Package 'classmap'

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```
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Author Jakob Raymaekers [aut, cre],
     Peter Rousseeuw [aut]
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Maintainer Jakob Raymaekers < jakob.raymaekers@kuleuven.be>
Description Tools to visualize the results of a classification or a regression.
       The graphical displays include stacked plots, silhouette plots, quasi resid-
     ual plots, class maps, predictions plots, and predictions correlation plots.
       Implements the techniques described and illustrated in Raymaekers J., Rousseeuw P.J., Hu-
     bert M. (2022). Class maps for visualizing classification re-
     sults. \emph{Technometrics}, 64(2), 151–165. \doi{10.1080/00401706.2021.1927849}
     (open access), Raymaekers J., Rousseeuw P.J.(2022). Silhouettes and quasi residual plots for neu-
     ral nets and tree-based classifiers. \emph{Journal of Computational and Graphical Statis-
     tics}, 31(4), 1332–1343. \doi{10.1080/10618600.2022.2050249}, and Rousseeuw, P.J. (2025). Ex-
     plainable Linear and Generalized Linear Models by the Predic-
     tions Plot. <doi:10.48550/arXiv.2412.16980> (open access).
     Examples can be found in the vignettes:
       ``Discriminant_analysis_examples", ``K_nearest_neighbors_examples",
       ``Support_vector_machine_examples", ``Rpart_examples", ``Random_forest_examples",
       ``Neural_net_examples", and ``predsplot_examples".
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```

2 classmap

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Contents

ciassmap	
confmat.vcr	 4
data_bookReviews	 6
data_floralbuds	 7
data_instagram	
data_titanic	
makeFV	
makeKernel	
predscor	
predsplot	
qresplot	
silplot	
stackedplot	
vcr.da.newdata	
vcr.da.train	
vcr.forest.newdata	
vcr.forest.train	
vcr.knn.newdata	
vcr.knn.train	
vcr.neural.newdata	
vcr.neural.train	
vcr.rpart.newdata	
vcr.rpart.train	
vcr.svm.newdata	
vcr.svm.train	
· · · · · · · · · · · · · · · · · · ·	10
	46

classmap

Index

Draw the class map to visualize classification results.

Description

Draw the class map to visualize classification results, based on the output of one of the vcr.*.* functions in this package. The vertical axis of the class map shows each case's PAC, the conditional probability that it belongs to an alternative class. The farness on the horizontal axis is the probability of a member of the given class being at most as far from the class as the case itself.

3 classmap

Usage

```
classmap(vcrout, whichclass, classLabels = NULL, classCols = NULL,
         main = NULL, cutoff = 0.99, plotcutoff = TRUE,
         identify = FALSE, cex = 1, cex.main = 1.2, cex.lab = NULL,
         cex.axis = NULL, opacity = 1,
         squareplot = TRUE, maxprob = NULL, maxfactor = NULL)
```

Arguments

vcrout

whichclass the number or level of the class to be displayed. Required. classLabels the labels (levels) of the classes. If NULL, they are taken from vcrout. classCols a list of colors for the class labels. There should be at least as many as there are levels. If NULL the classCols are taken as 2, 3, 4, ... main title for the plot. cutoff cases with overall farness vcrout\$ofarness > cutoff are flagged as outliers. plotcutoff If true, plots the cutoff on the farness values as a vertical line. if TRUE, left-click on a point to get its number, then ESC to exit. identify cex passed on to graphics::plot. cex.main same, for title. cex.lab same, for labels on horizontal and vertical axes. cex.axis same, for axes. opacity

output of vcr.*.train or vcr.*.newdata. Required.

determines opacity of plotted dots. Value between 0 and 1, where 0 is transpar-

ent and 1 is opaque.

squareplot If TRUE, makes the axes of the plot equally long.

maxprob draws the farness axis at least upto probability maxprob. If NULL, the limits are

obtained automatically.

maxfactor if not NULL, a number slightly higher than 1 to increase the space at the right

hand side of the plot, to make room for marking points.

Value

Executing the function plots the class map and returns

coordinates

a matrix with 2 columns containing the coordinates of the plotted points. The first coordinate is the quantile of the farness probability. This makes it easier to add text next to interesting points. If identify = T, the attribute ids of coordinates contains the row numbers of the identified points in the matrix coordinates.

Author(s)

Raymaekers J., Rousseeuw P.J.

4 confmat.vcr

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, 64(2), 151–165. doi:10.1080/00401706.2021.1927849

Raymaekers J., Rousseeuw P.J.(2021). Silhouettes and quasi residual plots for neural nets and tree-based classifiers. *Journal of Computational and Graphical Statistics*, 31(4), 1332–1343. doi:10.1080/10618600.2022.2050249

See Also

```
vcr.da.train, vcr.da.newdata,
vcr.knn.train, vcr.knn.newdata,
vcr.svm.train, vcr.svm.newdata,
vcr.rpart.train, vcr.rpart.newdata,
vcr.forest.train, vcr.forest.newdata,
vcr.neural.train, vcr.neural.newdata
```

Examples

```
vcrout <- vcr.da.train(iris[, 1:4], iris[, 5])
classmap(vcrout, "setosa", classCols = 2:4) # tight class
classmap(vcrout, "versicolor", classCols = 2:4) # less tight
# The cases misclassified as virginica are shown in blue.
classmap(vcrout, "virginica", classCols = 2:4)
# The case misclassified as versicolor is shown in green.
# For more examples, we refer to the vignettes:
## Not run:
vignette("Discriminant_analysis_examples")
vignette("K_nearest_neighbors_examples")
vignette("Support_vector_machine_examples")
vignette("Rpart_examples")
vignette("Random_forest_examples")
vignette("Neural_net_examples")
## End(Not run)</pre>
```

confmat.vcr

Build a confusion matrix from the output of a function vcr.*.*.

Description

Build a confusion matrix from the output of a function vcr.*.*. Optionally, a separate column for outliers can be added to the confusion matrix.

Usage

confmat.vcr 5

Arguments

vcrout output of vcr.*.train or vcr.*.newdata.

cutoff cases with overall farness vcrout\$ofarness > cutoff are flagged as outliers.

showClassNumbers

if TRUE, the row and column names are the number of each level instead of the

level itself. Useful for long level names.

showOutliers if TRUE and some points were flagged as outliers, it adds an extra column on the

right of the confusion matrix for these outliers, with label "outl".

silent if FALSE, the confusion matrix and accuracy are shown on the screen.

Value

A confusion matrix

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, 64(2), 151–165. doi:10.1080/00401706.2021.1927849

See Also

```
vcr.da.train, vcr.da.newdata,
vcr.knn.train, vcr.knn.newdata,
vcr.svm.train, vcr.svm.newdata,
vcr.rpart.train, vcr.rpart.newdata,
vcr.forest.train, vcr.forest.newdata,
vcr.neural.train, vcr.neural.newdata
```

```
vcrout <- vcr.knn.train(scale(iris[, 1:4]), iris[, 5], k = 5)
# The usual confusion matrix:
confmat.vcr(vcrout, showOutliers = FALSE)

# Cases with ofarness > cutoff are flagged as outliers:
confmat.vcr(vcrout, cutoff = 0.98)

# With the default cutoff = 0.99 only one case is flagged here:
confmat.vcr(vcrout)
# Note that the accuracy is computed before any cases
# are flagged, so it does not depend on the cutoff.

confmat.vcr(vcrout, showClassNumbers = TRUE)
# Shows class numbers instead of labels. This option can
# be useful for long level names.
```

6 data_bookReviews

```
# For more examples, we refer to the vignettes:
## Not run:
vignette("Discriminant_analysis_examples")
vignette("K_nearest_neighbors_examples")
vignette("Support_vector_machine_examples")
vignette("Rpart_examples")
vignette("Random_forest_examples")
vignette("Neural_net_examples")
## End(Not run)
```

data_bookReviews

Amazon book reviews data

Description

This is a subset of the data used in the paper, which was assembled by Prettenhofer and Stein (2010). It contains 1000 reviews of books on Amazon, of which 500 were selected from the original training data and 500 from the test data.

The full dataset has been used for a variety of things, including classification using svm. The subset was chosen small enough to keep the computation time low, while still containing the examples in the paper.

Usage

```
data("data_bookReviews")
```

Format

A data frame with 1000 observations on the following 2 variables.

```
review the review in text format (character)
sentiment factor indicating the sentiment of the review: negative (1) or positive (2)
```

Source

Prettenhofer, P., Stein, B. (2010). Cross-language text classification using structural correspondence learning. *Proceedings of the 48th annual meeting of the association for computational linguistics*, 1118-1127.

```
data(data_bookReviews)
# Example review:
data_bookReviews[5, 1]
# The data are used in:
## Not run:
```

data_floralbuds 7

```
vignette("Support_vector_machine_examples")
## End(Not run)
```

data_floralbuds

Floral buds data

Description

This data on floral pear bud detection was first described by Wouters et al. The goal is to classify the instances into buds, branches, scales and support. The numeric vectors resulted from a multispectral vision sensor and describe the scanned images.

Usage

```
data("data_floralbuds")
```

Format

A data frame with 550 observations on the following 7 variables.

