Package 'classmap'

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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 of cases.
The graphical displays include stacked plots, silhouette plots, quasi residual plots, and class maps.
Implements the techniques described and illustrated in Raymaekers, Rousseeuw and Hubert (2021), Class maps for visualizing classification results, Technometrics, appeared online.
<doi:10.1080/00401706.2021.1927849> (open access) and Raymaekers and Rousseeuw (2021),
Silhouettes and quasi residual plots for neural nets and tree-based classifiers,
<arXiv:2106.08814>. Examples can be found in the vignettes:
``Discriminant_analysis_examples",``K_nearest_neighbors_examples",
``Support_vector_machine_examples", ``Rpart_examples", ``Random_forest_examples",
and ``Neural_net_examples".

URL https://doi.org/10.1080/00401706.2021.1927849,
https://arxiv.org/abs/2106.08814

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R topics documented:

`classmap` *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.

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	output of vcr.*.train or vcr.*.newdata. Required.
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.
identify	if TRUE, left-click on a point to get its number, then ESC to exit.
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	determines opacity of plotted dots. Value between 0 and 1, where 0 is transparent 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.

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, appeared online. doi: 10.1080/00401706.2021.1927849(link to open access pdf)

Raymaekers J., Rousseeuw P.J.(2021). Silhouettes and quasi residual plots for neural nets and tree-based classifiers. (link to open access pdf)

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)
```

---

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(vcrout, cutoff = 0.99, showClassNumbers = FALSE,
            showOutliers = TRUE, silent = FALSE)
```

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*, appeared online. doi: 10.1080/00401706.2021.1927849(link to open access pdf)

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.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.

# 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.

Examples

```
data(data_bookReviews)
# Example review:
data_bookReviews[5, 1]

# The data are used in:
## Not run:
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>

Examples

```
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)
```

`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

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.

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)
```

---

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.

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_training'`.
`transfmat`	square matrix for transforming kmat to `Xf`. The actual transformation needs to be carried out by `makeFV` because it is not a simple matrix product.

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, appeared online. doi: 10.1080/00401706.2021.1927849(link to open access pdf)

See Also

`makeKernel`

Examples

```
library(e1071)
set.seed(1); X <- matrix(rnorm(200 * 2), ncol = 2)
X[1:100, ] <- X[1:100, ] + 2
X[101:150, ] <- X[101:150, ] - 2
y <- as.factor(c(rep("blue", 150), rep("red", 50)))
cols <- c("deepskyblue3", "red")
plot(X, col = cols[as.numeric(y)], pch = 19)
# We now fit an SVM with radial basis kernel to the data:
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)
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))))) # 6.167711e-11 # 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.
```

```
# 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*, appeared online. doi: 10.1080/00401706.2021.1927849(link to open access pdf)

See Also

`makeFV`

Examples

```
library(e1071)
set.seed(1); X <- matrix(rnorm(200 * 2), ncol = 2)
X[1:100, ] <- X[1:100, ] + 2
X[101:150, ] <- 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)
# 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)
```

`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.

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 transparent 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 plotLoess, plotErrorbars, or plotQuantiles can be selected.
grid	only used when plotErrorBars or plotQuantiles are selected. This is a vector 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).
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. (link to open access pdf)

Examples

```
library(rpart)
data("data_titanic")
traindata <- data_titanic[which(data_titanic$dataType == "train"), -13]
set.seed(123) # rpart is not deterministic
rpart.out <- rpart(y ~ Pclass + Sex + SibSp +
                     Parch + Fare + Embarked,
                   data = traindata, method = 'class', model = TRUE)
mytype <- list(nominal = c("Name", "Sex", "Ticket", "Cabin", "Embarked"), ordratio = c("Pclass"))
x_train <- traindata[, -12]
y_train <- traindata[,  12]
vcrtrain <- vcr.rpart.train(x_train, y_train, rpart.out, mytype)
# Quasi residual plot versus age, for males only:
PAC <- vcrtrain$PAC[which(x_train$Sex == "male")]
feat <- x_train$Age[which(x_train$Sex == "male")]
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)
```

`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

```
silplot(vcrout, classLabels = NULL, classCols = NULL,
        showLegend = TRUE, showClassNumbers = FALSE,
        showCases = FALSE, drawLineAtAverage = FALSE,
        topdown = TRUE, main = NULL, summary = TRUE)
```

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.

References

Raymaekers J., Rousseeuw P.J.(2021). Silhouettes and quasi residual plots for neural nets and tree-based classifiers. (link to open access pdf)

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)
```

`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)
```

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*, appeared online. doi: 10.1080/00401706.2021.1927849(link to open access pdf)

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

```
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)

# 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("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.
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.
lCurrent	log of mixture density of each case in its given class. Is NA for cases with missing ynew.
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 ynew.

