Package 'caret'

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Title Classification and Regression Training

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Description Misc functions for training and plotting classification and regression models

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Depends R (>= 2.10), stats, lattice (>= 0.20), ggplot2

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Suggests e1071, earth (>= 2.2-3), fastICA, gam, ipred, kernlab, klaR, MASS, ellipse, mda, mgcv, mlbench, nnet, party (>= 0.9-99992), pls, pROC, proxy, randomForest, RANN, spls, subselect, pamr, superpc, Cubist, testthat (>= 0.9.1)

License GPL (>= 2)

NeedsCompilation yes

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R topics documented:

`as.table.confusionMatrix` *Save Confusion Table Results*

Description

Conversion functions for class `confusionMatrix`

Usage

```
## S3 method for class 'confusionMatrix'
as.matrix(x, what = "xtabs", ...)

## S3 method for class 'confusionMatrix'
as.table(x, ...)
```

Arguments

x	an object of class confusionMatrix
what	data to conver to matrix. Either "xtabs", "overall" or "classes"
...	not currently used

Details

For as.table, the cross-tabulations are saved. For as.matrix, the three object types are saved in matrix format.

Value

A matrix or table

Author(s)

Max Kuhn

See Also

confusionMatrix

Examples

```
###################
## 2 class example

lvs <- c("normal", "abnormal")
truth <- factor(rep(lvs, times = c(86, 258)),
                levels = rev(lvs))
pred <- factor(
               c(
                 rep(lvs, times = c(54, 32)),
                 rep(lvs, times = c(27, 231))),
               levels = rev(lvs))

xtab <- table(pred, truth)

results <- confusionMatrix(xtab)
as.table(results)
as.matrix(results)
as.matrix(results, what = "overall")
```

```
as.matrix(results, what = "classes")

###################
## 3 class example

xtab <- confusionMatrix(iris$Species, sample(iris$Species))
as.matrix(xtab)
```

---

avNNet.default *Neural Networks Using Model Averaging*

Description

Aggregate several neural network models

Usage

```
## Default S3 method:
avNNet(x, y, repeats = 5, bag = FALSE, allowParallel = TRUE, ...)
## S3 method for class 'formula'
avNNet(formula, data, weights, ...,
        repeats = 5, bag = FALSE, allowParallel = TRUE,
        subset, na.action, contrasts = NULL)

## S3 method for class 'avNNet'
predict(object, newdata, type = c("raw", "class", "prob"), ...)
```

Arguments

formula	A formula of the form `class ~ x1 + x2 + ...`
x	matrix or data frame of `x` values for examples.
y	matrix or data frame of target values for examples.
weights	(case) weights for each example – if missing defaults to 1.
repeats	the number of neural networks with different random number seeds
bag	a logical for bagging for each repeat
allowParallel	if a parallel backend is loaded and available, should the function use it?
data	Data frame from which variables specified in `formula` are preferentially to be taken.
subset	An index vector specifying the cases to be used in the training sample. (NOTE: If given, this argument must be named.)
na.action	A function to specify the action to be taken if `NA`s are found. The default action is for the procedure to fail. An alternative is `na.omit`, which leads to rejection of cases with missing values on any required variable. (NOTE: If given, this argument must be named.)

contrasts	a list of contrasts to be used for some or all of the factors appearing as variables in the model formula.
object	an object of class avNNet as returned by avNNet.
newdata	matrix or data frame of test examples. A vector is considered to be a row vector comprising a single case.
type	Type of output, either: raw for the raw outputs, code for the predicted class or prob for the class probabilities.
...	arguments passed to nnet

Details

Following Ripley (1996), the same neural network model is fit using different random number seeds. All the resulting models are used for prediction. For regression, the output from each network are averaged. For classification, the model scores are first averaged, then translated to predicted classes. Bagging can also be used to create the models.

If a parallel backend is registered, the **foreach** package is used to train the networks in parallel.

Value

For avNNet, an object of "avNNet" or "avNNet.formula". Items of interest in the output are:

model	a list of the models generated from nnet
repeats	an echo of the model input
names	if any predictors had only one distinct value, this is a character string of the remaining columns. Otherwise a value of NULL

Author(s)

These are heavily based on the nnet code from Brian Ripley.

References

Ripley, B. D. (1996) *Pattern Recognition and Neural Networks.* Cambridge.

See Also

nnet, preProcess

Examples

```
data(BloodBrain)
## Not run:
modelFit <- avNNet(bbbDescr, logBBB, size = 5, linout = TRUE, trace = FALSE)
modelFit

predict(modelFit, bbbDescr)

## End(Not run)
```

bag.default *A General Framework For Bagging*

Description

bag provides a framework for bagging classification or regression models. The user can provide their own functions for model building, prediction and aggregation of predictions (see Details below).