- X1 numeric vector
- X2 numeric vector
- X3 numeric vector
- X4 numeric vector
- X5 numeric vector
- X6 numeric vector
- y a factor with levels branch bud scales support

Source

Wouters, N., De Ketelaere, B., Deckers, T. De Baerdemaeker, J., Saeys, W. (2015). Multispectral detection of floral buds for automated thinning of pear. *Comput. Electron. Agric.* 113, C, 93–103. <doi:10.1016/j.compag.2015.01.015>

```
data("data_floralbuds")
str(data_floralbuds)
summary(data_floralbuds)

# The data are used in:
## Not run:
vignette("Discriminant_analysis_examples")
vignette("Neural_net_examples")

## End(Not run)
```

8 data_instagram

data_instagram

Instagram data

Description

This dataset contains information on fake (spam) accounts on Instagram. The original source is https://www.kaggle.com/free4ever1/instagram-fake-spammer-genuine-accounts by Bardiya Bakhshandeh.

The data contains information on 696 Instagram accounts. For each account, 11 variables were recorded describing its characteristics. The goal is to detect fake instagram accounts, which are used for spamming.

Usage

```
data("data_instagram")
```

Format

A data frame with 696 observations on the following variables.

profile.pic binary, indicates whether profile has picture.

nums.length.username ratio of number of numerical chars in username to its length.

fullname.words number of words in full name.

nums.length.fullname ratio of number of numerical characters in full name to its length.

name..username binary, indicates whether the name and username of the profile are the same.

description.length length of the description/biography of the profile (in number of characters).

external.URL binary, indicates whether profile has external url.

private binary, indicates whether profile is private or not.

X.posts number of posts made by profile.

X.followers number of followers.

X.follows numbers of follows.

y whether profile is fake or not.

dataType vector taking the values "train" or "test" indicating whether the observation belongs to the training or the test data.

Source

https://www.kaggle.com/free4ever1/instagram-fake-spammer-genuine-accounts

data_titanic 9

Examples

```
data(data_instagram)
str(data_instagram)

# The data are used in:
## Not run:
vignette("Random_forest_examples")
## End(Not run)
```

data_titanic

Titanic data

Description

This dataset contains information on 1309 passengers of the RMS Titanic. The goal is to predict survival based on 11 characteristics such as the travel class, age and sex of the passengers.

The original data source is https://www.kaggle.com/c/titanic/data

The data is split up in a training data consisting of 891 observations and a test data of 418 observations. The response in the test set was obtained by combining information from other data files, and has been verified by submitting it as a 'prediction' to kaggle and getting perfect marks.

Usage

```
data("data_titanic")
```

Format

A data frame with 1309 observations on the following variables.

PassengerId a unique identified for each passenger.

Pclass travel class of the passenger.

Name name of the passenger.

Sex sex of the passenger.

Age age of the passenger.

SibSp number of siblings and spouses traveling with the passenger.

Parch number of parents and children traveling with the passenger.

Ticket Ticket number of the passenger.

Fare fare paid for the ticket.

Cabin cabin number of the passenger.

Embarked Port of embarkation. Takes the values C (Cherbourg), Q (Queenstown) and S (Southampton).

y factor indicating casualty or survivor.

dataType vector taking the values "train" or "test" indicating whether the observation belongs to the training or the test data.

10 makeFV

Source

https://www.kaggle.com/c/titanic/data

Examples

```
data("data_titanic")
traindata <- data_titanic[which(data_titanic$dataType == "train"), -13]
testdata <- data_titanic[which(data_titanic$dataType == "test"), -13]
str(traindata)
table(traindata$y)

# The data are used in:
## Not run:
vignette("Rpart_examples")

## End(Not run)</pre>
```

makeFV

Constructs feature vectors from a kernel matrix.

Description

Constructs feature vectors from a kernel matrix.

Usage

```
makeFV(kmat, transfmat = NULL, precS = 1e-12)
```

Arguments

kmat a kernel matrix. If transfmat is NULL, we are dealing with training data and

then kmat must be a square kernel matrix (of size n by n when there are n cases). Such a PSD matrix kmat can e.g. be produced by makeKernel or by kernlab::kernelMatrix. If on the other hand transfmat is not NULL, we are

dealing with a test set. See details for the precise working.

transfmat transformation matrix. If not NULL, it is the value transfmat of makeFV on

training data. It has to be a square matrix, with as many rows as there were

training data.

precS if not NULL, eigenvalues of kmat below precS will be set equal to precS.

Details

If transfmat is non-NULL, we are dealing with a test set. Denote the number of cases in the test set by $m \geq 1$. Each row of kmat of the test set then must contain the kernel values of a new case with all cases in the training set. Therefore the kernel matrix kmat must have dimensions m by n. The matrix kmat can e.g. be produced by makeKernel. It can also be obtained by running kernlab::kernelMatrix on the union of the training set and the test set, yielding an (n+m) by (n+m) matrix, from which one then takes the [(n+1):m,1:n] submatrix.

makeFV 11

Value

A list with components:

Xf

When makeKV is applied to the training set, Xf has coordinates of n points (vectors), the plain inner products of which equal the kernel matrix of the training set. That is, kmat = Xf Xf'. The Xf are expressed in an orthogonal basis in which the variance of the coordinates is decreasing, which is useful when plotting the first few coordinates. When makeFV is applied to a test set, Xf are coordinates of the feature vectors of the test set in the same space as those of the training set, and then kmat = Xf %*% Xf of training data.

transfmat

square matrix for transforming kmat to Xf.

Author(s)

Raymaekers J., Rousseeuw P.J., Hubert, M.

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, 64(2), 151–165. doi:10.1080/00401706.2021.1927849

See Also

makeKernel

```
library(e1071)
set.seed(1); X \leftarrow matrix(rnorm(200 * 2), ncol = 2)
X[1:100, ] \leftarrow X[1:100, ] + 2
X[101:150, ] \leftarrow X[101:150, ] - 2
y <- as.factor(c(rep("blue", 150), rep("red", 50)))</pre>
cols <- c("deepskyblue3", "red")</pre>
plot(X, col = cols[as.numeric(y)], pch = 19)
# We now fit an SVM with radial basis kernel to the data:
svmfit \leftarrow svm(y^{-}, data = data.frame(X = X, y = y), scale = FALSE,
             kernel = "radial", cost = 10, gamma = 1, probability = TRUE)
Kxx <- makeKernel(X, svfit = svmfit)</pre>
outFV <- makeFV(Kxx)
Xf <- outFV$Xf # The data matrix in this feature space.
dim(Xf) # The feature vectors are high dimensional.
# The inner products of Xf match the kernel matrix:
\max(abs(as.vector(Kxx - crossprod(t(Xf), t(Xf))))) # 3.005374e-13 # tiny, OK
range(rowSums(Xf^2)) # all points in Xf lie on the unit sphere.
pairs(Xf[, 1:5], col = cols[as.numeric(y)])
# In some of these we see spherical effects, e.g.
plot(Xf[, 1], Xf[, 5], col = cols[as.numeric(y)], pch = 19)
# The data look more separable here than in the original
# two-dimensional space.
```

12 makeKernel

```
# For more examples, we refer to the vignette:
## Not run:
vignette("Support_vector_machine_examples")
## End(Not run)
```

makeKernel

Compute kernel matrix

Description

Computes kernel value or kernel matrix, where the kernel type is extracted from an svm trained by e1071::svm.

Usage

```
makeKernel(X1, X2 = NULL, svfit)
```

Arguments

X1 first matrix (or vector) of coordinates.

X2 if not NULL, second data matrix or vector. If NULL, X2 is assumed equal to X1.

svfit output from e1071::svm

Value

the kernel matrix, of dimensions nrow(X1) by nrow(X2). When both X1 and X2 are vectors, the result is a single number.

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, 64(2), 151–165. doi:10.1080/00401706.2021.1927849

See Also

makeFV

predscor 13

Examples

```
library(e1071)
set.seed(1); X \leftarrow matrix(rnorm(200 * 2), ncol = 2)
X[1:100, ] \leftarrow X[1:100, ] + 2
X[101:150, ] \leftarrow X[101:150, ] - 2
y <- as.factor(c(rep("blue", 150), rep("red", 50))) # two classes
# We now fit an SVM with radial basis kernel to the data:
set.seed(1) # to make the result of svm() reproducible.
svmfit < -svm(y^{-}, data = data.frame(X = X, y = y), scale = FALSE,
             kernel = "radial", cost = 10, gamma = 1, probability = TRUE)
Kxx <- makeKernel(X, svfit = svmfit)</pre>
# The result is a square kernel matrix:
dim(Kxx) # 200 200
Kxx[1:5, 1:5]
# For more examples, we refer to the vignette:
## Not run:
vignette("Support_vector_machine_examples")
## End(Not run)
```

predscor

Draws a predictions correlation plot, which visualizes the correlations between the prediction terms in a regression fit.

Description

Computes the correlations between the prediction terms in a regression fit, and displays them graphically in a way that takes the standard deviations of the prediction terms into account. The input variables of the regression can be numerical, categorical, logical and character, and the regression model can be linear or generalized linear. The regression formula in 1m or g1m may contain transformations and interactions.

