one of "ks.test" (de-

fault), "stepclass" or "greedy.wilks".

niveau used niveau for "ks.test"

fold parameter for cross-validation, if "stepclass" is chosen 'vs.method'

28 locpvs

impr	least improvement of performance measure desired to include or exclude any variable (<=1), if "stepclass" is chosen 'vs.method'
direct	direction of variable selection, if "stepclass" is chosen 'vs.method'. Must be one if "forward", "backward" (default) or "both".
out	indicator (logical) for textoutput during computation (slows down computation!), if "stepclass" is chosen 'vs.method'
	further parameters passed to classification function ('method') or variable selection method ('vs.method')

#### **Details**

A call on pvs is performed using "subclasses" as grouping variable. See pvs for further details.

#### Value

```
An object of class 'locpvs' containing the following components:

pvs.result the complete output of the call to pvs (see pvs for further details subclass.labels the subclass.labels as specified in function call
```

#### Author(s)

Gero Szepannek, <szepannek@statistik.tu-dortmund.de>, Christian Neumann

#### References

Szepannek, G. and Weihs, C. (2006) Local Modelling in Classification on Different Feature Subspaces. In *Advances in Data Mining.*, ed Perner, P., LNAI 4065, pp. 226-234. Springer, Heidelberg.

#### See Also

```
predict.locpvs for predicting 'locpvs' models and pvs
```

```
## this example might be a bit artificial, but it sufficiently shows how locpvs has to be used
## learn a locpvs-model on the Vehicle dataset
library("mlbench")
data("Vehicle")

subclass <- Vehicle$Class # use four car-types in dataset as subclasses
## aggregate "bus" and "van" to upper-class "big" and "saab" and "opel" to upper-class "small"
subclass_class <- matrix(c("bus", "van", "saab", "opel", "big", "big", "small", "small"), ncol=2)

## learn now a locpvs-model for the subclasses:
model <- locpvs(Vehicle[,1:18], subclass, subclass_class)</pre>
```

meclight.default 29

```
model # short summary, showing the class-pairs of the submodels
# together with the selected variables and the relation of sub- to upperclasses
## predict:
pred <- predict(model, Vehicle[,1:18])
## now you can look at the predicted classes:
pred$class
## or at the posterior probabilities:
pred$posterior
## or at the posterior probabilities for the subclasses:
pred$subclass.posteriors</pre>
```

meclight.default

Minimal Error Classification

# **Description**

Computer intensive method for linear dimension reduction that minimizes the classification error directly.

#### Usage

```
meclight(x, ...)
## Default S3 method:
meclight(x, grouping, r = 1, fold = 10, ...)
## S3 method for class 'formula'
meclight(formula, data = NULL, ..., subset, na.action = na.fail)
## S3 method for class 'data.frame'
meclight(x, ...)
## S3 method for class 'matrix'
meclight(x, grouping, ..., subset, na.action = na.fail)
```

#### **Arguments**

X	(required if no formula is given as the principal argument.) A matrix or data frame containing the explanatory variables.
grouping	(required if no formula principal argument is given.) A factor specifying the class for each observation.
r	Dimension of projected subspace.
fold	Number of Bootstrap samples.
formula	A formula of the form groups $\sim x1 + x2 + \ldots$ That is, the response is the grouping factor and the right hand side specifies the (non-factor) discriminators.
data	Data frame from which variables specified in formula are preferentially to be taken.

30 meclight.default

subset An index vector specifying the cases to be used in the training sample. (NOTE:

If given, this argument must be named.)

na.action A function to specify the action to be taken if NAs are found. The default action

is for the procedure to fail. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable. (NOTE: If given, this

argument must be named.)

... Further arguments passed to lda.

#### **Details**

Computer intensive method for linear dimension reduction that minimizes the classification error in the projected subspace directly. Classification is done by lda. In contrast to the reference function minimization is done by Nelder-Mead in optim.

#### Value

method.model An object of class 'lda'.

Proj.matrix Projection matrix.

B. error Estimated bootstrap error rate.B. impro Improvement in 1da error rate.

# Author(s)

Maria Eveslage, Karsten Luebke, <karsten.luebke@fom.de>

#### References

Roehl, M.C., Weihs, C., and Theis, W. (2002): Direct Minimization in Multivariate Classification. *Computational Statistics*, 17, 29-46.

# See Also

```
predict.meclight
```

```
data(iris)
meclight.obj <- meclight(Species ~ ., data = iris)
meclight.obj</pre>
```

NaiveBayes 31

|--|

# **Description**

Computes the conditional a-posterior probabilities of a categorical class variable given independent predictor variables using the Bayes rule.

# Usage

```
## S3 method for class 'formula'
NaiveBayes(formula, data, ..., subset, na.action = na.pass)
## Default S3 method:
NaiveBayes(x, grouping, prior, usekernel = FALSE, fL = 0, ...)
```

# Arguments

х	a numeric matrix, or a data frame of categorical and/or numeric variables.
grouping	class vector (a factor).
formula	a formula of the form class $\sim$ x1 + x2 + Interactions are not allowed.
data	a data frame of predictors (caegorical and/or numeric).
prior	the prior probabilities of class membership. If unspecified, the class proportions for the training set are used. If present, the probabilities should be specified in the order of the factor levels.
usekernel	if TRUE a kernel density estimate ( $density$ ) is used for density estimation. If FALSE a normal density is estimated.
fL	Factor for Laplace correction, default factor is 0, i.e. no correction.
	arguments passed to density.
subset	for data given in a data frame, an index vector specifying the cases to be used in the training sample. (NOTE: If given, this argument must be named.)
na.action	a function to specify the action to be taken if NAs are found. The default action is not to count them for the computation of the probability factors. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable. (NOTE: If given, this argument must be named.)

# **Details**

This implementation of Naive Bayes as well as this help is based on the code by David Meyer in the package e1071 but extended for kernel estimated densities and user specified prior probabilities. The standard naive Bayes classifier (at least this implementation) assumes independence of the predictor variables.

nm

#### Value

An object of class "NaiveBayes" including components:

apriori Class distribution for the dependent variable.

tables A list of tables, one for each predictor variable. For each categorical variable a

table giving, for each attribute level, the conditional probabilities given the target class. For each numeric variable, a table giving, for each target class, mean and standard deviation of the (sub-)variable or a object of class density.

#### Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

#### See Also

```
predict.NaiveBayes,plot.NaiveBayes,naiveBayes,qda
```

# **Examples**

```
data(iris)
m <- NaiveBayes(Species ~ ., data = iris)</pre>
```

nm

Nearest Mean Classification

# Description

Function for nearest mean classification.

# Usage

```
nm(x, ...)
## Default S3 method:
nm(x, grouping, gamma = 0, ...)
## S3 method for class 'data.frame'
nm(x, ...)
## S3 method for class 'matrix'
nm(x, grouping, ..., subset, na.action = na.fail)
## S3 method for class 'formula'
nm(formula, data = NULL, ..., subset, na.action = na.fail)
```

nm 33

#### **Arguments**

Х	matrix or data frame containing the explanatory variables (required, if formula is not given)
grouping	factor specifying the class for each observation (required, if formula is not given) $\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$
formula	formula of the form groups $\sim x1 + x2 + \ldots$ . That is, the response is the grouping factor and the right hand side specifies the (non-factor) discriminators
data	Data frame from which variables specified in formula are preferentially to be taken
gamma	gamma parameter for rbf weight of the distance to mean. If gamma=0 the posterior is 1 for the nearest class (mean) and 0 else.
subset	An index vector specifying the cases to be used in the training sample. (Note: If given, this argument must be named!)
na.action	specify the action to be taken if NAs are found. The default action is for the procedure to fail. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable. (Note: If given, this argument must be named.)
	further arguments passed to the underlying sknn function

#### **Details**

nm is calling sknn with the class means as observations. If gamma>0 a gaussian like density is used to weight the distance to the class means weight=exp(-gamma\*distance). This is similar to an rbf kernel. If the distances are large it may be useful to scale the data first.

#### Value

A list containing the function call and the class means (learn)).

# Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

# See Also

```
sknn, rda, knn
```

```
data(B3)
x <- nm(PHASEN ~ ., data = B3)
x$learn
x <- nm(PHASEN ~ ., data = B3, gamma = 0.1)
predict(x)$post</pre>
```

34 partimat

partimat

Plotting the 2-d partitions of classification methods

# Description

Provides a multiple figure array which shows the classification of observations based on classification methods (e.g. 1da, qda) for every combination of two variables. Moreover, the classification borders are displayed and the apparent error rates are given in each title.