Usage

```
bag(x, ...)

## Default S3 method:
bag(x, y, B = 10, vars = ncol(x), bagControl = NULL, ...)

bagControl(fit = NULL,
           predict = NULL,
           aggregate = NULL,
           downSample = FALSE,
           oob = TRUE,
           allowParallel = TRUE)

ldaBag
plsBag
nbBag
ctreeBag
svmBag
nnetBag

## S3 method for class 'bag'
predict(object, newdata = NULL, ...)
```

Arguments

x	a matrix or data frame of predictors
y	a vector of outcomes
B	the number of bootstrap samples to train over.
bagControl	a list of options.
...	arguments to pass to the model function
fit	a function that has arguments x, y and ... and produces a model object that can later be used for prediction. Example functions are found in ldaBag, plsBag, nbBag, svmBag and nnetBag.

predict	a function that generates predictions for each sub-model. The function should have arguments object and x. The output of the function can be any type of object (see the example below where posterior probabilities are generated. Example functions are found in ldaBag, plsBag, nbBag, svmBag and nnetBag.)
aggregate	a function with arguments x and type. The function that takes the output of the predict function and reduces the bagged predictions to a single prediction per sample. the type argument can be used to switch between predicting classes or class probabilities for classification models. Example functions are found in ldaBag, plsBag, nbBag, svmBag and nnetBag.
downSample	a logical: for classification, should the data set be randomly sampled so that each class has the same number of samples as the smallest class?
oob	a logical: should out-of-bag statistics be computed and the predictions retained?
allowParallel	if a parallel backend is loaded and available, should the function use it?
vars	an integer. If this argument is not NULL, a random sample of size vars is taken of the predictors in each bagging iteration. If NULL, all predictors are used.
object	an object of class bag.
newdata	a matrix or data frame of samples for prediction. Note that this argument must have a non-null value

Details

The function is basically a framework where users can plug in any model in to assess the effect of bagging. Examples functions can be found in ldaBag, plsBag, nbBag, svmBag and nnetBag. Each has elements fit, pred and aggregate.

One note: when vars is not NULL, the sub-setting occurs prior to the fit and predict functions are called. In this way, the user probably does not need to account for the change in predictors in their functions.

When using bag with train, classification models should use type = "prob" inside of the predict function so that predict.train(object, newdata, type = "prob") will work.

If a parallel backend is registered, the **foreach** package is used to train the models in parallel.

Value

bag produces an object of class bag with elements

fits	a list with two sub-objects: the fit object has the actual model fit for that bagged samples and the vars object is either NULL or a vector of integers corresponding to which predictors were sampled for that model
control	a mirror of the arguments passed into bagControl
call	the call
B	the number of bagging iterations
dims	the dimensions of the training set

Author(s)

Max Kuhn

Examples

```
## A simple example of bagging conditional inference regression trees:
data(BloodBrain)

## treebag <- bag(bbbDescr, logBBB, B = 10,
##                bagControl = bagControl(fit = ctreeBag$fit,
##                                        predict = ctreeBag$pred,
##                                        aggregate = ctreeBag$aggregate))



## An example of pooling posterior probabilities to generate class predictions
data(mdrr)

## remove some zero variance predictors and linear dependencies
mdrrDescr <- mdrrDescr[, -nearZeroVar(mdrrDescr)]
mdrrDescr <- mdrrDescr[, -findCorrelation(cor(mdrrDescr), .95)]

## basicLDA <- train(mdrrDescr, mdrrClass, "lda")

## bagLDA2 <- train(mdrrDescr, mdrrClass,
##                  "bag",
##                  B = 10,
##                  bagControl = bagControl(fit = ldaBag$fit,
##                                          predict = ldaBag$pred,
##                                          aggregate = ldaBag$aggregate),
##                  tuneGrid = data.frame(vars = c((1:10)*10 , ncol(mdrrDescr))))
```

---

bagEarth *Bagged Earth*

Description

A bagging wrapper for multivariate adaptive regression splines (MARS) via the `earth` function

Usage

```
## S3 method for class 'formula'
bagEarth(formula, data = NULL, B = 50,
         summary = mean, keepX = TRUE,
         ..., subset, weights, na.action = na.omit)
## Default S3 method:
bagEarth(x, y, weights = NULL, B = 50,
         summary = mean, keepX = TRUE, ...)
```

Arguments

formula	A formula of the form y ~ x1 + x2 + ...
x	matrix or data frame of 'x' values for examples.
y	matrix or data frame of numeric values outcomes.
weights	(case) weights for each example - if missing defaults to 1.
data	Data frame from which variables specified in 'formula' are preferentially to be taken.
subset	An index vector specifying the cases to be used in the training sample. (NOTE: If given, this argument must be named.)
na.action	A function to specify the action to be taken if 'NA's are found. The default action is for the procedure to fail. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable. (NOTE: If given, this argument must be named.)
B	the number of bootstrap samples
summary	a function with a single argument specifying how the bagged predictions should be summarized
keepX	a logical: should the original training data be kept?
...	arguments passed to the earth function

Details

The function computes a Earth model for each bootstap sample.