Usage

```
predscor(fit, maxnpreds = 8, sort.by.stdev = TRUE, adj.order = FALSE,
cell.length = "stdev", plot.abs.cor = FALSE, palette = NULL,
diagonalcolor = "black")
```

Arguments

fit an output object of lm or glm.

maxnpreds the maximal number of prediction terms to plot. When there are more prediction

terms than this, those with smallest standard deviations are combined.

sort.by.stdev if TRUE, sorts the prediction terms by decreasing standard deviation.

adj.order if TRUE, this modifies the order of the prediction terms in an attempt to bring

highly correlated prediction terms close to each other in the predscor display.

If sort.by.stdev is TRUE, this happens after that sorting.

14 predscor

cell.length if "stdev", the sides of the square cells on the diagonal of the correlation matrix

are proportional to the standard deviation of their prediction term. If "sqrt" they are proportional to the square root of the standard deviation. If "equal" all

sides are the same.

plot.abs.cor if FALSE, the default, positive and negative correlations are shown in different

colors, typically red and blue. If TRUE the absolute values of the correlations are

shown.

palette a vector with colors to display correlations ranging from -1 to 1. If NULL, the

default palette shows positive correlations in red, negative correlations in blue,

and uses white for correlation zero.

diagonal color of the cells on the diagonal of the correlation matrix. The default is

"black".

Value

A list containing

cormat the correlation matrix of the prediction terms.

predterms matrix of cases by prediction terms.

predsummary data frame with the standard deviation of each prediction term and the total

linear prediction.

Author(s)

Rousseeuw, P.J.

References

Rousseeuw, P.J. (2025). Explainable Linear and Generalized Linear Models by the Predictions Plot https://arxiv.org/abs/2412.16980v2 (open access).

See Also

predsplot

```
data(data_titanic)
attach(data_titanic)
Pclass = factor(Pclass, unique(Pclass))
Sex = factor(Sex, labels = c("F","M"))
fit <- glm(y ~ Sex + Age + SibSp + Parch + Pclass, family=binomial)
predscor(fit)

# For more examples, we refer to the vignette:
## Not run:
vignette("predsplot_examples")

## End(Not run)</pre>
```

predsplot 15

predsplot Make a predictions plot

Description

Plots the prediction terms of a regression, together with the total prediction. The input variables of the regression can be numerical, categorical, logical and character, and are visualized by histograms, densities, or bar plots. The regression model can be linear or generalized linear. The regression formula in lm() or glm() may contain transformations and interactions. The plot shows all cases in the data, but can also be made for a single case, either in-sample or out-of-sample, to explain its prediction.

Usage

```
predsplot(fit, maxnpreds = 8, sort.by.stdev = TRUE, displaytype = "histogram",
totalpred.type = "response", trunc.totalpred = TRUE, casetoshow = NULL,
staircase = FALSE, verbose = TRUE, maxchar.level = 5, nfact = 8, main = NULL,
cex.main = 1, xlab = NULL, ylab = NULL, vlinewidth = 0.25, hlinewidth = 0.25,
drawborder = TRUE, borderwidth = 1.0, densitycolors = NULL, predupcolor = "red",
preddowncolor = "blue", predpointsize = 3, draw.segments = TRUE,
predsegmentwidth = 0.8, profile = FALSE, bw = "nrd0", adjust = 1)
```

Arguments

fit	an output object of lm or glm.	
maxnpreds	the maximal number of prediction terms to plot. When there are more prediction terms than this, those with smallest standard deviations are combined.	
sort.by.stdev	if TRUE, sorts the prediction terms by decreasing standard deviation.	
displaytype	when "histogram", the distributions of the numerical prediction terms and the total prediction are displayed as histograms. When "density", the default density estimate of R is plotted instead.	
totalpred.type	when fit is a glm object, option "response" plots labels of the total prediction that are obtained by the inverse link function. Option "linear" plots labels of the total linear prediction. When fit is an lm object, argument totalpred.type is ignored.	
trunc.totalpred		
	if TRUE, the default, the range of the total prediction is truncated so ymin and ymax are determined by the individual prediction terms. FALSE may make the prediction terms look small in the plot.	
casetoshow	if not NULL, the particular case to be displayed. This can be a case number or row name of a case in the dataset, or a list or vector with input values of a new case.	
staircase	if TRUE and case to show is not NULL, the prediction for the case is shown in staircase style. $ \\$	
verbose	if TRUE, some intermediate results are shown on the console.	

16 predsplot

maxchar.level only the first maxchar.level characters of the categorical levels are displayed.

nfact if a numeric input variable has at most nfact unique values, it will be displayed

as if it were a factor. This may be useful since R considers a binary variable to

be numeric.

main title of the plot.

cex.main its size.

xlab horizontal legend. Its size can be changed by setting the height and width of the

plot.

ylab vertical legend. Its size can be changed by setting the height and width of the

plot.

vlinewidth width of the vertical lines.
hlinewidth width of the horizontal line.

drawborder if TRUE, draws a box outside the entire plot.

borderwidth width of the border. Defaults to 1.

density colors a vector with 4 colors. The first is for numeric input variables pointing up, the

second for numeric input variables pointing down, the third for prediction terms without orientation and the total prediction, and the fourth for factors. If NULL,

the default colors are used.

predupcolor the color of a positive prediction for casetoshow.

preddowncolor the color of a negative prediction for casetoshow.

predpointsize the size of the points displaying the predictions for casetoshow.

draw. segments if TRUE, also plots a line segment from the center of each prediction term to the

prediction term for casetoshow, in the same color as the prediction.

predsegmentwidth

the width of that line segment.

profile when casetoshow is not NULL and staircase is FALSE, this plots the profile of the

case with a feint grey line.

bw the bandwidth of the density estimation, only used when displaytype = "density".

This is the argument 'bw' of the function density.

adjust multiplier of the bandwidth of the density estimation, only used when displaytype

= "density". This is the argument 'adjust' of the function density.

Value

A list with items

p the predictions plot, which is a ggplot2 object.

totpred vector with the total linear prediction of all cases for which it can be computed.

centercept the centercept, which is the total linear prediction when all prediction terms have

their average value.

predterms matrix of cases by prediction terms.

predsummary data frame with the standard deviation of each prediction term and the total

linear prediction.

qresplot 17

casetotpred a number, the total linear prediction for casetoshow if one is given. casepredterms a vector with the values of the prediction terms for casetoshow.

data frame which shows all prediction terms for casetoshow together with the centercept, total linear prediction, and for a glm fit also the total prediction in

response units.

Author(s)

Rousseeuw, P.J.

casesummary

References

Rousseeuw, P.J. (2025). Explainable Linear and Generalized Linear Models by the Predictions Plot https://arxiv.org/abs/2412.16980v2 (open access).

See Also

predscor

Examples

```
data(data_titanic)
attach(data_titanic)
survival = y
Pclass = factor(Pclass, unique(Pclass))
Sex = factor(Sex, labels = c("F","M"))
fit <- glm(survival ~ Sex + Age + SibSp + Parch + Pclass, family=binomial)
predsplot(fit, main = "Titanic data", displaytype = "density")

# For more examples, we refer to the vignette:
## Not run:
vignette("predsplot_examples")

## End(Not run)</pre>
```

qresplot

Draw a quasi residual plot of PAC versus a data feature

Description

Draw a quasi residual plot to visualize classification results. The vertical axis of the quasi residual plot shows each case's probability of alternative class (PAC). The horizontal axis shows the feature given as the second argument in the function call.

18 qresplot

Usage

```
qresplot(PAC, feat, xlab = NULL, xlim = NULL,
    main = NULL, identify = FALSE, gray = TRUE,
    opacity = 1, squareplot = FALSE, plotLoess = FALSE,
    plotErrorBars = FALSE, plotQuantiles = FALSE,
    grid = NULL, probs = c(0.5, 0.75),
    cols = NULL, fac = 1, cex = 1,
    cex.main = 1.2, cex.lab = 1,
    cex.axis = 1, pch = 19)
```

Arguments

PAC vector with the PAC values of a classification, typically the \$PAC in the return of

a call to a function vcr.*.*

feat the PAC will be plotted versus this data feature. Note that feat does not have to

be one of the explanatory variables of the model. It can be another variable, a combination of variables (like a sum or a principal component score), the row

number of the cases if they were recorded succesively, etc.

xlab label for the horizontal axis, i.e. the name of variable feat.

xlim limits for the horizontal axis. If NULL, the range of feat is used.

main title for the plot.

identify if TRUE, left-click on a point to get its number, then ESC to exit.

gray logical, if TRUE (the default) the plot region where PAC < 0.5 gets a light gray

background. Points in this region were classified into their given class, and the

points above this region were misclassified.

opacity determines opacity of plotted dots. Value between 0 and 1, where 0 is transpar-

ent and 1 is opaque.

squareplot if TRUE, the horizontal and vertical axis will get the same length.

plotLoess if TRUE, a standard loess curve is fitted and superimposed on the plot. May

not work well if feat is discrete with few values. At most one of the options

plotLoess, plotErrorbars, or plotQuantiles can be selected.