# Usage

# **Arguments**

X	matrix or data frame containing the explanatory variables (required, if formula is not given).
grouping	factor specifying the class for each observation (required, if formula is not given).
formula	formula of the form groups $\sim x1 + x2 + \ldots$ That is, the response is the grouping factor and the right hand side specifies the (non-factor) discriminators.
method	the method the classification is based on, currently supported are: lda, qda, rpart, naiveBayes, rda, sknn and svmlight.
prec	precision used to draw the classification borders (the higher the more precise; default: 100).
data	Data frame from which variables specified in formula are preferentially to be taken.
nplots.vert	number of rows in the multiple figure array
nplots.hor	number of columns in the multiple figure array
subset	index vector specifying the cases to be used in the training sample. (Note: If given, this argument must be named.)

partimat 35

na.action	specify the action to be taken if NAs are found. The default action is for the procedure to fail. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable. (Note: If given, this argument must be named.)
main	title
name	Variable names to be printed at the axis / into the diagonal.
mar	numerical vector of the form $c(bottom, left, top, right)$ which gives the lines of margin to be specified on the four sides of the plot. Defaults are $rep(0, 4)$ if $plot.matrix = TRUE, c(5, 4, 2, 1) + 0.1$ otherwise.
plot.matrix	logical; if TRUE, like a scatterplot matrix; if FALSE (default) uses less space and arranges the plots "optimal" (using a fuzzy algorithm) in an array by plotting each pair of variables once.
plot.control	A list containing further arguments passed to the underlying plot functions (and to drawparti).

#### Note

Warnings such as 'parameter "xyz" couldn't be set in high-level plot function' are expected, if making use of . . . .

Further arguments passed to the classification method (through drawparti).

# Author(s)

Karsten Luebke, <karsten.luebke@fom.de>, Uwe Ligges, Irina Czogiel

# See Also

for much more fine tuning see drawparti

36 plineplot

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Plotting marginal posterior class probabilities

# Description

For a given variable the posteriori probabilities of the classes given by a classification method are plotted. The variable need not be used for the actual classification.

# Usage

# Arguments

formula	formula of the form groups $\sim x1 + x2 + \ldots$ That is, the response is the grouping factor and the right hand side specifies the (non-factor) discriminators.
data	Data frame from which variables specified in formula are preferentially to be taken.
method	character, name of classification function (e.g. "lda").
x	variable that should be plotted. See examples.
col.wrong	color to use for missclassified objects.
ylim	ylim for the plot.
loo	logical, whether leave-one-out estimate is used for prediction
mfrow	number of rows and columns in the graphics device, see par. If missing, number of rows equals number of classes, and 1 column.
	further arguments passed to the underlying classification method or plot functions.

#### Value

The actual error rate.

# Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

# See Also

partimat

plot.NaiveBayes 37

#### **Examples**

plot.NaiveBayes

Naive Bayes Plot

## **Description**

Visualizes the marginal probabilities of predictor variables given the class.

## Usage

```
## S3 method for class 'NaiveBayes'
plot(x, vars, n = 1000, legendplot = TRUE, lty, col,
    ylab = "Density", main = "Naive Bayes Plot", ...)
```

## Arguments

X	an object of class NaiveBayes
vars	variables to be plotted. If missing, all predictor variables are plotted.
n	number of points used to plot the density line.
legendplot	logical, whether to print a legend
lty	line type for different classes, defaults to the first length(x\$apriori) colors of the current palette in use.
col	color for different classes, defaults to rainbow(length(x\$apriori)).
ylab	label for y-axis.
main	title of the plots.
	furhter arguments passed to the underlying plot functions.

## **Details**

For metric variables the estimated density is plotted. For categorial variables mosaicplot is called.

38 predict.loclda

#### Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

#### See Also

NaiveBayes

### **Examples**

```
data(iris)
mN <- NaiveBayes(Species ~ ., data = iris)
plot(mN)

mK <- NaiveBayes(Species ~ ., data = iris, usekernel = TRUE)
plot(mK)</pre>
```

predict.loclda

Localized Linear Discriminant Analysis (LocLDA)

## **Description**

Classifies new observations using parameters determined by the loclda-function.

## Usage

```
## S3 method for class 'loclda'
predict(object, newdata, ...)
```

## Arguments

object Object of class loclda.

newdata Data frame of cases to be classified.
... Further arguments are ignored.

## Value

A list with components:

class Vector (of class factor) of classifications.

posterior Posterior probabilities for the classes. For details of computation see loclda (+

normalization so posterior-values add up to 1 for each observation).

all.zero Vector (of class integer) indicating for which rows of newdata all correspond-

ing posterior-values are  $< 10^{-150}$  before normalization. Those observations are assigned to the class to whose (locally weighted) centroid they have the lowest

euclidian distance.

predict.locpvs 39

#### Author(s)

Marc Zentgraf (<marc-zentgraf@gmx.de>) and Karsten Luebke (<karsten.luebke@fom.de>)

#### See Also

loclda

#### **Examples**

```
data(B3)

x \leftarrow loclda(PHASEN \sim ., data = B3, subset = 1:80)

predict(x, B3[-(1:80),])
```

predict.locpvs

predict method for locpvs objects

#### Description

Prediction of class membership and posterior probabilities in local models using pairwise variable selection.

## Usage

```
## S3 method for class 'locpvs'
predict(object,newdata, quick = FALSE, return.subclass.prediction = TRUE, ...)
```

#### **Arguments**

object an object of class 'locpvs', as that created by the function "locpvs"

newdata a data frame or matrix containing new data. If not given the same datas as used

for training the 'pvs'-model are used.

quick indicator (logical), whether a quick, but less accurate computation of posterior

probabalities should be used or not.

return.subclass.prediction

indicator (logical), whether the returned object includes posterior probabilities

for each date in each subclass

... Further arguments are passed to underlying predict calls.

#### **Details**

Posterior probabilities are predicted as if object is a standard 'pvs'-model with the subclasses as classes. Then the posterior probabilities are summed over all subclasses for each class. The class with the highest value becomes the prediction.

If "quick=FALSE" the posterior probabilities for each case are computed using the pairwise coupling algorithm presented by Hastie, Tibshirani (1998). If "quick=FALSE" a much quicker solution is used, which leads to less accurate posterior probabilities. In almost all cases it doesn't has a negative effect on the classification result.

40 predict.meclight

#### Value

a list with components:

class the predicted (upper) classes

posterior posterior probabilities for the (upper) classes

subclass.posteriors

(only if "return. subclass.prediction=TRUE". A matrix containing posterior

probabilities for the subclasses.

#### Author(s)

Gero Szepannek, <szepannek@statistik.tu-dortmund.de>, Christian Neumann

#### References

Szepannek, G. and Weihs, C. (2006) Local Modelling in Classification on Different Feature Subspaces. In *Advances in Data Mining.*, ed Perner, P., LNAI 4065, pp. 226-234. Springer, Heidelberg.

#### See Also

locpvs for learning 'locpvs'-models and examples for applying this predict method, pvs for pairwise variable selection without modeling subclasses, predict.pvs for predicting 'pvs'-models

predict.meclight

Prediction of Minimal Error Classification

## **Description**

Classify multivariate observations in conjunction with meclight and lda.

## Usage

```
## S3 method for class 'meclight'
predict(object, newdata,...)
```

## **Arguments**

object Object of class meclight.

newdata Data frame of cases to be classified or, if object has a formula, a data frame with

columns of the same names as the variables used. A vector will be interpreted

as a row vector.

... currently ignored

#### **Details**

Classify multivariate observations in conjunction with meclight and lda.

predict.NaiveBayes 41

## Value

class The estimated class (factor).

posterior Posterior probabilities for the classes.

## Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

#### References

Roehl, M.C., Weihs, C., and Theis, W. (2002): Direct Minimization in Multivariate Classification. *Computational Statistics*, 17, 29-46.

#### See Also

```
meclight
```

## **Examples**

```
data(iris)
meclight.obj <- meclight(Species ~ ., data = iris)
predict(meclight.obj, iris)</pre>
```

predict.NaiveBayes

Naive Bayes Classifier

## **Description**

Computes the conditional a-posterior probabilities of a categorical class variable given independent predictor variables using the Bayes rule.

#### Usage

```
## S3 method for class 'NaiveBayes'
predict(object, newdata, threshold = 0.001, ...)
```

#### **Arguments**

object An object of class "naiveBayes".

newdata A dataframe with new predictors.

threshold Value replacing cells with 0 probabilities.
... passed to dkernel function if neccessary.