Value

A list with elements

fit	a list of B Earth fits
B	the number of bootstrap samples
call	the function call
x	either NULL or the value of x, depending on the value of keepX
oob	a matrix of performance estimates for each bootstrap sample

Author(s)

Max Kuhn (bagEarth.formula is based on Ripley's nnet.formula)

References

J. Friedman, "Multivariate Adaptive Regression Splines" (with discussion) (1991). Annals of Statistics, 19/1, 1-141.

See Also

earth, predict.bagEarth

Examples

```
## Not run:
library(mda)
library(earth)
data(trees)
fit1 <- earth(trees[,-3], trees[,3])
fit2 <- bagEarth(trees[,-3], trees[,3], B = 10)

## End(Not run)
```

---

bagFDA *Bagged FDA*

Description

A bagging wrapper for flexible discriminant analysis (FDA) using multivariate adaptive regression splines (MARS) basis functions

Usage

```
bagFDA(x, ...)
## S3 method for class 'formula'
bagFDA(formula, data = NULL, B = 50, keepX = TRUE,
       ..., subset, weights, na.action = na.omit)
## Default S3 method:
bagFDA(x, y, weights = NULL, B = 50, keepX = TRUE, ...)
```

Arguments

formula	A formula of the form `y ~ x1 + x2 + ...`
x	matrix or data frame of 'x' values for examples.
y	matrix or data frame of numeric values outcomes.
weights	(case) weights for each example - if missing defaults to 1.
data	Data frame from which variables specified in 'formula' are preferentially to be taken.
subset	An index vector specifying the cases to be used in the training sample. (NOTE: If given, this argument must be named.)
na.action	A function to specify the action to be taken if 'NA's are found. The default action is for the procedure to fail. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable. (NOTE: If given, this argument must be named.)
B	the number of bootstrap samples
keepX	a logical: should the original training data be kept?
...	arguments passed to the `mars` function

Details

The function computes a FDA model for each bootstap sample.

Value

A list with elements

`fit`	a list of `B` FDA fits
`B`	the number of bootstrap samples
`call`	the function call
`x`	either `NULL` or the value of `x`, depending on the value of `keepX`
`oob`	a matrix of performance estimates for each bootstrap sample

Author(s)

Max Kuhn (`bagFDA.formula` is based on Ripley's `nnet.formula`)

References

J. Friedman, "Multivariate Adaptive Regression Splines" (with discussion) (1991). Annals of Statistics, 19/1, 1-141.

See Also

`fda`, `predict.bagFDA`

Examples

```
library(mlbench)
library(earth)
data(Glass)

set.seed(36)
inTrain <- sample(1:dim(Glass)[1], 150)

trainData <- Glass[ inTrain, ]
testData  <- Glass[-inTrain, ]


baggedFit <- bagFDA(Type ~ ., trainData)
confusionMatrix(predict(baggedFit, testData[, -10]),
                testData[, 10])
```

BloodBrain *Blood Brain Barrier Data*

Description

Mente and Lombardo (2005) develop models to predict the log of the ratio of the concentration of a compound in the brain and the concentration in blood. For each compound, they computed three sets of molecular descriptors: MOE 2D, rule-of-five and Charge Polar Surface Area (CPSA). In all, 134 descriptors were calculated. Included in this package are 208 non-proprietary literature compounds. The vector `logBBB` contains the concentration ratio and the data fame `bbbDescr` contains the descriptor values.

Usage

```
data(BloodBrain)
```

Value

`bbbDescr`	data frame of chemical descriptors
`logBBB`	vector of assay results

Source

Mente, S.R. and Lombardo, F. (2005). A recursive-partitioning model for blood-brain barrier permeation, *Journal of Computer-Aided Molecular Design*, Vol. 19, pg. 465–481.