plotErrorBars if TRUE, the average PAC and its standard error are computed on the intervals

of a grid (see option grid). Then a red curve connecting the averages is plotted, as well as two blue curves corresponding to the average plus or minus one standard error. At most one of the options plotLoess, plotErrorbars,

or plotQuantiles can be selected.

plotQuantiles if TRUE, one or more quantiles of the PAC are computed on the intervals of

a grid (see option grid). The quantiles correspond the probabilities in option probs. Then the curves connecting the quantiles are plotted. At most one of the options plottlesses plotErrorbars or plotOuantiles can be selected.

options plotLoess, plotErrorbars, or plotQuantiles can be selected.

grid only used when plotErrorBars or plotQuantiles are selected. This is a vec-

tor with increasing feat values, forming the grid. If NULL, the grid consists of the minimum and the maximum of feat, with 9 equispaced points between them.

probs only used when plotQuantiles is selected. This is a vector with probabilities

determining the quantiles. If NULL, defaults to c(0.5, 0.75).

qresplot 19

cols	only used when plotquantiles is selected. A vector with the colors of the quantile curves. If NULL the cols are taken as 2, 3,
fac	only used when plotLoess, plotErrorBars or plotQuantiles are selected. A real number to multiply the resulting curves. A value fac > 1 can be useful to better visualize the curves when they would be too close to zero. By default (fac = 1) this is not done.
cex	passed on to plot.
cex.main	same, for title.
cex.lab	same, for labels on horizontal and vertical axes.
cex.axis	same, for axes.
pch	plot character for the points, defaults to 19.

Value

coordinates

a matrix with 2 columns containing the coordinates of the plotted points. This makes it easier to add text next to interesting points. If identify = TRUE, the attribute ids of coordinates contains the row numbers of the identified points in the matrix coordinates.

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J.(2021). Silhouettes and quasi residual plots for neural nets and tree-based classifiers. *Journal of Computational and Graphical Statistics*, 31(4), 1332–1343. doi:10.1080/10618600.2022.2050249

```
library(rpart)
data("data_titanic")
traindata <- data_titanic[which(data_titanic$dataType == "train"), -13]</pre>
set.seed(123) # rpart is not deterministic
rpart.out <- rpart(y ~ Pclass + Sex + SibSp +</pre>
                     Parch + Fare + Embarked,
                   data = traindata, method = 'class', model = TRUE)
mytype <- list(nominal = c("Name", "Sex", "Ticket", "Cabin", "Embarked"), ordratio = c("Pclass"))</pre>
x_train <- traindata[, -12]</pre>
y_train <- traindata[, 12]</pre>
vcrtrain <- vcr.rpart.train(x_train, y_train, rpart.out, mytype)</pre>
# Quasi residual plot versus age, for males only:
PAC <- vcrtrain$PAC[which(x_train$Sex == "male")]
feat <- x_train$Age[which(x_train$Sex == "male")]</pre>
qresplot(PAC, feat, xlab = "Age (years)", opacity = 0.5,
         main = "quasi residual plot for male passengers",
         plotLoess = TRUE)
text(x = 14, y = 0.60, "loess curve", col = "red", cex = 1)
```

20 silplot

silplot	Draw the silhouette plot of a classification	

Description

Draw the silhouette plot to visualize classification results, based on the output of one of the vcr.*.* functions in this package. The horizontal axis of the silhouette plot shows each case's s(i).

Usage

Arguments

vcrout output of vcr.*.train or vcr.*.newdata. Required.

classLabels the labels (levels) of the classes. If NULL, they are taken from vcrout.

classCols a list of colors for the classes. There should be at least as many as there are

levels. If NULL a default palette is used.

showLegend if TRUE, a legend is shown to the right of the plot.

showClassNumbers

if TRUE, the legend will show the class numbers instead of the class labels.

showCases if TRUE, the plot shows the numbers of the cases. They are only readable when

the number of cases is relatively small.

topdown if TRUE (the default), the silhouettes are plotted from top to bottom. Otherwise

they are plotted from left to right.

drawLineAtAverage

if TRUE, drwas a line at the average value of the s(i).

main title for the plot. If NULL, a default title is used.

summary if TRUE, puts a summary table on the screen with for each class its number, label,

number of class members, and the average of its s(i).

Value

A ggplot object containing the silhouette plot.

Author(s)

Raymaekers J., Rousseeuw P.J.

stackedplot 21

References

Raymaekers J., Rousseeuw P.J.(2021). Silhouettes and quasi residual plots for neural nets and tree-based classifiers. *Journal of Computational and Graphical Statistics*, 31(4), 1332–1343. doi:10.1080/10618600.2022.2050249

See Also

```
vcr.da.train, vcr.da.newdata,
vcr.knn.train, vcr.knn.newdata,
vcr.svm.train, vcr.svm.newdata,
vcr.rpart.train, vcr.rpart.newdata,
vcr.forest.train, vcr.forest.newdata,
vcr.neural.train, vcr.neural.newdata
```

Examples

```
vcrout <- vcr.da.train(iris[, 1:4], iris[, 5])
silplot(vcrout)
# For more examples, we refer to the vignettes:
## Not run:
vignette("Discriminant_analysis_examples")
vignette("K_nearest_neighbors_examples")
vignette("Support_vector_machine_examples")
vignette("Rpart_examples")
vignette("Forest_examples")
vignette("Neural_net_examples")
## End(Not run)</pre>
```

stackedplot

Make a vertically stacked mosaic plot of class predictions.

Description

Make a vertically stacked mosaic plot of class predictions from the output of vcr.*.train or vcr.*.newdata. Optionally, the outliers for each class can be shown as a gray rectangle at the top.

Usage

```
stackedplot(vcrout, cutoff = 0.99, classCols = NULL,
classLabels = NULL, separSize=1, minSize=1.5,
showOutliers = TRUE, showLegend = FALSE, main = NULL,
htitle = NULL, vtitle = NULL)
```

22 stackedplot

Arguments

vcrout output of vcr.*.train or vcr.*.newdata.

cutoff cases with overall farness vcrout\$ofarness > cutoff are flagged as outliers.

classCols user-specified colors for the classes. If NULL a default palette is used.

classLabels names of given labels. If NULL they are taken from vcrout.

separSize how much white between rectangles.

minSize rectangles describing less than minSize percent of the data, are shown as minSize

percent.

showOutliers if TRUE, shows a separate class in gray with the outliers, always at the top.

showLegend if TRUE, a legend is shown to the right of the plot. Default FALSE, since the

legend is not necessary as the colors are already visible in the bottom part of

each stack.

main title for the plot.

htitle title for horizontal axis (given labels). If NULL, a default title is shown.

vtitle title for vertical axis (predicted labels). If NULL, a default title is shown.

Value

A ggplot object.

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, 64(2), 151–165. doi:10.1080/00401706.2021.1927849

See Also

```
vcr.da.train, vcr.da.newdata,
vcr.knn.train, vcr.knn.newdata,
vcr.svm.train, vcr.svm.newdata,
vcr.rpart.train, vcr.rpart.newdata,
vcr.forest.train, vcr.forest.newdata,
vcr.neural.train, vcr.neural.newdata
```

```
data("data_floralbuds")
X <- data_floralbuds[, 1:6]; y <- data_floralbuds[, 7]
vcrout <- vcr.da.train(X, y)
cols <- c("saddlebrown", "orange", "olivedrab4", "royalblue3")
stackedplot(vcrout, classCols = cols, showLegend = TRUE)</pre>
```

vcr.da.newdata 23

```
# The legend is not really needed, since we can read the
# color of a class from the bottom of its vertical bar:
stackedplot(vcrout, classCols = cols, main = "Stacked plot of QDA on foral buds data")

# If we do not wish to show outliers:
stackedplot(vcrout, classCols = cols, showOutliers = FALSE)

# For more examples, we refer to the vignettes:
## Not run:
vignette("Discriminant_analysis_examples")
vignette("K_nearest_neighbors_examples")
vignette("Support_vector_machine_examples")
vignette("Rpart_examples")
vignette("Random_forest_examples")
vignette("Random_forest_examples")
vignette("Neural_net_examples")

## End(Not run)
```

vcr.da.newdata

Carry out discriminant analysis on new data, and prepare to visualize its results.

Description

Predicts class labels for new data by discriminant analysis, using the output of vcr.da.train on the training data. For new data cases whose label in yintnew is non-missing, additional output is produced for constructing graphical displays such as the classmap.

Usage

```
vcr.da.newdata(Xnew, ynew=NULL, vcr.da.train.out)
```

Arguments

Xnew data matrix of the new data, with the same number of columns as in the training

data. Missing values are not allowed.

ynew factor with class membership of each new case. Can be NA for some or all cases.

If NULL, is assumed to be NA everywhere.

vcr.da.train.out

output of vcr.da.train on the training data.

Value

A list with components:

yintnew number of the given class of each case. Can contain NA's.

ynew given class label of each case. Can contain NA's.