42 predict.pvs

## **Details**

This implementation of Naive Bayes as well as this help is based on the code by David Meyer in the package e1071 but extended for kernel estimated densities. The standard naive Bayes classifier (at least this implementation) assumes independence of the predictor variables. For attributes with missing values, the corresponding table entries are omitted for prediction.

#### Value

A list with the conditional a-posterior probabilities for each class and the estimated class are returned.

#### Author(s)

```
Karsten Luebke, <karsten.luebke@fom.de>
```

## See Also

NaiveBayes,dkernelnaiveBayes,qda

#### **Examples**

```
data(iris)
m <- NaiveBayes(Species ~ ., data = iris)
predict(m)</pre>
```

predict.pvs

predict method for pvs objects

## **Description**

Prediction of class membership and posterior probabilities using pairwise variable selection.

## Usage

```
## S3 method for class 'pvs'
predict(object, newdata, quick = FALSE, detail = FALSE, ...)
```

## **Arguments**

C	bject	an object of class 'pvs', as that created by the function "pvs"
r	newdata	a data frame or matrix containing new data. If not given the same datas as used for training the 'pvs'-model are used.
C	quick	indicator (logical), whether a quick, but less accurate computation of posterior probabalities should be used or not.
C	letail	indicator (logical), whether the returned object includes additional information about the posterior probabilities for each date in each submodel.
		Further arguments are passed to underlying predict calls.

predict.rda 43

#### **Details**

If "quick=FALSE" the posterior probabilities for each case are computed using the pairwise coupling algorithm presented by Hastie, Tibshirani (1998). If "quick=FALSE" a much quicker solution is used, which leads to less accurate posterior probabilities. In almost all cases it doesn't has a negative effect on the classification result.

#### Value

a list with components:

class the predicted classes

posterior posterior probabilities for the classes

details (only if "details=TRUE". A list containing matrices of posterior probabilities

computated by the classification method for each case and classpair.

## Author(s)

Gero Szepannek, <szepannek@statistik.tu-dortmund.de>, Christian Neumann

#### References

Szepannek, G. and Weihs, C. (2006) Variable Selection for Classification of More than Two Classes Where the Data are Sparse. In *From Data and Information Analysis to Kwnowledge Engineering.*, eds Spiliopolou, M., Kruse, R., Borgelt, C., Nuernberger, A. and Gaul, W. pp. 700-708. Springer, Heidelberg.

#### See Also

For more details and examples how to use this predict method, see pvs.

predict.rda

Regularized Discriminant Analysis (RDA)

## Description

Classifies new observations using parameters determined by the rda-function.

#### Usage

44 predict.sknn

#### **Arguments**

object Object of class rda.

newdata Data frame (or matrix) of cases to be classified.

posterior Logical; indicates whether a matrix of posterior probabilites over all classes for

each observation shall be returned in addition to classifications.

aslist Logical; if TRUE, a list containing classifications and posterior probabilities is

returned, otherwise a vector with an attribute 'posterior'.

... currently unused

#### Value

Depends on the value of argument 'aslist':

Either a vector (of class factor) of classifications that (optionally) has an attribute 'posterior' containing the posterior probability matrix, or

A list with elements 'class' and 'posterior'.

## Author(s)

Christian Röver, <roever@statistik.tu-dortmund.de>

#### See Also

rda

#### **Examples**

```
data(iris)
x <- rda(Species ~ ., data = iris, gamma = 0.05, lambda = 0.2)
predict(x, iris[, 1:4])</pre>
```

predict.sknn

Simple k Nearest Neighbours Classification

## Description

Classifies new observations using the sknn learned by the sknn-function.

## Usage

```
## S3 method for class 'sknn'
predict(object, newdata,...)
```

#### **Arguments**

object Object of class sknn.

newdata Data frame (or matrix) of cases to be classified.

predict.svmlight 45

## Value

A list with elements 'class' and 'posterior'.

#### Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

#### See Also

```
sknn, knn
```

## **Examples**

```
data(iris)
x <- sknn(Species ~ ., data = iris)
predict(x, iris)
x <- sknn(Species ~ ., gamma = 10, kn = 10, data = iris)
predict(x, iris)</pre>
```

predict.svmlight

Interface to SVMlight

## **Description**

Predicts new observations using the SVM learned by the symlight-function.

## Usage

```
## S3 method for class 'svmlight'
predict(object, newdata, scal = TRUE, ...)
```

## **Arguments**

object Object of class symlight.

newdata Data frame (or matrix) of cases to be predicted.

scal Logical, whether to scale membership values via e. scal.

...

## Value

If a classification is learned (type="C") in svmlight a list with elements 'class' and 'posterior' (scaled, if scal = TRUE).

If a Regression is learned (type="R") in symlight the predicted values.

#### Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

46 pvs

#### See Also

```
svmlight, svm
```

## **Examples**

```
## Not run:
data(iris)
x <- symlight(Species ~ ., data = iris)
predict(x, iris)
## End(Not run)</pre>
```

pvs

Pairwise variable selection for classification

## Description

Pairwise variable selection for numerical data, allowing the use of different classifiers and different variable selection methods.

## Usage

```
pvs(x, ...)
## Default S3 method:
pvs(x, grouping, prior=NULL, method="lda",
    vs.method=c("ks.test","stepclass","greedy.wilks"), niveau=0.05,
    fold=10, impr=0.1, direct="backward", out=FALSE, ...)
## S3 method for class 'formula'
pvs(formula, data = NULL, ...)
```

## Arguments

X	matrix or data frame containing the explanatory variables (required, if formula is not given). x must consist of numerical data only.
formula	A formula of the form groups $\sim x1 + x2 + \ldots$ . That is, the response is the grouping factor (the classes) and the right hand side specifies the (numerical) discriminators. Interaction terms are not supported.
data	data matrix (rows=cases, columns=variables)
grouping	class indicator vector (a factor)
prior	prior probabilites for the classes. If not specified the prior probabilities will be set according to proportion in "grouping". If specified the order of prior probabilities must be the same as in "grouping".
method	character, name of classification function (e.g. "lda" (default)).

47 pvs

vs.method character, name of variable selection method. Must be one of "ks.test" (default), "stepclass" or "greedy.wilks". used niveau for "ks. test" niveau fold parameter for cross-validation, if "stepclass" is chosen 'vs.method' least improvement of performance measure desired to include or exclude any impr variable (<=1), if "stepclass" is chosen 'vs.method' direct direction of variable selection, if "stepclass" is chosen 'vs.method'. Must be one if "forward", "backward" (default) or "both". indicator (logical) for textoutput during computation (slows down computaout tion!), if "stepclass" is chosen 'vs.method'

further parameters passed to classification function ('method') or variable selec-

tion method ('vs.method')

#### **Details**

The classification "method" (e.g. 'lda') must have its own 'predict' method (like 'predict.lda' for 'lda') returns a list with an element 'posterior' containing the posterior probabilties. It must be able to deal with matrices as in method(x, grouping, ...). Examples of such classification methods are 'lda', 'qda', 'rda', 'NaiveBayes' or 'sknn'.\ For the classification methods "svm" and "randomForest" there are special routines implemented, to make them work with 'pvs' method even though their 'predict' methods don't provide the demanded posteriors. However those two classfiers can not be used together with variable selection method "stepclass".

'pvs' performs a variable selection using the selection method chosen in 'vs.method' for each pair of classes in 'x'. Then for each pair of classes a submodel using 'method' is trained (using only the earlier selected variables for this class-pair).

If 'method' is "ks.test", then for each variable the empirical distribution functions of the cases of both classes are compared via "ks.test". Only variables with a p-values below 'niveau' are used for training the submodel for this pair of classes.

If 'method' is "stepclass" the variable selection is performed using the "stepclass" method.

If 'method' is "greedy.wilks" the variable selection is performed using Wilk's lambda criterion.

## Value

An object of class 'pvs' containing the following components:

classes the classes in grouping used prior probabilities prior

name of used classification function method

vs.method name of used function for variable selection

submodels containing a list of submodels. For each pair of classes there is a list element

> being another list of 3 containing the class-pair of this submodel, the selected variables for the subspace of classes and the result of the trained classification

function.

call the (matched) function call 48 pvs

#### Author(s)

Gero Szepannek, <szepannek@statistik.tu-dortmund.de>, Christian Neumann

#### References

- Szepannek, G. and Weihs, C. (2006) Variable Selection for Classification of More than Two Classes Where the Data are Sparse. In *From Data and Information Analysis to Kwnowledge Engineering.*, eds Spiliopolou, M., Kruse, R., Borgelt, C., Nuernberger, A. and Gaul, W. pp. 700-708. Springer, Heidelberg.
- Szepannek, G. (2008): Different Subspace Classification Datenanalyse, -interpretation, visualisierung und Vorhersage in hochdimensionalen Raeumen, ISBN 978-3-8364-6302-7, vdm, Saarbruecken.