BoxCoxTrans.default *Box-Cox and Exponential Transformations*

Description

These classes can be used to estimate transformations and apply them to existing and future data

Usage

```
BoxCoxTrans(y, ...)
expoTrans(y, ...)

## Default S3 method:
BoxCoxTrans(y, x = rep(1, length(y)),
            fudge = 0.2, numUnique = 3, na.rm = FALSE, ...)
## Default S3 method:
expoTrans(y, na.rm  = TRUE, init = 0,
     lim = c(-4, 4), method = "Brent",
     numUnique = 3, ...)
```

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

Arguments

y	a numeric vector of data to be transformed. For BoxCoxTrans, the data must be strictly positive.
x	an optional dependent variable to be used in a linear model.
fudge	a tolerance value: lambda values within +/-fudge will be coerced to 0 and within 1+/-fudge will be coerced to 1.
numUnique	how many unique values should y have to estimate the transformation?
na.rm	a logical value indicating whether NA values should be stripped from y and x before the computation proceeds.
init, lim, method	initial values, limits and optimization method for optim.
...	for BoxCoxTrans: options to pass to boxcox. plotit should not be passed through. For predict.BoxCoxTrans, additional arguments are ignored.
object	an object of class BoxCoxTrans or expoTrans.
newdata	a numeric vector of values to transform.

Details

BoxCoxTrans function is basically a wrapper for the boxcox function in the MASS library. It can be used to estimate the transformation and apply it to new data.

expoTrans estimates the exponential transformation of Manly (1976) but assumes a common mean for the data. The transformation parameter is estimated by directly maximizing the likelihood.

If any(y <= 0) or if length(unique(y)) < numUnique, lambda is not estimated and no transformation is applied.

Value

Both functions returns a list of class of either BoxCoxTrans or expoTrans with elements

lambda	estimated transformation value
fudge	value of fudge
n	number of data points used to estimate lambda
summary	the results of summary(y)
ratio	max(y)/min(y)
skewness	sample skewness statistic

BoxCoxTrans also returns:

fudge	value of fudge

The predict functions returns numeric vectors of transformed values

Author(s)

Max Kuhn

References

Box, G. E. P. and Cox, D. R. (1964) An analysis of transformations (with discussion). Journal of the Royal Statistical Society B, 26, 211-252.

Manly, B. L. (1976) Exponential data transformations. The Statistician, 25, 37 - 42.

See Also

boxcox, preProcess, optim

Examples

```
data(BloodBrain)

ratio <- exp(logBBB)
bc <- BoxCoxTrans(ratio)
bc

predict(bc, ratio[1:5])

ratio[5] <- NA
bc2 <- BoxCoxTrans(ratio, bbbDescr$tpsa, na.rm = TRUE)
bc2

manly <- expoTrans(ratio)
manly
```

---

calibration *Probability Calibration Plot*

Description

For classification models, this function creates a 'calibration plot' that describes how consistent model probabilities are with observed event rates.

Usage

```
calibration(x, ...)

## S3 method for class 'formula'
calibration(x, data = NULL,
            class = NULL,
```

```
            cuts = 11, subset = TRUE,
            lattice.options = NULL, ...)

## S3 method for class 'calibration'
xyplot(x, data, ...)

panel.calibration(...)
```

Arguments

x	a lattice formula (see xyplot for syntax) where the left-hand side of the formula is a factor class variable of the observed outcome and the right-hand side specifies one or model columns corresponding to a numeric ranking variable for a model (e.g. class probabilities). The classification variable should have two levels.
data	For calibration.formula, a data frame (or more precisely, anything that is a valid envir argument in eval, e.g., a list or an environment) containing values for any variables in the formula, as well as groups and subset if applicable. If not found in data, or if data is unspecified, the variables are looked for in the environment of the formula. This argument is not used for xyplot.calibration.
class	a character string for the class of interest
cuts	the number of splits of the data are used to create the plot. By default, it uses as many cuts as there are rows in data
subset	An expression that evaluates to a logical or integer indexing vector. It is evaluated in data. Only the resulting rows of data are used for the plot.
lattice.options	A list that could be supplied to lattice.options
...	options to pass through to xyplot or the panel function (not used in calibration.formula).

Details

calibration.formula is used to process the data and xyplot.calibration is used to create the plot.

To construct the calibration plot, the following steps are used for each model:

1. The data are split into cuts - 1 roughly equal groups by their class probabilities
2. the number of samples with true results equal to class are determined
3. the event rate is determined for each bin

xyplot.calibration produces a plot of the observed event rate by the mid-point of the bins.

This implementation uses the **lattice** function xyplot, so plot elements can be changed via panel functions, trellis.par.set or other means. calibration uses the panel function panel.calibration by default, but it can be changed by passing that argument into xyplot.calibration.