24 vcr.da.newdata

levels levels of the response, from vcr.da.train.out.

predint predicted class number of each case. Always exists.

pred predicted label of each case.

altint number of the alternative class. Among the classes different from the given

class, it is the one with the highest posterior probability. Is NA for cases whose

ynew is missing.

altlab label of the alternative class. Is NA for cases whose ynew is missing.

PAC probability of the alternative class. Is NA for cases whose ynew is missing.

fig distance of each case i to each class g. Always exists.

farness farness of each case i from its given class. Is NA for cases whose ynew is missing.

ofarness For each case i, its lowest fig[i,g] to any class g. Always exists.

classMS list with center and covariance matrix of each class, from vcr.da.train.out.

1Current log of mixture density of each case in its given class. Is NA for cases with missing

ynew.

1Pred log of mixture density of each case in its predicted class. Always exists.

lAlt log of mixture density of each case in its alternative class. Is NA for cases with

missing ynew.

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, 64(2), 151–165. doi:10.1080/00401706.2021.1927849

See Also

```
vcr.da.train, classmap, silplot, stackedplot
```

```
vcr.train <- vcr.da.train(iris[, 1:4], iris[, 5])
inds <- c(51:150) # a subset, containing only 2 classes
iris2 <- iris[inds, ] # fake "new" data
iris2[c(1:10, 51:60), 5] <- NA
vcr.test <- vcr.da.newdata(iris2[, 1:4], iris2[, 5], vcr.train)
vcr.test$PAC[1:25] # between 0 and 1. Is NA where the response is.
plot(vcr.test$PAC, vcr.train$PAC[inds]); abline(0, 1) # match
plot(vcr.test$farness, vcr.train$farness[inds]); abline(0, 1) # match
confmat.vcr(vcr.train) # for comparison
confmat.vcr(vcr.test)
stackedplot(vcr.train) # for comparison
stackedplot(vcr.train, "versicolor", classCols = 2:4) # for comparison
classmap(vcr.test, "versicolor", classCols = 2:4) # has fewer points</pre>
```

vcr.da.train 25

```
# For more examples, we refer to the vignette:
## Not run:
vignette("Discriminant_analysis_examples")
## End(Not run)
```

vcr.da.train

Carry out discriminant analysis on training data, and prepare to visualize its results.

Description

Custom DA function which prepares for graphical displays such as the classmap. The disciminant analysis itself is carried out by the maximum a posteriori rule, which maximizes the density of the mixture.

Usage

```
vcr.da.train(X, y, rule = "QDA", estmethod = "meancov")
```

Arguments

X a numerical matrix containing the predictors in its columns. Missing values are

not allowed.

y a factor with the given class labels.

rule either "QDA" for quadratic discriminant analysis or "LDA" for linear discriminant

analysis.

estmethod function for location and covariance estimation. Should return a list with the

center m and the covariance matrix S. The default is "meancov" (classical

mean and covariance matrix), and the option "DetMCD" (based on robustbase::covMcd)

is also provided.

Value

A list with components:

yint number of the given class of each case. Can contain NA's.

y given class label of each case. Can contain NA's.

levels levels of y

predint predicted class number of each case. For each case this is the class with the

highest posterior probability. Always exists.

pred predicted label of each case.

26 vcr.da.train

altint	number of the alternative class. Among the classes different from the given
	class, it is the one with the highest posterior probability. Is NA for cases whose y
	is missing.

altlab label of the alternative class. Is NA for cases whose y is missing.

PAC probability of the alternative class. Is NA for cases whose y is missing.

figparams parameters for computing fig, can be used for new data. fig distance of each case i from each class q. Always exists.

farness farness of each case from its given class. Is NA for cases whose y is missing.

ofarness for each case i, its lowest fig[i,g] to any class g. Always exists.

classMS list with center and covariance matrix of each class

1Current log of mixture density of each case in its given class. Is NA for cases with missing

у.

lPred log of mixture density of each case in its predicted class. Always exists.

lalt log of mixture density of each case in its alternative class. Is NA for cases with

missing y.

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, 64(2), 151–165. doi:10.1080/00401706.2021.1927849

See Also

```
vcr.da.newdata, classmap, silplot, stackedplot
```

```
data("data_floralbuds")
X <- data_floralbuds[, 1:6]; y <- data_floralbuds[, 7]
vcrout <- vcr.da.train(X, y, rule = "QDA")
# For linear discriminant analysis, put rule = "LDA".
confmat.vcr(vcrout) # There are a few outliers
cols <- c("saddlebrown", "orange", "olivedrab4", "royalblue3")
stackedplot(vcrout, classCols = cols)
classmap(vcrout, "bud", classCols = cols)
# For more examples, we refer to the vignette:
## Not run:
vignette("Discriminant_analysis_examples")
## End(Not run)</pre>
```

vcr.forest.newdata 27

vcr.f	orest.	newdata
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Prepare for visualization of a random forest classification on new data.

Description

Produces output for the purpose of constructing graphical displays such as the classmap on new data. Requires the output of vcr. forest.train as an argument.

Usage

Arguments

Xnew data matrix of the new data, with the same number of columns d as in the training

data. Missing values are not allowed.

ynew factor with class membership of each new case. Can be NA for some or all cases.

If NULL, is assumed to be NA everywhere.

vcr.forest.train.out

output of vcr. forest. train on the training data.

LOO leave one out. Only used when testing this function on a subset of the training

data. Default is LOO=FALSE.

Value

yintnew

A list with components:

ynew	given class label of each case. Can contain NA's.
levels	levels of the response, from vcr.forest.train.out.
predint	predicted class number of each case. Always exists.
pred	predicted label of each case.
altint	number of the alternative class. Among the classes different from the given class, it is the one with the highest posterior probability. Is NA for cases whose ynew is missing.
altlab	alternative label if yintnew was given, else NA.
PAC	probability of the alternative class. Is NA for cases whose ynew is missing.

number of the given class of each case. Can contain NA's.

fig distance of each case i from each class g. Always exists.

farness of each case from its given class. Is NA for cases whose ynew is missing.

ofarness for each case i, its lowest fig[i,g] to any class g. Always exists.

28 vcr.forest.train

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J.(2021). Silhouettes and quasi residual plots for neural nets and tree-based classifiers. *Journal of Computational and Graphical Statistics*, 31(4), 1332–1343. doi:10.1080/10618600.2022.2050249

See Also

```
vcr.forest.train, classmap, silplot, stackedplot
```

Examples

```
library(randomForest)
data("data_instagram")
traindata <- data_instagram[which(data_instagram$dataType == "train"), -13]</pre>
set.seed(71) # randomForest is not deterministic
rfout <- randomForest(y ~ ., data = traindata, keep.forest = TRUE)</pre>
mytype \leftarrow list(symm = c(1, 5, 7, 8)) # These 4 columns are
# (symmetric) binary variables. The variables that are not
# listed are interval-scaled by default.
x_train <- traindata[, -12]</pre>
y_train <- traindata[, 12]</pre>
vcrtrain <- vcr.forest.train(X = x_train, y = y_train,</pre>
                              trainfit = rfout, type = mytype)
testdata <- data_instagram[which(data_instagram$dataType == "test"), -13]</pre>
Xnew <- testdata[, -12]</pre>
ynew <- testdata[, 12]</pre>
vcrtest <- vcr.forest.newdata(Xnew, ynew, vcrtrain)</pre>
confmat.vcr(vcrtest)
stackedplot(vcrtest, classCol = c(4, 2))
silplot(vcrtest, classCols = c(4, 2))
classmap(vcrtest, "genuine", classCols = c(4, 2))
classmap(vcrtest, "fake", classCols = c(4, 2))
# For more examples, we refer to the vignette:
## Not run:
vignette("Random_forest_examples")
## End(Not run)
```

Prepare for visualization of a random forest classification on training data

vcr.forest.train 29

Description

Produces output for the purpose of constructing graphical displays such as the classmap and silplot. The user first needs to train a random forest on the data by randomForest::randomForest. This then serves as an argument to vcr.forest.train.

Usage

Arguments

X A rectangular matrix or data frame, where the columns (variables) may be of

mixed type.

y factor with the given class labels. It is crucial that X and y are exactly the same

as in the call to randomForest::randomForest. y is allowed to contain NA's.

trainfit the output of a randomForest::randomForest training run.

k the number of nearest neighbors used in the farness computation.

type list for specifying some (or all) of the types of the variables (columns) in X,

used for computing the dissimilarity matrix, as in cluster::daisy. The list may contain the following components: "ordratio" (ratio scaled variables to be treated as ordinal variables), "logratio" (ratio scaled variables that must be logarithmically transformed), "asymm" (asymmetric binary) and "symm" (symmetric binary variables). Each component's value is a vector, containing the names or the numbers of the corresponding columns of X. Variables not men-

tioned in the type list are interpreted as usual (see argument X).

stand whether or not to standardize numerical (interval scaled) variables by their range

as in the original cluster::daisy code for the farness computation. Defaults

to TRUE.

Value

A list with components:

X The data used to train the forest.

yint number of the given class of each case. Can contain NA's.

y given class label of each case. Can contain NA's.

levels levels of y

predint predicted class number of each case. For each case this is the class with the

highest posterior probability. Always exists.

pred predicted label of each case.

altint number of the alternative class. Among the classes different from the given

class, it is the one with the highest posterior probability. Is NA for cases whose y

is missing.