#### See Also

predict.pvs for predicting 'pvs' models and locpvs for pairwisevariable selection in local models
of several subclasses

```
## Example 1: learn an "lda" model on the waveform data using pairwise variable selection (pvs) using "ks.test
## and compare it to using lda without pvs
library("mlbench")
trainset <- mlbench.waveform(300)</pre>
pvsmodel <- pvs(trainset$x, trainset$classes, niveau=0.05) # default: using method="lda"</pre>
pvsmodel # short summary, showing the class-pairs of the submodels and the selected variables
testset <- mlbench.waveform(500)</pre>
## prediction of the test data set:
prediction <- predict(pvsmodel, testset$x)</pre>
## calculating the test error rate
1-sum(testset$classes==prediction$class)/length(testset$classes)
## Bayes error is 0.149
## comparison to performance of simple lda
ldamodel <- lda(trainset$x, trainset$classes)</pre>
LDAprediction <- predict(ldamodel, testset$x)
## test error rate
1-sum(testset$classes==LDAprediction$class)/length(testset$classes)
## Example 2: learn a "qda" model with pvs on half of the Satellite dataset, using "ks.test"
library("mlbench")
data("Satellite")
model <- pvs(classes ~ ., Satellite[1:3218,], method="qda", vs.method="ks.test")</pre>
model # short summary, showing the class-pairs of the submodels and the selected variables
```

quadplot 49

```
## now predict on the rest of the data set:
## pred <- predict(model,Satellite[3219:6435,]) # takes some time
pred <- predict(model,Satellite[3219:6435,], quick=TRUE) # that's much quicker

## now you can look at the predicted classes:
pred$class
## or the posterior probabilities:
pred$posterior</pre>
```

quadplot

Plotting of 4 dimensional membership representation simplex

## **Description**

For a 4 class discrimination problem the membership values of each class are visualized in a 3 dimensional barycentric coordinate system.

## Usage

```
quadplot(e = NULL, f = NULL, g = NULL, h = NULL, angle = 75,
    scale.y = 0.6, label = 1:4, labelcol = rainbow(4),
    labelpch = 19, labelcex = 1.5, main = "", s3d.control = list(),
    simplex.control = list(), legend.control = list(), ...)
```

## **Arguments**

е	either a matrix with 4 columns representing the membership values or a vector with the membership values of the first class
f	vector with the membership values of the second class
g	vector with the membership values of the third class
h	vector with the membership values of the forth class
angle	angle between x and y axis
scale.y	scale of y axis related to x- and z axis
label	label for the classes
labelcol	colors to use for the labels
labelpch	pch for the labels
labelcex	cex for the labels
main	main title of the plot
s3d.control	a <i>list</i> with further arguments passed to the underlying scatterplot3d function call that sets up the plot
simplex.control	
	a <i>list</i> with further arguments passed to the underlying function call that draws

the barycentric coordinate system

50 quadplot

legend.control a *list* with further arguments passed to the underlying function call that adds the legend

... further arguments passed to the underlying plot function that draws the data points

#### **Details**

The membership values are calculated with quadtrafo and plotted with scatterplot3d.

#### Value

A scatterplot3d object.

#### Author(s)

Karsten Luebke, <karsten.luebke@fom.de>, and Uwe Ligges

#### References

Garczarek, Ursula Maria (2002): Classification rules in standardized partition spaces. Dissertation, University of Dortmund. URL http://hdl.handle.net/2003/2789

## See Also

```
triplot, scatterplot3d
```

```
library("MASS")
data(B3)
opar <- par(mfrow = c(1, 2), pty = "s")
posterior <- predict(lda(PHASEN \sim ., data = B3))post
s3d <- quadplot(posterior, col = rainbow(4)[B3$PHASEN],</pre>
        labelpch = 22:25, labelcex = 0.8,
        pch = (22:25)[apply(posterior, 1, which.max)],
        main = "LDA posterior assignments")
quadlines(centerlines(4), sp = s3d, lty = "dashed")
posterior <- predict(qda(PHASEN ~ ., data = B3))$post</pre>
s3d <- quadplot(posterior, col = rainbow(4)[B3$PHASEN],
        labelpch = 22:25, labelcex = 0.8,
        pch = (22:25)[apply(posterior, 1, which.max)],
        main = "QDA posterior assignments")
quadlines(centerlines(4), sp = s3d, lty = "dashed")
par(opar)
```

rda 51

rda

Regularized Discriminant Analysis (RDA)

## Description

Builds a classification rule using regularized group covariance matrices that are supposed to be more robust against multicollinearity in the data.

## Usage

```
rda(x, ...)
## Default S3 method:
rda(x, grouping = NULL, prior = NULL, gamma = NA,
    lambda = NA, regularization = c(gamma = gamma, lambda = lambda),
    crossval = TRUE, fold = 10, train.fraction = 0.5,
    estimate.error = TRUE, output = FALSE, startsimplex = NULL,
    max.iter = 100, trafo = TRUE, simAnn = FALSE, schedule = 2,
    T.start = 0.1, halflife = 50, zero.temp = 0.01, alpha = 2,
    K = 100, ...)
## S3 method for class 'formula'
rda(formula, data, ...)
```

## **Arguments**

X	Matrix or data frame containing the explanatory variables (required, if formula is not given).
formula	Formula of the form 'groups $\sim x1 + x2 +$ '.
data	A data frame (or matrix) containing the explanatory variables.
grouping	(Optional) a vector specifying the class for each observation; if not specified, the first column of 'data' is taken.
prior	(Optional) prior probabilities for the classes. Default: proportional to training sample sizes. "prior=1" indicates equally likely classes.
gamma, lambda,	regularization
	One or both of the rda-parameters may be fixed manually. Unspecified parameters are determined by minimizing the estimated error rate (see below).
crossval	Logical. If TRUE, in the optimization step the error rate is estimated by Cross-Validation, otherwise by drawing several training- and test-samples.
fold	The number of Cross-Validation- or Bootstrap-samples to be drawn.
train.fraction	In case of Bootstrapping: the fraction of the data to be used for training in each Bootstrap-sample; the remainder is used to estimate the misclassification rate.
estimate.error	Logical. If TRUE, the apparent error rate for the final parameter set is estimated.
output	Logical flag to indicate whether text output during computation is desired.
startsimplex	(Optional) a starting simplex for the Nelder-Mead-minimization.

52 rda

max.iter Maximum number of iterations for Nelder-Mead.

trafo Logical; indicates whether minimization is carrried out using transformed pa-

rameters.

simAnn Logical; indicates whether Simulated Annealing shall be used.

schedule Annealing schedule 1 or 2 (exponential or polynomial).

T. start Starting temperature for Simulated Annealing.

halflife Number of iterations until temperature is reduced to a half (schedule 1).

zero.temp Temperature at which it is set to zero (schedule 1).

alpha Power of temperature reduction (linear, quadratic, cubic,...) (schedule 2).

K Number of iterations until temperature = 0 (schedule 2).

... currently unused

#### **Details**

J.H. Friedman (see references below) suggested a method to fix almost singular covariance matrices in discriminant analysis. Basically, individual covariances as in QDA are used, but depending on two parameters ( $\gamma$  and  $\lambda$ ), these can be shifted towards a diagonal matrix and/or the pooled covariance matrix. For ( $\gamma = 0$ ,  $\lambda = 0$ ) it equals QDA, for ( $\gamma = 0$ ,  $\lambda = 1$ ) it equals LDA.

You may fix these parameters at certain values or leave it to the function to try to find "optimal" values. If one parameter is given, the other one is determined using the R-function 'optimize'. If no parameter is given, both are determined numerically by a Nelder-Mead-(Simplex-)algorithm with the option of using Simulated Annealing. The goal function to be minimized is the (estimated) misclassification rate; the misclassification rate is estimated either by Cross-Validation or by repeatedly dividing the data into training- and test-sets (Boostrapping).