The following elements are set by default in the plot but can be changed by passing new values into xyplot.calibration: xlab = "Bin Midpoint", ylab = "Observed Event Percentage", type = "o", ylim = extendrange(c(0, 100)),xlim = extendrange(c(0, 100)) and panel = panel.calibration

Value

`calibration.formula` returns a list with elements:

`data`	the data used for plotting
`cuts`	the number of cuts
`class`	the event class
`probNames`	the names of the model probabilities

`xyplot.calibration` returns a **lattice** object

Author(s)

Max Kuhn, some **lattice** code and documentation by Deepayan Sarkar

See Also

`xyplot`, `trellis.par.set`

Examples

```
## Not run:
data(mdrr)
mdrrDescr <- mdrrDescr[, -nearZeroVar(mdrrDescr)]
mdrrDescr <- mdrrDescr[, -findCorrelation(cor(mdrrDescr), .5)]


inTrain <- createDataPartition(mdrrClass)
trainX <- mdrrDescr[inTrain[[1]], ]
trainY <- mdrrClass[inTrain[[1]]]
testX <- mdrrDescr[-inTrain[[1]], ]
testY <- mdrrClass[-inTrain[[1]]]

library(MASS)

ldaFit <- lda(trainX, trainY)
qdaFit <- qda(trainX, trainY)

testProbs <- data.frame(obs = testY,
                        lda = predict(ldaFit, testX)$posterior[,1],
                        qda = predict(qdaFit, testX)$posterior[,1])

calibration(obs ~ lda + qda, data = testProbs)

calPlotData <- calibration(obs ~ lda + qda, data = testProbs)
calPlotData

xyplot(calPlotData, auto.key = list(columns = 2))

## End(Not run)
```

caretFuncs *Backwards Feature Selection Helper Functions*

Description

Ancillary functions for backwards selection

Usage

```
pickSizeTolerance(x, metric, tol = 1.5, maximize)
pickSizeBest(x, metric, maximize)

pickVars(y, size)

caretFuncs
lmFuncs
rfFuncs
treebagFuncs
ldaFuncs
nbFuncs
gamFuncs
lrFuncs
```

Arguments

x	a matrix or data frame with the performance metric of interest
metric	a character string with the name of the performance metric that should be used to choose the appropriate number of variables
maximize	a logical; should the metric be maximized?
tol	a scalar to denote the acceptable difference in optimal performance (see Details below)
y	a list of data frames with variables Overall and var
size	an integer for the number of variables to retain

Details

This page describes the functions that are used in backwards selection (aka recursive feature elimination). The functions described here are passed to the algorithm via the functions argument of rfeControl.

See rfeControl for details on how these functions should be defined.

The 'pick' functions are used to find the appropriate subset size for different situations. pickBest will find the position associated with the numerically best value (see the maximize argument to help define this).

pickSizeTolerance picks the lowest position (i.e. the smallest subset size) that has no more of an X percent loss in performances. When maximizing, it calculates (O-X)/O*100, where X is the

set of performance values and O is max(X). This is the percent loss. When X is to be minimized, it uses (X-O)/O*100 (so that values greater than X have a positive "loss"). The function finds the smallest subset size that has a percent loss less than `tol`.

Both of the 'pick' functions assume that the data are sorted from smallest subset size to largest.

Author(s)

Max Kuhn

See Also

`rfeControl`, `rfe`

Examples

```
## For picking subset sizes:
## Minimize the RMSE
example <- data.frame(RMSE = c(1.2, 1.1, 1.05, 1.01, 1.01, 1.03, 1.00),
                      Variables = 1:7)
## Percent Loss in performance (positive)
example$PctLoss <- (example$RMSE - min(example$RMSE))/min(example$RMSE)*100

xyplot(RMSE ~ Variables, data= example)
xyplot(PctLoss ~ Variables, data= example)

absoluteBest <- pickSizeBest(example, metric = "RMSE", maximize = FALSE)
within5Pct <- pickSizeTolerance(example, metric = "RMSE", maximize = FALSE)

cat("numerically optimal:",
    example$RMSE[absoluteBest],
    "RMSE in position",
    absoluteBest, "\n")
cat("Accepting a 1.5 pct loss:",
    example$RMSE[within5Pct],
    "RMSE in position",
    within5Pct, "\n")

## Example where we would like to maximize
example2 <- data.frame(Rsquared = c(0.4, 0.6, 0.94, 0.95, 0.95, 0.95, 0.95),
                      Variables = 1:7)
## Percent Loss in performance (positive)
example2$PctLoss <- (max(example2$Rsquared) - example2$Rsquared)/max(example2$Rsquared)*100

xyplot(Rsquared ~ Variables, data= example2)
xyplot(PctLoss ~ Variables, data= example2)

absoluteBest2 <- pickSizeBest(example2, metric = "Rsquared", maximize = TRUE)
within5Pct2 <- pickSizeTolerance(example2, metric = "Rsquared", maximize = TRUE)

cat("numerically optimal:",
    example2$Rsquared[absoluteBest2],
    "R^2 in position",
```

```
    absoluteBest2, "\n")
cat("Accepting a 1.5 pct loss:",
    example2$Rsquared[within5Pct2],
    "R^2 in position",
    within5Pct2, "\n")
```