30 vcr.forest.train

altlab	label of the alternative class. Is NA for cases whose y is missing.
PAC	probability of the alternative class. Is NA for cases whose y is missing.
figparams	parameters for computing fig, can be used for new data.
fig	distance of each case i from each class g . Always exists.
farness	farness of each case from its given class. Is NA for cases whose y is missing.
ofarness	for each case i, its lowest fig[i,g] to any class g. Always exists.
trainfit	The trained random forest which was given as an input to this function.

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J.(2021). Silhouettes and quasi residual plots for neural nets and tree-based classifiers. *Journal of Computational and Graphical Statistics*, 31(4), 1332–1343. doi:10.1080/10618600.2022.2050249

See Also

```
vcr.forest.newdata, classmap, silplot, stackedplot
```

```
library(randomForest)
data("data_instagram")
traindata <- data_instagram[which(data_instagram$dataType == "train"), -13]</pre>
set.seed(71) # randomForest is not deterministic
rfout <- randomForest(y~., data = traindata, keep.forest = TRUE)</pre>
mytype <- list(symm = c(1, 5, 7, 8)) # These 4 columns are
# (symmetric) binary variables. The variables that are not
# listed are interval-scaled by default.
x_train <- traindata[, -12]</pre>
y_train <- traindata[, 12]</pre>
# Prepare for visualization:
vcrtrain <- vcr.forest.train(X = x_train, y = y_train,</pre>
                             trainfit = rfout, type = mytype)
confmat.vcr(vcrtrain)
stackedplot(vcrtrain, classCols = c(4, 2))
silplot(vcrtrain, classCols = c(4, 2))
classmap(vcrtrain, "genuine", classCols = c(4, 2))
classmap(vcrtrain, "fake", classCols = c(4, 2))
# For more examples, we refer to the vignette:
## Not run:
vignette("Random_forest_examples")
## End(Not run)
```

vcr.knn.newdata 31

vcr.knn.newdata	Carry out a k-nearest neighbor classification on new data, and prepare to visualize its results.
	to visualize its results.

Description

Predicts class labels for new data by k nearest neighbors, using the output of vcr.knn.train on the training data. For cases in the new data whose given label ynew is not NA, additional output is produced for constructing graphical displays such as the classmap.

Usage

```
vcr.knn.newdata(Xnew, ynew = NULL, vcr.knn.train.out, LOO = FALSE)
```

Arguments

0	6 ** - ***			
	Xnew	If the training data was a matrix of coordinates, Xnew must be such a matrix with the same number of columns. If the training data was a set of dissimilarities, Xnew must be a rectangular matrix of dissimilarities, with each row containing the dissmilarities of a new case to all training cases. Missing values are not allowed.		
	ynew	factor with class membership of each new case. Can be NA for some or all cases. If $NULL$, is assumed to be NA everywhere.		
vcr.knn.train.out				
		output of vcr.knn.train on the training data.		
-	L00	leave one out. Only used when testing this function on a subset of the training data. Default is L00=FALSE.		

Value

A list with components:

yintnew	number of the given class of each case. Can contain NA's.
ynew	given class label of each case. Can contain NA's.
levels	levels of the response, from vcr.knn.train.out.
predint	predicted class number of each case. Always exists.
pred	predicted label of each case.
altint	number of the alternative class. Among the classes different from the given class, it is the one with the highest posterior probability. Is NA for cases whose ynew is missing.
altlab	label of the alternative class. Is NA for cases whose ynew is missing.
PAC	probability of the alternative class. Is NA for cases whose ynew is missing.
fig	distance of each case i from each class g . Always exists.

32 vcr.knn.newdata

farness of each case from its given class. Is NA for cases whose ynew is missing.

for each case i, its lowest fig[i,g] to any class g. Always exists.

k the requested number of nearest neighbors, from vcr.knn.train.out.

ktrues for each case this contains the actual number of elements in its neighborhood. This can be higher than k due to ties.

counts a matrix with 3 columns, each row representing a case. For the neighborhood of each case it says how many members it has from the given class, the predicted class, and the alternative class. The first and third entry is NA for cases whose ynew is missing.

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, 64(2), 151–165. doi:10.1080/00401706.2021.1927849

See Also

```
vcr.knn.train, classmap, silplot, stackedplot
```

```
data("data_floralbuds")
X <- data_floralbuds[, 1:6]; y <- data_floralbuds[, 7]</pre>
set.seed(12345); trainset <- sample(1:550, 275)
vcr.train <- vcr.knn.train(X[trainset, ], y[trainset], k = 5)</pre>
vcr.test <- vcr.knn.newdata(X[-trainset, ], y[-trainset], vcr.train)</pre>
confmat.vcr(vcr.train) # for comparison
confmat.vcr(vcr.test)
cols <- c("saddlebrown", "orange", "olivedrab4", "royalblue3")</pre>
stackedplot(vcr.train, classCols = cols) # for comparison
stackedplot(vcr.test, classCols = cols)
classmap(vcr.train, "bud", classCols = cols) # for comparison
classmap(vcr.test, "bud", classCols = cols)
# For more examples, we refer to the vignette:
## Not run:
vignette("K_nearest_neighbors_examples")
## End(Not run)
```

vcr.knn.train 33

I I	vcr.knn.train	Carry out a k-nearest neighbor classification on training data, and prepare to visualize its results.
-------	---------------	-------------------------------------------------------------------------------------------------------

Description

Carries out a k-nearest neighbor classification on the training data. Various additional output is produced for the purpose of constructing graphical displays such as the classmap.

Usage

```
vcr.knn.train(X, y, k)
```

Arguments

X	This can be a rectangular matrix or data frame of (already standardized) measurements, or a dist object obtained from stats::dist or cluster::daisy. Missing values are not allowed.
У	factor with the given (observed) class labels. There need to be non-missing y in order to be able to train the classifier.
k	the number of nearest neighbors used. It can be selected by running cross-validation using a different package.

Value

A list with components:

yint	number of the given class of each case. Can contain NA's.
у	given class label of each case. Can contain NA's.
levels	levels of y
predint	predicted class number of each case. Always exists.
pred	predicted label of each case.
altint	number of the alternative class. Among the classes different from the given class, it is the one with the highest posterior probability. Is NA for cases whose y is missing.
altlab	label of the alternative class. Is NA for cases whose y is missing.
PAC	probability of the alternative class. Is NA for cases whose y is missing.
figparams	parameters used to compute fig.
fig	distance of each case i from each class g . Always exists.
farness	farness of each case from its given class. Is NA for cases whose y is missing.
ofarness	for each case i , its lowest fig[i,g] to any class g . Always exists.

34 vcr.neural.newdata

k	the requested number of nearest neighbors, from the arguments. Will also be used for classifying new data.
ktrues	for each case this contains the actual number of elements in its neighborhood. This can be higher than k due to ties.
counts	a matrix with 3 columns, each row representing a case. For the neighborhood of each case it says how many members it has from the given class, the predicted class, and the alternative class. The first and third entry is NA for cases whose y is missing.
X	If the argument X was a data frame or matrix of coordinates, as.matrix(X) is returned here. This is useful for classifying new data.

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, 64(2), 151–165. doi:10.1080/00401706.2021.1927849

See Also

```
vcr.knn.newdata, classmap, silplot, stackedplot
```

Examples

```
vcrout <- vcr.knn.train(iris[, 1:4], iris[, 5], k = 5)
confmat.vcr(vcrout)
stackedplot(vcrout)
classmap(vcrout, "versicolor", classCols = 2:4)
# The cases misclassified as virginica are shown in blue.
# For more examples, we refer to the vignette:
## Not run:
vignette("K_nearest_neighbors_examples")
## End(Not run)</pre>
```

vcr.neural.newdata

Prepare for visualization of a neural network classification on new data.

Description

Prepares graphical display of new data fitted by a neural net that was modeled on the training data, using the output of vcr.neural.train on the training data.

vcr.neural.newdata 35

Usage

Arguments

Xnew data matrix of the new data, with the same number of columns as in the training

data. Missing values in Xnew are not allowed.

ynew factor with class membership of each new case. Can be NA for some or all cases.

If NULL, is assumed to be NA everywhere.

probs posterior probabilities obtained by running the neural net on the new data.

vcr.neural.train.out

output of vcr.neural.train on the training data.

Value

A list with components:

number of the given class of each case. Can contain NA's. yintnew given class label of each case. Can contain NA's. vnew levels of the response, from vcr.svm.train.out. levels predint predicted class number of each case. Always exists. pred predicted label of each case. altint number of the alternative class. Among the classes different from the given class, it is the one with the highest posterior probability. Is NA for cases whose ynew is missing. altlab alternative label if yintnew was given, else NA. PAC probability of the alternative class. Is NA for cases whose ynew is missing. fig distance of each case i from each class g. Always exists. farness of each case from its given class. Is NA for cases whose ynew is missing. farness

Author(s)

ofarness

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J.(2021). Silhouettes and quasi residual plots for neural nets and tree-based classifiers. *Journal of Computational and Graphical Statistics*, 31(4), 1332–1343. doi:10.1080/10618600.2022.2050249

for each case i, its lowest fig[i,g] to any class g. Always exists.