*Warning*: If these sets are small, optimization is expected to produce almost random results. We recommend to adjust the parameters manually in such a case. In all other cases it is recommended to run the optimization several times in order to see whether stable results are gained.

Since the Nelder-Mead-algorithm is actually intended for *continuous* functions while the observed error rate by its nature is *discrete*, a greater number of Boostrap-samples might improve the optimization by increasing the smoothness of the response surface (and, of course, by reducing variance and bias). If a set of parameters leads to singular covariance matrices, a penalty term is added to the misclassification rate which will hopefully help to maneuver back out of singularity (so do not worry about error rates greater than one during optimization).

#### Value

A list of class rda containing the following components:

call The (matched) function call.

regularization vector containing the two regularization parameters (gamma, lambda)

classes the names of the classes

prior the prior probabilities for the classes

error.rate apparent error rate (if computation was not suppressed), and, if any optimization

took place, the final (cross-validated or bootstrapped) error rate estimate as well.

rda 53

means Group means.

covariances Array of group covariances.

covpooled Pooled covariance.

converged (Logical) indicator of convergence (only for Nelder-Mead).

iter Number of iterations actually performed (only for Nelder-Mead).

#### More details

The explicit defintion of  $\gamma$ ,  $\lambda$  and the resulting covariance estimates is as follows:

The pooled covariance estimate  $\hat{\Sigma}$  is given as well as the individual covariance estimates  $\hat{\Sigma}_k$  for each group.

First, using  $\lambda$ , a convex combination of these two is computed:

$$\hat{\Sigma}_k(\lambda) := (1 - \lambda)\hat{\Sigma}_k + \lambda\hat{\Sigma}.$$

Then, another convex combination is constructed using the above estimate and a (scaled) identity matrix:

$$\hat{\Sigma}_k(\lambda, \gamma) = (1 - \gamma)\hat{\Sigma}_k(\lambda) + \gamma \frac{1}{d} \text{tr}[\hat{\Sigma}_k(\lambda)] I.$$

The factor  $\frac{1}{d} \operatorname{tr}[\hat{\Sigma}_k(\lambda)]$  in front of the identity matrix I is the mean of the diagonal elements of  $\hat{\Sigma}_k(\lambda)$ , so it is the mean variance of all d variables assuming the group covariance  $\hat{\Sigma}_k(\lambda)$ .

For the four extremes of  $(\gamma, \lambda)$  the covariance structure reduces to special cases:

- ( $\gamma=0,\,\lambda=0$ ): QDA individual covariance for each group.
- $(\gamma = 0, \lambda = 1)$ : LDA a common covariance matrix.
- $(\gamma = 1, \lambda = 0)$ : Conditional independent variables similar to Naive Bayes, but variable variances within group (main diagonal elements) are equal.
- $(\gamma = 1, \lambda = 1)$ : Classification using euclidean distance as in previous case, but variances are the same for all groups. Objects are assigned to group with nearest mean.

## Author(s)

Christian Röver, <roever@statistik.tu-dortmund.de>

#### References

Friedman, J.H. (1989): Regularized Discriminant Analysis. In: *Journal of the American Statistical Association* 84, 165-175.

Press, W.H., Flannery, B.P., Teukolsky, S.A., Vetterling, W.T. (1992): *Numerical Recipes in C.* Cambridge: Cambridge University Press.

#### See Also

predict.rda, lda, qda

54 shardsplot

#### **Examples**

```
data(iris)
x <- rda(Species ~ ., data = iris, gamma = 0.05, lambda = 0.2)
predict(x, iris)</pre>
```

shardsplot

Plotting Eight Direction Arranged Maps or Self-Organizing Maps

## **Description**

Plotting method for objects of class EDAM or som.

## Usage

```
shardsplot(object, plot.type = c("eight", "four", "points", "n"),
   expand = 1, stck = TRUE, grd = FALSE, standardize = FALSE,
   data.or = NA, label = FALSE, plot = TRUE, classes = 0,
   vertices = TRUE, classcolors = "rainbow", wghts = 0,
   xlab = "Dimension 1", ylab = "Dimension 2", xaxs = "i",
   yaxs = "i", plot.data.column = NA,
    log.classes = FALSE, revert.colors = FALSE, ...)
level_shardsplot(object, par.names, rows = 1:NCOL(object$data),
   centers = rep(NA, length(par.names)), class.labels = NA,
    revert.colors = rep(FALSE, length(par.names)),
   log.classes = rep(FALSE, length(par.names)),
    centeredcolors = colorRamp(c("red", "white", "blue")),
   mfrow = c(2, 2), plot.type = c("eight", "four", "points", "n"),
   expand = 1, stck = TRUE, grd = FALSE, standardize = FALSE,
   label = FALSE, plot = TRUE, vertices = TRUE, classcolors = "topo",
   wghts = 0, xlab = "Dimension 1", ylab = "Dimension 2",
   xaxs = "i", yaxs = "i", ...)
## S3 method for class 'EDAM'
plot(...)
```

#### **Arguments**

object an object of class EDAM or som.

par.names names used to lable the data columns

rows vector with indices of colomns to be plotted

centers vector of type numeric defining the class centers for the data. NA if data does not have a center.

class.labels matrix of type text and dimension(3, NROW(object\$data)) defining the lables to be used for maximum, minimum and central value.

shardsplot 55

centeredcolors colors to represent the classes with a central value

mfrow parameter defining number of plots on a page. see par

plot.type a character giving the shape of the shards. Available are "eight" and "four"

for octagons resp. rectangles, and "points" for points. If plot. type is "n", no

shards are plotted at all.

expand a numeric giving the relative expansion of the axes. A value greater than one

implies smaller shards. Varying expand can be sensible for visual reasons.

stck logical. If TRUE the cells are varied continously corresponding to the differences

of direct neighbors in the origin space. Within this variation the relative order of

the cells is always preserved.

grd logical. If TRUE (which automatically sets stck to TRUE), the variation of cells

is restricted to their original discrete values.

standardize logical. If TRUE, then the measurements in object\$preimages are standard-

ized before calculating Euclidean distances. Measurements are standardized for each variable by dividing by the variable's standard deviation. Meaningless if

object\$preimages is a dissimilarity matrix.

data.or original data and classes where the first k columns are variables and the (k+1)-th

column are the classes. If defined and class of object is som, data.or is used to assign a class to each codebook. There a codebook receives the class, from

which the majority of its assigned objects origins.

label logical. If TRUE, the shards are labeled by the rownames of the preimages.

plot logical. If FALSE, all graphical output is suppressed.

classes a vector giving alternative classes for objects of class EDAM; classes have to be

given in the original order of the data to which EDAM was applied.

vertices logical. If TRUE the grid is drawn.

classcolors colors to represent the classes, or a character giving the *colorscale* for the classes.

Since now available scales are rainbow, topo and gray.

wghts an optional vector of length k giving relative weights of the variables in comput-

ing Euclidean distances. Meaningless if object\$preimages is a dissimilarity

matrix.

xaxs see par
yaxs see par
xlab see par
ylab see par

... further plotting parameters.

plot.data.column

column index defining from data.or providing the data used to calculate the

coloring of the cells.

log.classes boolean indicating that the data should be transformed with the logarithmic

function before calculating the cell coloring

revert.colors boolean indicating that the colorscale should be reverted.

56 shardsplot

#### **Details**

level\_shardsplot uses multiple shardsplot representations of a SOM in order to depict how the data used to calculate the SOM is distribution across the map. Two representations are possible for the data, first with a single color ramp from the minimum value to the maximum value. The second representation is usefull for data for which a basic value exists some where between minimum and maximum for which a special color representation should be used (e.g. 0 is indicated with white).

If plot.type is "four" or "eight", the shape of each shard depends on the relative distances of the actual object or codebook to its up to eight neighbours. If plot.type is "eight", shardsplot corresponds to the representation method suggested by Cottrell and de Bodt (1996) for Kohonen Self-Organizing Maps. If plot.type is "points", shardsplot reduces to a usual scatter plot.

#### Value

The following list is (invisibly) returned:

```
Cells.ex the images of the visualized data
S the criterion of the visualization
```

#### Author(s)

Nils Raabe, level\_shardsplot function from Dominik Reusser

#### References

Cottrell, M., and de Bodt, E. (1996). A Kohonen Map Representation to Avoid Misleading Interpretations. *Proceedings of the European Symposium on Atrificial Neural Networks*, D-Facto, pp. 103–110.