---

caretSBF *Selection By Filtering (SBF) Helper Functions*

Description

Ancillary functions for univariate feature selection

Usage

```
anovaScores(x, y)
gamScores(x, y)

caretSBF
lmSBF
rfSBF
treebagSBF
ldaSBF
nbSBF
```

Arguments

x	a matrix or data frame of numeric predictors
y	a numeric or factor vector of outcomes

Details

More details on these functions can be found at http://topepo.github.io/caret/featureselection.html#filter.

This page documents the functions that are used in selection by filtering (SBF). The functions described here are passed to the algorithm via the `functions` argument of `sbfControl`.

See `sbfControl` for details on how these functions should be defined.

`anovaScores` and `gamScores` are two examples of univariate filtering functions. `anovaScores` fits a simple linear model between a single feature and the outcome, then the p-value for the whole model F-test is returned. `gamScores` fits a generalized additive model between a single predictor and the outcome using a smoothing spline basis function. A p-value is generated using the whole model test from `summary.gam` and is returned.

If a particular model fails for `lm` or `gam`, a p-value of 1 is returned.

Author(s)

Max Kuhn

See Also

sbfControl, sbf, summary.gam

---

cars *Kelly Blue Book resale data for 2005 model year GM cars*

Description

Kuiper (2008) collected data on Kelly Blue Book resale data for 804 GM cars (2005 model year).

Usage

```
data(cars)
```

Value

cars	data frame of the suggested retail price (column Price) and various characteristics of each car (columns Mileage, Cylinder, Doors, Cruise, Sound, Leather, Buick, Cadillac, Chevy, Pontiac, Saab, Saturn, convertible, coupe, hatchback, sedan and wagon)

Source

Kuiper, S. (2008). Introduction to Multiple Regression: How Much Is Your Car Worth?, *Journal of Statistics Education*, Vol. 16, www.amstat.org/publications/jse/v16n3/datasets.kuiper.html

---

classDist *Compute and predict the distances to class centroids*

Description

This function computes the class centroids and covariance matrix for a training set for determining Mahalanobis distances of samples to each class centroid.

Usage

```
classDist(x, ...)

## Default S3 method:
classDist(x, y, groups = 5, pca = FALSE, keep = NULL, ...)

## S3 method for class 'classDist'
predict(object, newdata, trans = log, ...)
```

Arguments

x	a matrix or data frame of predictor variables
y	a numeric or factor vector of class labels
groups	an integer for the number of bins for splitting a numeric outcome
pca	a logical: should principal components analysis be applied to the dataset prior to splitting the data by class?
keep	an integer for the number of PCA components that should by used to predict new samples (NULL uses all within a tolerance of sqrt(.Machine$double.eps))
object	an object of class classDist
newdata	a matrix or data frame. If vars was previously specified, these columns should be in newdata
trans	an optional function that can be applied to each class distance. trans = NULL will not apply a function
...	optional arguments to pass (not currently used)

Details

For factor outcomes, the data are split into groups for each class and the mean and covariance matrix are calculated. These are then used to compute Mahalanobis distances to the class centers (using predict.classDist The function will check for non-singular matrices.

For numeric outcomes, the data are split into roughly equal sized bins based on groups. Percentiles are used to split the data.

Value

for classDist, an object of class classDist with elements:

values	a list with elements for each class. Each element contains a mean vector for the class centroid and the inverse of the class covariance matrix
classes	a character vector of class labels
pca	the results of prcomp when pca = TRUE
call	the function call
p	the number of variables
n	a vector of samples sizes per class

For predict.classDist, a matrix with columns for each class. The columns names are the names of the class with the prefix dist.. In the case of numeric y, the class labels are the percentiles. For example, of groups = 9, the variable names would be dist.11.11, dist.22.22, etc.