See Also

```
vcr.neural.train, classmap, silplot, stackedplot
```

36 vcr.neural.train

Examples

```
# For examples, we refer to the vignette:
## Not run:
vignette("Neural_net_examples")
## End(Not run)
```

vcr.neural.train

Prepare for visualization of a neural network classification on training data.

Description

Produces output for the purpose of constructing graphical displays such as the classmap. The user first needs train a neural network. The representation of the data in a given layer (e.g. the final layer before applying the softmax function) then serves as the argument X to vcr.neural.train.

Usage

```
vcr.neural.train(X, y, probs, estmethod = meancov)
```

Arguments

C	
X	the coordinates of the n objects of the training data, in the layer chosen by the user. Missing values are not allowed.
у	factor with the given class labels of the objects. Make sure that the levels are in the same order as used in the neural net, i.e. the columns of its binary "oncehot-encoded" response vectors.
probs	posterior probabilities obtained by the neural net, e.g. in keras. For each case (row of X), the classes have probabilities that add up to 1. Each row of the matrix probs contains these probabilities. The columns of probs must be in the same order as the levels of y.
estmethod	function for location and covariance estimation. Should return a list with \$m and \$S. Can be meancov (classical mean and covariance matrix) or DetMCD. If one or more classes have a singular covariance matrix, the function automatically

switches to the PCA-based farness used in vcr.svm.train.

Value

A list with components:

X	the coordinates of the n objects of the training data, in the layer chosen by the user.
yint	number of the given class of each case. Can contain NA's.
у	given class label of each case. Can contain NA's.

vcr.neural.train 37

levels of y predicted class number of each case. For each case this is the class with the predint highest posterior probability. Always exists.

pred predicted label of each case.

altint number of the alternative class. Among the classes different from the given

class, it is the one with the highest posterior probability. Is NA for cases whose y

is missing.

altlab label of the alternative class. Is NA for cases whose y is missing.

number of columns in X. Keep?? ncolX

PAC probability of the alternative class. Is NA for cases whose y is missing. Whether or not the farness is computed using the Mahalanobis distance. computeMD

classMS list with center and covariance matrix of each class

PCAfits if not NULL, PCA fits to each class, estimated from the training data but also

useful for new data.

figparams parameters for computing fig, can be used for new data. fig distance of each case i from each class g. Always exists.

farness farness of each case from its given class. Is NA for cases whose y is missing.

ofarness for each case i, its lowest fig[i,g] to any class g. Always exists.

Author(s)

levels

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J. (2021). Silhouettes and quasi residual plots for neural nets and treebased classifiers. Journal of Computational and Graphical Statistics, 31(4), 1332-1343. doi:10.1080/ 10618600.2022.2050249

See Also

```
vcr.neural.newdata, classmap, silplot, stackedplot
```

```
# For examples, we refer to the vignette:
## Not run:
vignette("Neural_net_examples")
## End(Not run)
```

38 vcr.rpart.newdata

vcr.rpart.newdata	Prepare for visualization of an rpart classification on new data.
ver par c.menaaca	Trepare for visualization of an ipart elassification on new data.

Description

Produces output for the purpose of constructing graphical displays such as the classmap on new data. Requires the output of vcr.rpart.train as an argument.

Usage

Arguments

Xnew data matrix of the new data, with the same number of columns d as in the training

data. Missing values are not allowed.

ynew factor with class membership of each new case. Can be NA for some or all cases.

If NULL, is assumed to be NA everywhere.

vcr.rpart.train.out

output of vcr.rpart.train on the training data.

LOO leave one out. Only used when testing this function on a subset of the training

data. Default is LOO=FALSE.

Value

A list with components:

ofarness

yintnew	number of the given class of each case. Can contain NA's.
ynew	given class label of each case. Can contain NA's.
levels	levels of the response, from vcr.rpart.train.out.
predint	predicted class number of each case. Always exists.
pred	predicted label of each case.
altint	number of the alternative class. Among the classes different from the given class, it is the one with the highest posterior probability. Is NA for cases whose ynew is missing.
altlab	alternative label if yintnew was given, else NA.
PAC	probability of the alternative class. Is NA for cases whose ynew is missing.
fig	distance of each case i from each class g . Always exists.
farness	farness of each case from its given class. Is NA for cases whose ynew is missing.

for each case i, its lowest fig[i,g] to any class g. Always exists.

vcr.rpart.train 39

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J.(2021). Silhouettes and quasi residual plots for neural nets and tree-based classifiers. *Journal of Computational and Graphical Statistics*, 31(4), 1332–1343. doi:10.1080/10618600.2022.2050249

See Also

```
vcr.rpart.train, classmap, silplot, stackedplot
```

```
library(rpart)
data("data_titanic")
traindata <- data_titanic[which(data_titanic$dataType == "train"), -13]</pre>
str(traindata); table(traindata$y)
set.seed(123) # rpart is not deterministic
rpart.out <- rpart(y ~ Pclass + Sex + SibSp +</pre>
                     Parch + Fare + Embarked,
                   data = traindata, method = 'class', model = TRUE)
y_train <- traindata[, 12]</pre>
x_train <- traindata[, -12]</pre>
mytype <- list(nominal = c("Name", "Sex", "Ticket", "Cabin", "Embarked"), ordratio = c("Pclass"))</pre>
# These are 5 nominal columns, and one ordinal.
# The variables not listed are by default interval-scaled.
vcrtrain <- vcr.rpart.train(x_train, y_train, rpart.out, mytype)</pre>
testdata <- data_titanic[which(data_titanic$dataType == "test"), -13]</pre>
dim(testdata)
x_test <- testdata[, -12]</pre>
y_test <- testdata[, 12]</pre>
vcrtest <- vcr.rpart.newdata(x_test, y_test, vcrtrain)</pre>
confmat.vcr(vcrtest)
silplot(vcrtest, classCols = c(2, 4))
classmap(vcrtest, "casualty", classCols = c(2, 4))
classmap(vcrtest, "survived", classCols = c(2, 4))
# For more examples, we refer to the vignette:
## Not run:
vignette("Rpart_examples")
## End(Not run)
```

40 vcr.rpart.train

Description

Produces output for the purpose of constructing graphical displays such as the classmap. The user first needs to train a classification tree on the data by rpart::rpart. This then serves as an argument to vcr.rpart.train.

Usage

Arguments

X A rectangular matrix or data frame, where the columns (variables) may be of

mixed type and may contain NA's.

y factor with the given class labels. It is crucial that X and y are exactly the same

as in the call to rpart::rpart. y is allowed to contain NA's.

k the number of nearest neighbors used in the farness computation.

trainfit the output of an rpart::rpart training cycle.

type list for specifying some (or all) of the types of the variables (columns) in X,

used for computing the dissimilarity matrix, as in cluster::daisy. The list may contain the following components: "ordratio" (ratio scaled variables to be treated as ordinal variables), "logratio" (ratio scaled variables that must be logarithmically transformed), "asymm" (asymmetric binary) and "symm" (symmetric binary variables). Each component's value is a vector, containing the names or the numbers of the corresponding columns of X. Variables not men-

tioned in the type list are interpreted as usual (see argument X).

stand whether or not to standardize numerical (interval scaled) variables by their range

as in the original cluster::daisy code for the farness computation. Defaults

to TRUE.

Value

A list with components:

X The input data X. Keep??

yint number of the given class of each case. Can contain NA's.

y given class label of each case. Can contain NA's.

levels levels of y

predint predicted class number of each case. For each case this is the class with the

highest posterior probability. Always exists.

pred predicted label of each case.

altint number of the alternative class. Among the classes different from the given

class, it is the one with the highest posterior probability. Is NA for cases whose y

is missing.

vcr.rpart.train 41

altlab	label of the alternative class. Is NA for cases whose y is missing.
PAC	probability of the alternative class. Is NA for cases whose y is missing.
figparams	parameters for computing fig, can be used for new data.
fig	distance of each case i from each class g . Always exists.
farness	farness of each case from its given class. Is NA for cases whose y is missing.
ofarness	for each case i, its lowest fig[i,g] to any class g. Always exists.
trainfit	the trainfit used to build the VCR object.

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J.(2021). Silhouettes and quasi residual plots for neural nets and tree-based classifiers. *Journal of Computational and Graphical Statistics*, 31(4), 1332–1343. doi:10.1080/10618600.2022.2050249

See Also

```
vcr.rpart.newdata, classmap, silplot, stackedplot
```

```
library(rpart)
data("data_titanic")
traindata <- data_titanic[which(data_titanic$dataType == "train"), -13]</pre>
str(traindata); table(traindata$y)
set.seed(123) # rpart is not deterministic
rpart.out <- rpart(y ~ Pclass + Sex + SibSp +</pre>
                    Parch + Fare + Embarked,
                   data = traindata, method = 'class', model = TRUE)
y_train <- traindata[, 12]</pre>
x_train <- traindata[, -12]</pre>
mytype <- list(nominal = c("Name", "Sex", "Ticket", "Cabin", "Embarked"), ordratio = c("Pclass"))</pre>
# These are 5 nominal columns, and one ordinal.
# The variables not listed are by default interval-scaled.
vcrtrain <- vcr.rpart.train(x_train, y_train, rpart.out, mytype)</pre>
confmat.vcr(vcrtrain)
silplot(vcrtrain, classCols = c(2, 4))
classmap(vcrtrain, "casualty", classCols = c(2, 4))
classmap(vcrtrain, "survived", classCols = c(2, 4))
# For more examples, we refer to the vignette:
## Not run:
vignette("Rpart_examples")
## End(Not run)
```

42 vcr.svm.newdata

new data.	vcr.svm.newdata	Prepare for visualization of a support vector machine classification on new data.
-----------	-----------------	-----------------------------------------------------------------------------------

Description

Carries out a support vector machine classification of new data using the output of vcr.svm.train on the training data, and computes the quantities needed for its visualization.