Author(s)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, appeared online. doi: 10.1080/00401706.2021.1927849(link to open access pdf)

See Also

vcr.da.train, classmap, silplot, stackedplot

Examples

```
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.test)
classmap(vcr.train, "versicolor", classCols = 2:4) # for comparison
classmap(vcr.test, "versicolor", classCols = 2:4) # has fewer points

# 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.
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 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.
classMS	list with center and covariance matrix of each class
lCurrent	log of mixture density of each case in its given class. Is NA for cases with missing y.
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*, appeared online. doi: 10.1080/00401706.2021.1927849(link to open access pdf)

See Also

vcr.da.newdata, classmap, silplot, stackedplot

Examples

```
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)
```

---

vcr.forest.newdata *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

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

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

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.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.
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.

References

Raymaekers J., Rousseeuw P.J.(2021). Silhouettes and quasi residual plots for neural nets and tree-based classifiers. (link to open access pdf)

See Also

vcr.forest.train, classmap, silplot, stackedplot

Examples

```
library(randomForest)
data("data_instagram")
traindata <- data_instagram[which(data_instagram$dataType == "train"), -13]
set.seed(71) # randomForest is not deterministic
rfout <- randomForest(y ~ ., data = traindata, keep.forest = TRUE)
mytype <- list(symm = c(1, 5, 7, 8)) # These 4 columns are
# (symmetric) binary variables. The variables that are not
# listed are interval-scaled by default.
x_train <- traindata[, -12]
y_train <- traindata[, 12]
vcrtrain <- vcr.forest.train(X = x_train, y = y_train,
                             trainfit = rfout, type = mytype)
testdata <- data_instagram[which(data_instagram$dataType == "test"), -13]
Xnew <- testdata[, -12]
```

```
ynew <- testdata[, 12]
vcrtest <- vcr.forest.newdata(Xnew, ynew, vcrtrain)
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)
```

`vcr.forest.train` *Prepare for visualization of a random forest classification on training data*

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

```
vcr.forest.train(X, y, trainfit, type = list(),
                 k = 5, stand = TRUE)
```

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 mentioned 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.
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. (link to open access pdf)

See Also

vcr.forest.newdata, classmap, silplot, stackedplot

Examples

```
library(randomForest)
data("data_instagram")
traindata <- data_instagram[which(data_instagram$dataType == "train"), -13]
set.seed(71) # randomForest is not deterministic
rfout <- randomForest(y~., data = traindata, keep.forest = TRUE)
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]
```

```
y_train <- traindata[, 12]
# Prepare for visualization:
vcrtrain <- vcr.forest.train(X = x_train, y = y_train,
                             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` *Carry out a k-nearest neighbor classification on new data, and prepare 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

`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.
`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:

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.
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.
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*, appeared online. doi: 10.1080/00401706.2021.1927849(link to open access pdf)

See Also

vcr.knn.train, classmap, silplot, stackedplot

Examples

```
data("data_floralbuds")
X <- data_floralbuds[, 1:6]; y <- data_floralbuds[, 7]
set.seed(12345); trainset <- sample(1:550, 275)
vcr.train <- vcr.knn.train(X[trainset, ], y[trainset], k = 5)
vcr.test <- vcr.knn.newdata(X[-trainset, ], y[-trainset], vcr.train)
```

```
confmat.vcr(vcr.train) # for comparison
confmat.vcr(vcr.test)
cols <- c("saddlebrown", "orange", "olivedrab4", "royalblue3")
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` *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.
`y`	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.
`y`	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.
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*, appeared online. doi: 10.1080/00401706.2021.1927849(link to open access pdf)

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)
```

`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.