#### See Also

```
EDAM, TopoS, som
```

```
# Compute clusters and an Eight Directions Arranged Map for the
# country data. Plotting the result.
data(countries)
logcount <- log(countries[,2:7])
sdlogcount <- apply(logcount, 2, sd)
logstand <- t((t(logcount) / sdlogcount) * c(1,2,6,5,5,3))
cclasses <- cutree(hclust(dist(logstand)), k = 6)
countryEDAM <- EDAM(logstand, classes = cclasses, sa = FALSE,
    iter.max = 10, random = FALSE)
plot(countryEDAM, vertices = FALSE, label = TRUE, stck = FALSE)
# Compute and plot a Self-Organizing Map for the iris data
data(iris)
library(som)
irissom <- som(iris[,1:4], xdim = 6, ydim = 14)
shardsplot(irissom, data.or = iris, vertices = FALSE)</pre>
```

sknn 57

```
opar <- par(xpd = NA)
legend(7.5, 6.1, col = rainbow(3), xjust = 0.5, yjust = 0,
    legend = levels(iris[, 5]), pch = 16, horiz = TRUE)
par(opar)

level_shardsplot(irissom, par.names = names(iris),
    class.labels = NA, mfrow = c(2,2))</pre>
```

sknn

Simple k nearest Neighbours

## **Description**

Function for simple knn classification.

## Usage

```
sknn(x, ...)
## Default S3 method:
sknn(x, grouping, kn = 3, gamma=0, ...)
## S3 method for class 'data.frame'
sknn(x, ...)
## S3 method for class 'matrix'
sknn(x, grouping, ..., subset, na.action = na.fail)
## S3 method for class 'formula'
sknn(formula, data = NULL, ..., subset, na.action = na.fail)
```

## Arguments

X	matrix or data frame containing the explanatory variables (required, if formula is not given).
grouping	factor specifying the class for each observation (required, if formula is not given). $ \\$
formula	formula of the form groups $\sim x1 + x2 + \ldots$ That is, the response is the grouping factor and the right hand side specifies the (non-factor) discriminators.
data	Data frame from which variables specified in formula are preferentially to be taken.
kn	Number of nearest neighbours to use.
gamma	$gamma\ parameter\ for\ rbf\ in\ knn.\ If\ gamma=0\ ordinary\ knn\ classification\ is\ used.$
subset	An index vector specifying the cases to be used in the training sample. (Note: If given, this argument must be named.)
na.action	specify the action to be taken if NAs are found. The default action is for the procedure to fail. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable. (Note: If given, this argument must be named.)
• • •	currently unused

58 stepclass

#### **Details**

If gamma>0 an gaussian like density is used to weight the classes of the kn nearest neighbors. weight=exp(-gamma\*distance). This is similar to an rbf kernel. If the distances are large it may be useful to scale the data first.

## Value

A list containing the function call.

#### Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

#### See Also

```
predict.sknn,knn
```

## **Examples**

```
data(iris)
x <- sknn(Species ~ ., data = iris)
x <- sknn(Species ~ ., gamma = 4, data = iris)</pre>
```

stepclass

Stepwise variable selection for classification

## **Description**

Forward/backward variable selection for classification using any specified classification function and selecting by estimated classification performance measure from ucpm.

## Usage

```
## Default S3 method:
stepclass(x, grouping, method, improvement = 0.05, maxvar = Inf,
    start.vars = NULL, direction = c("both", "forward", "backward"),
    criterion = "CR", fold = 10, cv.groups = NULL, output = TRUE,
    min1var = TRUE, ...)
## S3 method for class 'formula'
stepclass(formula, data, method, ...)
```

stepclass 59

#### **Arguments**

x matrix or data frame containing the explanatory variables (required, if formula

is not given).

formula A formula of the form groups  $\sim x1 + x2 + \dots$  That is, the response is the

grouping factor and the right hand side specifies the (non-factor) discriminators.

Interaction terms are not supported.

data matrix (rows=cases, columns=variables)

grouping class indicator vector (a factor)

method character, name of classification function (e.g. "lda").

improvement least improvement of performance measure desired to include or exclude any

variable (<=1)

maxvar maximum number of variables in model

start.vars set variables to start with (indices or names). Default is no variables if 'direction'

is "forward" or "both", and all variables if 'direction' is "backward".

direction "forward", "backward" or "both" (default)

criterion performance measure taken from ucpm.

fold parameter for cross-validation; omitted if 'cv.groups' is specified.

cv.groups vector of group indicators for cross-validation. By default assigned automati-

cally.

output indicator (logical) for textoutput during computation (slows down computation!)
min1var logical, whether to include at least one variable in the model, even if the prior

itself already is a reasonable model.

... further parameters passed to classification function ('method'), e.g. priors etc.

## Details

The classification "method" (e.g. 'lda') must have its own 'predict' method (like 'predict.lda' for 'lda') that either returns a matrix of posterior probabilities or a list with an element 'posterior' containing that matrix instead. It must be able to deal with matrices as in method(x, grouping, ...)

Then a stepwise variable selection is performed. The initial model is defined by the provided starting variables; in every step new models are generated by including every single variable that is not in the model, and by excluding every single variable that is in the model. The resulting performance measure for these models are estimated (by cross-validation), and if the maximum value of the chosen criterion is better than 'improvement' plus the value so far, the corresponding variable is in- or excluded. The procedure stops, if the new best value is not good enough, or if the specified maximum number of variables is reached.

If 'direction' is "forward", the model is only extended (by including further variables), if 'direction' is "backward", the model is only reduced (by excluding variables from the model).

#### Value

An object of class 'stepclass' containing the following components:

call the (matched) function call.

60 symlight

```
method name of classification function used (e.g. "lda").

start.variables

vector of starting variables.

process data frame showing selection process (included/excluded variables and performance measure).

model the final model: data frame with 2 columns; indices and names of variables.

perfomance.measure

value of the criterion used by ucpm

formula formula of the form 'response ~ list + of + selected + variables'
```

#### Author(s)

Christian Röver, <roever@statistik.tu-dortmund.de>, Irina Czogiel

#### See Also

step, stepAIC, and greedy.wilks for stepwise variable selection according to Wilk's lambda

## **Examples**

svmlight

Interface to SVMlight

## **Description**

Function to call SVMlight from R for classification. Multiple group classification is done with the one-against-rest partition of data.

symlight 61

## Usage

```
svmlight(x, ...)
## Default S3 method:
svmlight(x, grouping, temp.dir = NULL, pathsvm = NULL,
    del = TRUE, type = "C", class.type = "oaa", svm.options = NULL,
    prior = NULL, out = FALSE, ...)
## S3 method for class 'data.frame'
svmlight(x, ...)
## S3 method for class 'matrix'
svmlight(x, grouping, ..., subset, na.action = na.fail)
## S3 method for class 'formula'
svmlight(formula, data = NULL, ..., subset,
    na.action = na.fail)
```

## Arguments

3	
х	matrix or data frame containing the explanatory variables (required, if formula is not given).
grouping	factor specifying the class for each observation (required, if formula is not given).
formula	formula of the form groups $\sim x1 + x2 + \ldots$ That is, the response is the grouping factor and the right hand side specifies the (non-factor) discriminators.
data	Data frame from which variables specified in formula are preferentially to be taken.
temp.dir	directory for temporary files.
pathsvm	Path to SVMlight binaries (required, if path is unknown by the OS).
del	Logical: whether to delete temporary files
type	Perform "C"=Classification or "R"=Regression
class.type	Multiclass scheme to use. See details.
svm.options	Optional parameters to SVMlight.  For further details see: "How to use" on http://svmlight.joachims.org/.
prior	A Priori probabilities of classes.
out	Logical: whether SVMlight output ahouild be printed on console (only for Windows OS.)
subset	An index vector specifying the cases to be used in the training sample. (Note: If given, this argument must be named.)
na.action	specify the action to be taken if NAs are found. The default action is for the procedure to fail. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable. (Note: If given, this argument

... currently unused

must be named.)

62 symlight

#### **Details**

Function to call SVMlight from R for classification (type="C"). SVMlight is an implementation of Vapnik's Support Vector Machine. It is written in C by Thorsten Joachims. On the homepage (see below) the source-code and several binaries for SVMlight are available. If more then two classes are given the SVM is learned by the one-against-all scheme (class.type="oaa"). That means that each class is trained against the other K-1 classes. The class with the highest decision function in the SVM wins. So K SVMs have to be learned. If class.type="oao" each class is tested against every other and the final class is elected by a majority vote.

If type="R" a SVM Regression is performed.

#### Value

A list containing the function call and the result of SVMlight.