Author(s)

Max Kuhn

References

Forina et al. CAIMAN brothers: A family of powerful classification and class modeling techniques. Chemometrics and Intelligent Laboratory Systems (2009) vol. 96 (2) pp. 239-245

See Also

mahalanobis

Examples

```
trainSet <- sample(1:150, 100)

distData <- classDist(iris[trainSet, 1:4],
                      iris$Species[trainSet])

newDist <- predict(distData,
                   iris[-trainSet, 1:4])

splom(newDist, groups = iris$Species[-trainSet])
```

---

confusionMatrix *Create a confusion matrix*

Description

Calculates a cross-tabulation of observed and predicted classes with associated statistics.

Usage

```
confusionMatrix(data, ...)

## Default S3 method:
confusionMatrix(data, reference, positive = NULL,
                dnn = c("Prediction", "Reference"),
                prevalence = NULL, ...)

## S3 method for class 'table'
confusionMatrix(data, positive = NULL, prevalence = NULL, ...)
```

Arguments

data	a factor of predicted classes (for the default method) or an object of class table.
reference	a factor of classes to be used as the true results
positive	an optional character string for the factor level that corresponds to a "positive" result (if that makes sense for your data). If there are only two factor levels, the first level will be used as the "positive" result.

dnn	a character vector of dimnames for the table
prevalence	a numeric value or matrix for the rate of the "positive" class of the data. When data has two levels, prevalence should be a single numeric value. Otherwise, it should be a vector of numeric values with elements for each class. The vector should have names corresponding to the classes.
...	options to be passed to table. NOTE: do not include dnn here

Details

The functions requires that the factors have exactly the same levels.

For two class problems, the sensitivity, specificity, positive predictive value and negative predictive value is calculated using the positive argument. Also, the prevalence of the "event" is computed from the data (unless passed in as an argument), the detection rate (the rate of true events also predicted to be events) and the detection prevalence (the prevalence of predicted events).

Suppose a 2x2 table with notation

	Reference	
Predicted	Event	No Event
Event	A	B
No Event	C	D

The formulas used here are:

$$Sensitivity = A/(A+C)$$

$$Specificity = D/(B+D)$$

$$Prevalence = (A+C)/(A+B+C+D)$$

$$PPV = (sensitivity*Prevalence)/((sensitivity*Prevalence)+((1-specificity)*(1-Prevalence)))$$

$$NPV = (specificity*(1-Prevalence))/(((1-sensitivity)*Prevalence)+((specificity)*(1-Prevalence)))$$

$$DetectionRate = A/(A+B+C+D)$$

$$DetectionPrevalence = (A+B)/(A+B+C+D)$$

$$BalancedAccuracy = (Sensitivity+Specificity)/2$$

See the references for discussions of the first five formulas.

For more than two classes, these results are calculated comparing each factor level to the remaining levels (i.e. a "one versus all" approach).

The overall accuracy and unweighted Kappa statistic are calculated. A p-value from McNemar's test is also computed using mcnemar.test (which can produce NA values with sparse tables).

The overall accuracy rate is computed along with a 95 percent confidence interval for this rate (using binom.test) and a one-sided test to see if the accuracy is better than the "no information rate," which is taken to be the largest class percentage in the data.

Value

a list with elements

`table`	the results of `table` on `data` and `reference`
`positive`	the positive result level
`overall`	a numeric vector with overall accuracy and Kappa statistic values
`byClass`	the sensitivity, specificity, positive predictive value, negative predictive value, prevalence, detection rate, detection prevalence and balanced accuracy for each class. For two class systems, this is calculated once using the `positive` argument

Author(s)

Max Kuhn

References

Kuhn, M. (2008), "Building predictive models in R using the caret package, " *Journal of Statistical Software*, (http://www.jstatsoft.org/v28/i05/).

Altman, D.G., Bland, J.M. (1994) "Diagnostic tests 1: sensitivity and specificity," *British Medical Journal*, vol 308, 1552.

Altman, D.G., Bland, J.M. (1994) "Diagnostic tests 2: predictive values," *British Medical Journal*, vol 309, 102.

Velez, D.R., et. al. (2008) "A balanced accuracy function for epistasis modeling in imbalanced datasets using multifactor dimensionality reduction.," *Genetic Epidemiology*, vol 4, 306.