Usage

```
vcr.neural.newdata(Xnew, ynew = NULL, probs,
                   vcr.neural.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.
`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:

`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.

References

Raymaekers J., Rousseeuw P.J.(2021). Silhouettes and quasi residual plots for neural nets and tree-based classifiers. (link to open access pdf)

See Also

vcr.neural.train, classmap, silplot, stackedplot

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

X	the coordinates of the n objects of the training data, in the layer chosen by the user. Missing values are not allowed.
y	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 "once-hot-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.
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.
altlab	label of the alternative class. Is NA for cases whose y is missing.
ncolX	number of columns in X. Keep??
PAC	probability of the alternative class. Is NA for cases whose y is missing.
computeMD	Whether or not the farness is computed using the Mahalanobis distance.
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)

Raymaekers J., Rousseeuw P.J.

References

Raymaekers J., Rousseeuw P.J.(2021). Silhouettes and quasi residual plots for neural nets and tree-based classifiers. (link to open access pdf)

See Also

vcr.neural.newdata, classmap, silplot, stackedplot

Examples

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

## End(Not run)
```

`vcr.rpart.newdata` *Prepare for visualization of an rpart 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.rpart.train` as an argument.

Usage

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

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:

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

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. (link to open access pdf)

See Also

vcr.rpart.train, classmap, silplot, stackedplot

Examples

```
library(rpart)
data("data_titanic")
traindata <- data_titanic[which(data_titanic$dataType == "train"), -13]
str(traindata); table(traindata$y)
set.seed(123) # rpart is not deterministic
rpart.out <- rpart(y ~ Pclass + Sex + SibSp +
                     Parch + Fare + Embarked,
                   data = traindata, method = 'class', model = TRUE)
y_train <- traindata[, 12]
x_train <- traindata[, -12]
mytype <- list(nominal = c("Name", "Sex", "Ticket", "Cabin", "Embarked"), ordratio = c("Pclass"))
# 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)
testdata <- data_titanic[which(data_titanic$dataType == "test"), -13]
dim(testdata)
x_test <- testdata[, -12]
y_test <- testdata[, 12]
vcrtest <- vcr.rpart.newdata(x_test, y_test, vcrtrain)
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)
```

---

vcr.rpart.train *Prepare for visualization of an rpart classification on training data.*

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

```
vcr.rpart.train(X, y, trainfit, type = list(),
                k = 5, stand = TRUE)
```

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 mentioned 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.

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. (link to open access pdf)

See Also

vcr.rpart.newdata, classmap, silplot, stackedplot

Examples

```
library(rpart)
data("data_titanic")
traindata <- data_titanic[which(data_titanic$dataType == "train"), -13]
str(traindata); table(traindata$y)
set.seed(123) # rpart is not deterministic
rpart.out <- rpart(y ~ Pclass + Sex + SibSp +
                     Parch + Fare + Embarked,
                   data = traindata, method = 'class', model = TRUE)
y_train <- traindata[, 12]
x_train <- traindata[, -12]
mytype <- list(nominal = c("Name", "Sex", "Ticket", "Cabin", "Embarked"), ordratio = c("Pclass"))
# 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)
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)
```

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.

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, appeared online. doi: 10.1080/00401706.2021.1927849(link to open access pdf)

See Also

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

Examples

```
library(e1071)
set.seed(1); X <- matrix(rnorm(200 * 2), ncol = 2)
X[1:100, ] <- X[1:100, ] + 2
X[101:150, ] <- X[101:150, ] - 2
y <- as.factor(c(rep("blue", 150), rep("red", 50)))
# 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)
vcr.train <- vcr.svm.train(X, y, svfit = svmfit)
# 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)
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")
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 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.
y	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.
y	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.

References

Raymaekers J., Rousseeuw P.J., Hubert M. (2021). Class maps for visualizing classification results. *Technometrics*, appeared online. doi: 10.1080/00401706.2021.1927849(link to open access pdf)

See Also

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

Examples

```
library(e1071)
set.seed(1); X <- matrix(rnorm(200 * 2), ncol = 2)
X[1:100, ] <- X[1:100, ] + 2
X[101:150, ] <- X[101:150, ] - 2
y <- as.factor(c(rep("blue", 150), rep("red", 50)))
cols <- c("deepskyblue3", "red")
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 <- svm(y~., data = data.frame(X = X, y = y),
scale = FALSE, kernel = "radial", cost = 10,
gamma = 1, probability = TRUE)
plot(svmfit$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)
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:
## Not run:
vignette("Support_vector_machine_examples")

## End(Not run)
```

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