#### Requirements

```
SVMlight (http://svmlight.joachims.org/) must be installed before using this interface.
```

## Author(s)

Karsten Luebke, <karsten.luebke@fom.de>, Andrea Preusser

#### References

```
http://svmlight.joachims.org/
```

#### See Also

```
predict.svmlight,svm,
```

```
## Not run:
## Only works if the svmlight binaries are in the path.
data(iris)
x <- svmlight(Species ~ ., data = iris)
## Using RBF-Kernel with gamma=0.1:
data(B3)
x <- svmlight(PHASEN ~ ., data = B3, svm.options = "-t 2 -g 0.1")
## End(Not run)</pre>
```

triframe 63

triframe

Barycentric plots

## Description

Function to add a frame to an existing (barycentric) plot.

#### Usage

```
triframe(label = 1:3, label.col = 1, cex = 1, ...)
```

#### **Arguments**

label labels for the three corners of the plot.
label.col text color for labels.

cex Magnification factor for label text relative to the default.

... Further graphical parameters passed to trilines.

#### Author(s)

Christian Röver, <roever@statistik.tu-dortmund.de>

#### See Also

```
triplot, trilines, trigrid, centerlines
```

## **Examples**

trigrid

Barycentric plots

## **Description**

Function to add a grid to an existing (barycentric) plot.

#### Usage

```
trigrid(x = seq(0.1, 0.9, by = 0.1), y = NULL, z = NULL, lty = "dashed", col = "grey", ...)
```

64 trigrid

## **Arguments**

X	Values along which to draw grid lines for first dimension (or all dimensions if y and z omitted). For NO grid lines in some dimensions just supply an NA.
у	Grid lines for second dimension.
Z	Grid lines for third dimension.
lty	Line type (see par).
col	Line colour (see par).
	Further graphical parameters passed to trilines.

#### **Details**

Grid lines illustrate the set of points for which one of the dimensions is held constant; e.g. horizontal lines contain all points with a certain value y for the second dimension, connecting the two extreme points (0,y,1-y) and (1-y,y,0).

Grids may be designed more flexible than with triplot's grid option.

## Author(s)

Christian Röver, <roever@statistik.tu-dortmund.de>

## See Also

```
triplot, trilines, triframe, centerlines
```

```
triplot(grid = FALSE)
trigrid(c(1/3, 0.5)) # same grid for all 3 dimensions

triplot(grid = c(1/3, 0.5)) # (same effect)

triplot(grid = FALSE)
# different grids for all dimensions:
trigrid(x = 1/3, y = 0.5, z = seq(0.2, 0.8, by=0.2))

triplot(grid = FALSE)
# grid for third dimension only:
trigrid(x = NA, y = NA, z = c(0.1, 0.2, 0.4, 0.8))
```

triperplines 65

## **Description**

Function to add a point and the corresponding perpendicular lines to all three sides to an existing (barycentric) plot.

## Usage

```
triperplines(x, y = NULL, z = NULL, lcol = "red", pch = 17, ...)
```

## **Arguments**

X	fraction of first component OR 3-element vector (for all three components, omitting y and z).
у	(optional) fraction of second component.
Z	(optional) fraction of third component.
lcol	line color
pch	plotting character. pch = 0 for no point
	Further graphical parameters (see points, lines and par).

#### **Details**

Adds a (single!) point and lines to an existing plot (generated by triplot). The lines originate from the point and run (perpendicular) towards all three sides. The lengths (and proportions) of these lines are identical to those of x, y and z.

## Value

a 2-column-matrix containing plot coordinates.

#### Author(s)

Christian Röver, <roever@statistik.tu-dortmund.de>

#### See Also

```
triplot, tripoints, trilines, tritrafo
```

```
triplot() # empty plot
triperplines(1/2, 1/3, 1/6)
```

66 triplot

#### **Description**

Function to produce triangular (barycentric) plots illustrating proportions of 3 components, e.g. discrete 3D-distributions or mixture fractions that sum up to 1.

## Usage

```
triplot(x = NULL, y = NULL, z = NULL, main = "", frame = TRUE,
    label = 1:3, grid = seq(0.1, 0.9, by = 0.1), center = FALSE,
    set.par = TRUE, ...)
```

#### **Arguments**

X	Vector of fractions of first component OR 3-column matrix containing all three components (omitting y and z) OR 3-element vector (for all three components, omitting y and z).
у	(Optional) vector of fractions of second component.
Z	(Optional) vector of fractions of third component.
main	Main title
frame	Controls whether a frame (triangle) and labels are drawn.
label	(Character) vector of labels for the three corners.
grid	Values along which grid lines are to be drawn (or FALSE for no grid at all). Default is steps of 10 percent.
center	Controls whether or not to draw centerlines at which there is a 'tie' between any two dimensions (see also centerlines).
set.par	Controls whether graphical parameter mar is set so the plot fills the window (see par).
	Further graphical parameters passed to trilines.

#### **Details**

The barycentric plot illustrates the set of points (x,y,z) with x,y,z between 0 and 1 and x+y+z=1; that is, the triangle spanned by (1,0,0), (0,1,0) and (0,0,1) in 3-dimensional space. The three dimensions x, y and z correspond to lower left, upper and lower right corner of the plot. The greater the share of x in the proportion, the closer the point is to the lower left corner; Points on the opposite (upper right) side have a zero x-fraction. The grid lines show the points at which one dimension is held constant, horizontal lines for example contain points with a constant second dimension.

#### Author(s)

Christian Röver, <roever@statistik.tu-dortmund.de>

tripoints 67

#### See Also

tripoints, trilines, triperplines, trigrid, triframe for points, lines and layout, tritrafo for placing labels, and quadplot for the same in 4 dimensions.

## **Examples**

```
# illustrating probabilities:
triplot(label = c("1, 2 or 3", "4 or 5", "6"),
    main = "die rolls: probabilities", pch = 17)
triperplines(1/2, 1/3, 1/6)
# expected...
triplot(1/2, 1/3, 1/6, label = c("1, 2 or 3", "4 or 5", "6"),
    main = "die rolls: expected and observed frequencies", pch = 17)
# ... and observed frequencies.
dierolls <- matrix(sample(1:3, size = 50*20, prob = c(1/2, 1/3, 1/6),
                           replace = TRUE), ncol = 50)
frequencies <- t(apply(dierolls, 1,</pre>
    function(x)(summary(factor(x, levels = 1:3)))) / 50)
tripoints(frequencies)
# LDA classification posterior:
data(iris)
require(MASS)
pred <- predict(lda(Species ~ ., data = iris),iris)</pre>
plotchar \leftarrow rep(1,150)
plotchar[pred$class != iris$Species] <- 19</pre>
triplot(pred$posterior, label = colnames(pred$posterior),
        main = "LDA posterior assignments", center = TRUE,
        pch = plotchar, col = rep(c("blue", "green3", "red"), rep(50, 3)),
        grid = TRUE)
legend(x = -0.6, y = 0.7, col = c("blue", "green3", "red"),
    pch = 15, legend = colnames(pred$posterior))
```

tripoints

Barycentric plots

## **Description**

Function to add points or lines to an existing (barycentric) plot.

## Usage

```
tripoints(x, y = NULL, z = NULL, ...)
trilines(x, y = NULL, z = NULL, ...)
```

68 tritrafo

## **Arguments**

Х	Vector of fractions of first component OR 3-column matrix containing all three components (omitting y and z) OR 3-element vector (for all three components, omitting y and z).
у	(optional) vector of fractions of second component.
z	(optional) vector of fractions of third component.
	Further graphical parameters (see points and par).

#### **Details**

Adds points or lines to an existing plot (generated by triplot).

#### Author(s)

Christian Röver, <roever@statistik.tu-dortmund.de>

#### See Also

```
points, lines, triplot, tritrafo, centerlines
```

## **Examples**

```
triplot() # empty plot
tripoints(0.1, 0.2, 0.7)  # a point
tripoints(c(0.2, 0.6), c(0.3, 0.3), c(0.5, 0.1),
    pch = c(2, 6))  # two points
trilines(c(0.1, 0.6), c(0.2, 0.3), c(0.7, 0.1),
    col = "blue", lty = "dotted")  # a line
trilines(centerlines(3))
```

tritrafo

Barycentric plots

## **Description**

Function to carry out the transformation into 2D space for triplot, trilines etc.