Usage

```
vcr.svm.newdata(Xnew, ynew = NULL, vcr.svm.train.out)
```

Arguments

Xnew data matrix of the new data, with the same number of columns as in the training

data. Missing values in Xnew are not allowed.

ynew factor with class membership of each new case. Can be NA for some or all cases.

If NULL, is assumed to be NA everywhere.

vcr.svm.train.out

output of vcr.svm.train on the training data.

Value

A list with components:

yintnew	number of the given class of each case. Can contain NA's.
ynew	given class label of each case. Can contain NA's.
levels	levels of the response, from vcr.svm.train.out.
predint	predicted class number of each case. Always exists.
pred	predicted label of each case.
altint	number of the alternative class. Among the classes different from the given class, it is the one with the highest posterior probability. Is NA for cases whose ynew is missing.
altlab	alternative label if yintnew was given, else NA.
PAC	probability of the alternative class. Is NA for cases whose ynew is missing.
fig	distance of each case i from each class g . Always exists.
farness	farness of each case from its given class. Is NA for cases whose ynew is missing.
ofarness	for each case i , its lowest fig[i,g] to any class g . Always exists.

Author(s)

Raymaekers J., Rousseeuw P.J.

vcr.svm.train 43

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, 64(2), 151–165. doi:10.1080/00401706.2021.1927849

See Also

```
vcr.svm.train, classmap, silplot, stackedplot, e1071::svm
```

Examples

```
library(e1071)
set.seed(1); X \leftarrow matrix(rnorm(200 * 2), ncol = 2)
X[1:100, ] \leftarrow X[1:100, ] + 2
X[101:150, ] \leftarrow X[101:150, ] - 2
y <- as.factor(c(rep("blue", 150), rep("red", 50)))</pre>
# We now fit an SVM with radial basis kernel to the data:
set.seed(1) # to make the result of svm() reproducible.
svmfit \leftarrow svm(y^{-}, data = data.frame(X = X, y = y),
scale = FALSE, kernel = "radial", cost = 10,
gamma = 1, probability = TRUE)
vcr.train <- vcr.svm.train(X, y, svfit = svmfit)</pre>
# As "new" data we take a subset of the training data:
inds <- c(1:25, 101:125, 151:175)
vcr.test <- vcr.svm.newdata(X[inds, ], y[inds], vcr.train)</pre>
plot(vcr.test$PAC, vcr.train$PAC[inds]); abline(0, 1) # match
plot(vcr.test$farness, vcr.train$farness[inds]); abline(0, 1)
confmat.vcr(vcr.test)
cols <- c("deepskyblue3", "red")</pre>
stackedplot(vcr.test, classCols = cols)
classmap(vcr.train, "blue", classCols = cols) # for comparison
classmap(vcr.test, "blue", classCols = cols)
classmap(vcr.train, "red", classCols = cols) # for comparison
classmap(vcr.test, "red", classCols = cols)
# For more examples, we refer to the vignette:
## Not run:
vignette("Support_vector_machine_examples")
## End(Not run)
```

vcr.svm.train

Prepare for visualization of a support vector machine classification on training data.

Description

Produces output for the purpose of constructing graphical displays such as the classmap. The user first needs to run a support vector machine classification on the data by e1071::svm, with

44 vcr.svm.train

the option probability = TRUE. This classification can be with two or more classes. The output of e1071::svm is then an argument to vcr.svm.train. As e1071::svm does not output the data itself, it needs to be given as well, in the arguments X and y.

Usage

```
vcr.svm.train(X, y, svfit, ortho = FALSE)
```

Arguments

X	matrix of data coordinates, as used in e1071::svm. Missing values are not allowed.
У	factor with the given (observed) class labels. It is crucial that X and y are exactly the same as in the call to e1071::svm.
svfit	an object returned by $e1071::svm$, called with exactly the same X and y as above.
ortho	If TRUE, will compute farness in the orthogonal complement of the vector beta given by e1071::svm. Is only possible for 2 classes, else there would be several beta vectors.

Value

A list with components:

yint	number of the given class of each case. Can contain NA's.
у	given class label of each case. Can contain NA's.
levels	levels of the response y.
predint	predicted class number of each case. Always exists.
pred	predicted label of each case.
altint	number of the alternative class. Among the classes different from the given class, it is the one with the highest posterior probability. Is NA for cases whose y is missing.
altlab	label of the alternative class. Is NA for cases whose y is missing.
PAC	probability of the alternative class. Is NA for cases whose y is missing.
figparams	parameters used in fig, can be used for new data.
fig	distance of each case i from each class g . Always exists.
farness	farness of each case from its given class. Is NA for cases whose y is missing.
ofarness	for each case i , its lowest fig[i,g] to any class g. Always exists.
svfit	as it was input, will be useful for new data.
X	the matrix of data coordinates from the arguments. This is useful for classifying new data.

Author(s)

Raymaekers J., Rousseeuw P.J.

vcr.svm.train 45

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, 64(2), 151–165. doi:10.1080/00401706.2021.1927849

See Also

```
vcr.knn.newdata, classmap, silplot, stackedplot, e1071::svm
```

```
library(e1071)
set.seed(1); X \leftarrow matrix(rnorm(200 * 2), ncol = 2)
X[1:100, ] \leftarrow X[1:100, ] + 2
X[101:150, ] \leftarrow X[101:150, ] - 2
y <- as.factor(c(rep("blue", 150), rep("red", 50)))</pre>
cols <- c("deepskyblue3", "red")</pre>
plot(X, col = cols[as.numeric(y)], pch = 19)
# We now fit an SVM with radial basis kernel to the data:
set.seed(1) # to make the result of svm() reproducible.
svmfit \leftarrow svm(y^{-}, data = data.frame(X = X, y = y),
scale = FALSE, kernel = "radial", cost = 10,
gamma = 1, probability = TRUE)
plot(svmfit\ensuremath{\$} decision.values, col = cols[as.numeric(y)]); abline(h = 0)
# so the decision values separate the classes reasonably well.
plot(svmfit, data = data.frame(X = X, y = y), X.2~X.1, col = cols)
# The boundary is far from linear (but in feature space it is).
vcr.train <- vcr.svm.train(X, y, svfit = svmfit)</pre>
confmat.vcr(vcr.train)
stackedplot(vcr.train, classCols = cols)
classmap(vcr.train, "blue", classCols = cols)
classmap(vcr.train, "red", classCols = cols)
# For more examples, we refer to the vignette:
vignette("Support_vector_machine_examples")
## End(Not run)
```

Index

```
classmap, 2, 23–41, 43, 45
cluster::daisy, 29, 33, 40
confmat.vcr, 4
data_bookReviews, 6
data_floralbuds, 7
data_instagram, 8
data_titanic, 9
density, 16
e1071::svm, 12, 43-45
glm, 13, 15
graphics::plot, 3
kernlab::kernelMatrix, 10
lm, 13, 15
makeFV, 10, 10, 11, 12
makeKernel, 10, 11, 12
plot, 19
predscor, 13, 13, 17
predsplot, 14, 15
qresplot, 17
randomForest::randomForest, 29
robustbase::covMcd, 25
rpart::rpart, 40
silplot, 20, 24, 26, 28-30, 32, 34, 35, 37, 39,
         41, 43, 45
stackedplot, 21, 24, 26, 28, 30, 32, 34, 35,
         37, 39, 41, 43, 45
stats::dist, 33
vcr.da.newdata, 4, 5, 21, 22, 23, 26
vcr.da.train, 4, 5, 21-24, 25
vcr.forest.newdata, 4, 5, 21, 22, 27, 30
vcr.forest.train, 4, 5, 21, 22, 27, 28, 28, 29
```

```
vcr.knn.newdata, 4, 5, 21, 22, 31, 34, 45 vcr.knn.train, 4, 5, 21, 22, 31, 32, 33 vcr.neural.newdata, 4, 5, 21, 22, 34, 37 vcr.neural.train, 4, 5, 21, 22, 34–36, 36 vcr.rpart.newdata, 4, 5, 21, 22, 38, 41 vcr.rpart.train, 4, 5, 21, 22, 38, 39, 39, 40 vcr.svm.newdata, 4, 5, 21, 22, 42 vcr.svm.train, 4, 5, 21, 22, 36, 42, 43, 43, 44
```