## Usage

```
tritrafo(x, y = NULL, z = NULL, check = TRUE, tolerance = 0.0001)
```

tritrafo 69

## **Arguments**

x	Vector of fractions of first component OR 3-column matrix containing all three components (omitting y and z) OR 3-element vector (for all three components, omitting y and z).
у	(optional) vector of fractions of second component.
z	(optional) vector of fractions of third component.
check	if TRUE, it is checked whether $x+y+z=1$ and $x$ , $y$ , $z>=0$ for all cases.
tolerance	tolerance for above sum check.

#### **Details**

Projects the mixture given by x, y, and z with x, y, z between one and zero and x+y+z=1 into a two-dimensional space.

For further details see triplot.

#### Value

A matrix with two columns corresponding to the two dimensions.

## Author(s)

Christian Röver, <roever@statistik.tu-dortmund.de>

#### See Also

```
triplot, tripoints, trilines, trigrid
```

```
tritrafo(0.1, 0.2, 0.7)
tritrafo(0.1, 0.2, 0.6) # warning

triplot()
points(tritrafo(0.1, 0.2, 0.7), col="red")
tripoints(0.1, 0.2, 0.7, col="green") # the same

tritrafo(c(0.1,0.2), c(0.3,0.4), c(0.6,0.4))
tritrafo(diag(3))

point <- c(0.25,0.6,0.15)
triplot(point, pch=16)
text(tritrafo(point), "(0.25, 0.60, 0.15)", adj=c(0.5,2)) # add a label</pre>
```

70 ucpm

ucpm

Uschi's classification performance measures

## **Description**

Function to calculate the Correctness Rate, the Accuracy, the Ability to Seperate and the Confidence of a classification rule.

## Usage

```
ucpm(m, tc, ec = NULL)
```

## **Arguments**

m matrix of (scaled) membership values

tc vector of true classes

ec vector of estimated classes (only required if scaled membership values are used)

#### **Details**

- The *correctness rate* is the estimator for the correctness of a classification rule (1-error rate).
- The *accuracy* is based on the euclidean distances between (scaled) membership vectors and the vectors representing the true class corner. These distances are standardized so that a measure of 1 is achieved if all vectors lie in the correct corners and 0 if they all lie in the center.
- Analougously, the *ability to seperate* is based on the distances between (scaled) membership vectors and the vector representing the corresponding assigned class corner.
- The *confidence* is the mean of the membership values of the assigned classes.

#### Value

A list with elements:

CR Correctness Rate

AC Accuracy

AS Ability to Seperate

CF Confidence

CFvec Confidence for each (true) class

## Author(s)

Karsten Luebke, <karsten.luebke@fom.de>

#### References

Garczarek, Ursula Maria (2002): Classification rules in standardized partition spaces. Dissertation, University of Dortmund. URL http://hdl.handle.net/2003/2789

ucpm 71

```
library(MASS)
data(iris)
ucpm(predict(lda(Species ~ ., data = iris))$posterior, iris$Species)
```

# **Index**

m :1-4	70
*Topic aplot	ucpm, 70
triframe, 63	*Topic <b>cluster</b>
trigrid, 63	corclust, 9
triperplines, 65	kmodes, 23
triplot, 66	*Topic datasets
tripoints, 67	B3, 4
*Topic attribute	countries, 11
corclust, 9	*Topic distribution
*Topic category	dkernel, 11
kmodes, 23	*Topic <b>dplot</b>
NaiveBayes, 31	centerlines, $8$
predict.NaiveBayes,41	classscatter, 8
*Topic <b>classif</b>	drawparti, 12
b.scal, 3	partimat, 34
benchB3, 5	plineplot, 36
betascale, 6	plot.NaiveBayes, 37
centerlines, $8$	quadplot, 49
classscatter, 8	tritrafo,68
corclust, 9	*Topic <b>hplot</b>
drawparti, 12	shardsplot, 54
e.scal, 14	*Topic <b>manip</b>
hmm.sop, 22	corclust, 9
locpvs, 27	*Topic <b>multivariate</b>
meclight.default,29	corclust, 9
NaiveBayes, 31	EDAM, 15
nm, 32	errormatrix, 17
partimat, 34	friedman.data,19
plineplot, 36	greedy.wilks,20
plot.NaiveBayes, 37	kmodes, 23
predict.locpvs, 39	loclda, 25
predict.meclight, 40	predict.loclda,38
predict.NaiveBayes,41	predict.rda,43
predict.pvs, 42	pvs, 46
predict.sknn,44	rda, 51
predict.svmlight, 45	stepclass, 58
pvs, 46	*Topic <b>nonparametric</b>
quadplot, 49	dkernel, 11
sknn, 57	*Topic <b>ts</b>
symlight, 60	calc.trans,7

INDEX 73

hmm.sop, 22	naiveBayes, <i>13</i> , <i>32</i> , <i>34</i> , <i>42</i>
	nm, 32
b.scal, 3, 6, 7	
B3, 4, 5, 6	optim, <i>30</i>
benchB3, 5, 5	optimize, 52
betascale, <i>3</i> , <i>4</i> , 6	
	par, <i>36</i> , <i>55</i> , <i>64–66</i> , <i>68</i>
calc.trans, 7, 22	partimat, <i>13</i> , <i>34</i> , <i>36</i>
centerlines, 8, 63, 64, 66, 68	pbeta, 3
classscatter, 8	plineplot, 36
contour, 13	plot, 9
corclust, 9	plot.EDAM(shardsplot), 54
countries, 11	plot.NaiveBayes, 32, 37
	plot.rda(rda), 51
density, <i>12</i> , <i>31</i> , <i>32</i>	plot. stepclass (stepclass), 58
dkernel, 11, 41, 42	points, 65, 68
drawparti, 12, <i>35</i>	predict.lda, 47, 59
	predict.loclda, 26, 27, 38
e.scal, 4, 7, 14, 45	predict.locida, 20, 27, 38 predict.locpvs, 28, 39
EDAM, 15, 54–56	predict. lochys, 28, 39 predict.meclight, 30, 40
errormatrix, 17	•
	predict.NaiveBayes, 32, 41
friedman.data, 19	predict.pvs, 40, 42, 48
1 11 20 27 47 60	predict.rda, 43, 53
greedy.wilks, 20, 27, 47, 60	predict.sknn, 44, 58
halust 10	predict.svmlight, 45, 62
hclust, 10	print.greedy.wilks(greedy.wilks), 20
hmm.sop, 22	print.kmodes(kmodes), 23
image, <i>13</i>	print.loclda(loclda),25
Illiage, 13	<pre>print.meclight(meclight.default), 29</pre>
kmodes, 23	print.pvs(pvs),46
knn, 33, 45, 58	print.rda(rda),51
ks. test, 27, 47	print.stepclass(stepclass),58
K3. cc3c, 27, 77	pvs, 28, 40, 42, 43, 46
1da, 3, 9, 13, 19, 27, 30, 34, 36, 40, 46, 47, 53,	
59	qbeta, $3$
legend, 37, 50	qda, 13, 19, 32, 34, 42, 47, 53
level_shardsplot (shardsplot), 54	quadplot, 8, 49, 67
lines, 65, 68	quadtrafo, 50
loclda, 25, 38, 39	
locpvs, 27, 39, 40, 48	randomForest, 47
10cpv3, 27, 39, 40, 40	rda, 13, 19, 20, 33, 34, 44, 47, 51
manova, 21	rpart, <i>13</i> , <i>34</i>
meclight, 40, 41	1 / /
meclight (meclight.default), 29	sammon, <i>16</i>
meclight.default, 29	scale, 5, 33, 58
mosaicplot, 37	scatterplot3d, <i>49</i> , <i>50</i>
mosarchiot, 3/	shardsplot, 16, 54
na.omit, 33, 35, 57, 61	sknn, 13, 33, 34, 44, 45, 47, 57
NaiveBayes, 12, 31, 37, 38, 42, 47	som, 54, 56
NaiveDayes, 12, 31, 37, 30, 42, 47	30iii, J <b>T</b> , JU

74 INDEX

```
step, <u>60</u>
stepAIC, 60
stepclass, 21, 27, 28, 47, 58
svm, 46, 47, 62
svmlight, 13, 34, 45, 46, 60
table, 18
TopoS, 16, 56
triframe, 63, 64, 67
trigrid, 63, 63, 67, 69
trilines, 63–69
trilines (tripoints), 67
triperplines, 65, 67
triplot, 8, 50, 63-65, 66, 68, 69
tripoints, 65, 67, 67, 69
tritrafo, 65, 67, 68, 68
ucpm, 58–60, 70
```