See Also

`as.table.confusionMatrix`, `as.matrix.confusionMatrix`, `sensitivity`, `specificity`, `posPredValue`, `negPredValue`, `print.confusionMatrix`, `binom.test`

Examples

```
###################
## 2 class example

lvs <- c("normal", "abnormal")
truth <- factor(rep(lvs, times = c(86, 258)),
                levels = rev(lvs))
pred <- factor(
               c(
                 rep(lvs, times = c(54, 32)),
                 rep(lvs, times = c(27, 231))),
               levels = rev(lvs))

xtab <- table(pred, truth)

confusionMatrix(xtab)
confusionMatrix(pred, truth)
```

```
confusionMatrix(xtab, prevalence = 0.25)

###################
## 3 class example

confusionMatrix(iris$Species, sample(iris$Species))

newPrior <- c(.05, .8, .15)
names(newPrior) <- levels(iris$Species)

confusionMatrix(iris$Species, sample(iris$Species))
```

`confusionMatrix.train` *Estimate a Resampled Confusion Matrix*

Description

Using a `train`, `rfe`, `sbf` object, determine a confusion matrix based on the resampling procedure

Usage

```
## S3 method for class 'train'
confusionMatrix(data, norm = "overall",
                dnn = c("Prediction", "Reference"), ...)

## S3 method for class 'rfe'
confusionMatrix(data, norm = "overall",
                dnn = c("Prediction", "Reference"), ...)

## S3 method for class 'sbf'
confusionMatrix(data, norm = "overall",
                dnn = c("Prediction", "Reference"), ...)
```

Arguments

`data`	an object of class `train`, `rfe`, `sbf` that did not use out-of-bag resampling or leave-one-out cross-validation.
`norm`	a character string indicating how the table entries should be normalized. Valid values are "none", "overall" or "average".
`dnn`	a character vector of dimnames for the table
`...`	not used here

Details

When train is used for tuning a model, it tracks the confusion matrix cell entries for the hold-out samples. These can be aggregated and used for diagnostic purposes. For train, the matrix is estimated for the final model tuning parameters determined by train. For rfe, the matrix is associated with the optimal number of variables.

There are several ways to show the table entries. Using `norm = "none"` will show the frequencies of samples on each of the cells (across all resamples). `norm = "overall"` first divides the cell entries by the total number of data points in the table, then averages these percentages. `norm = "average"` takes the raw, aggregate cell counts across resamples and divides by the number of resamples (i.e. to yield an average count for each cell).

Value

a list of class `confusionMatrix.train`, `confusionMatrix.rfe` or `confusionMatrix.sbf` with elements

`table`	the normalized matrix
`norm`	an echo fo the call
`text`	a character string with details about the resampling procedure (e.g. "Bootstrapped (25 reps) Confusion Matrix"

Author(s)

Max Kuhn

See Also

confusionMatrix, train, rfe, sbf, trainControl

Examples

```
data(iris)
TrainData <- iris[,1:4]
TrainClasses <- iris[,5]

knnFit <- train(TrainData, TrainClasses,
                method = "knn",
                preProcess = c("center", "scale"),
                tuneLength = 10,
                trControl = trainControl(method = "cv"))
confusionMatrix(knnFit)
confusionMatrix(knnFit, "average")
confusionMatrix(knnFit, "none")
```

cox2 *COX-2 Activity Data*

Description

From Sutherland, O'Brien, and Weaver (2003): "A set of 467 cyclooxygenase-2 (COX-2) inhibitors has been assembled from the published work of a single research group, with in vitro activities against human recombinant enzyme expressed as IC50 values ranging from 1 nM to >100 uM (53 compounds have indeterminate IC50 values)."

The data are in the Supplemental Data file for the article.

A set of 255 descriptors (MOE2D and QikProp) were generated. To classify the data, we used a cutoff of $2^2.5$ to determine activity

Usage

```
data(cox2)
```

Value

`cox2Descr`	the descriptors
`cox2IC50`	the IC50 data used to determine activity
`cox2Class`	the categorical outcome ("Active" or "Inactive") based on the $2^2.5$ cutoff

Source

Sutherland, J. J., O'Brien, L. A. and Weaver, D. F. (2003). Spline-Fitting with a Genetic Algorithm: A Method for Developing Classification Structure-Activity Relationships, *Journal of Chemical Information and Computer Sciences*, Vol. 43, pg. 1906–1915.

createDataPartition *Data Splitting functions*

Description

A series of test/training partitions are created using `createDataPartition` while `createResample` creates one or more bootstrap samples. `createFolds` splits the data into k groups while `createTimeSlices` creates cross-validation sample information to be used with time series data.

Usage

```
createDataPartition(y,
                    times = 1,
                    p = 0.5,
                    list = TRUE,
                    groups = min(5, length(y)))
createResample(y, times = 10, list = TRUE)
createFolds(y, k = 10, list = TRUE, returnTrain = FALSE)
createMultiFolds(y, k = 10, times = 5)
createTimeSlices(y, initialWindow, horizon = 1, fixedWindow = TRUE)
```

Arguments

y	a vector of outcomes. For createTimeSlices, these should be in chronological order.
times	the number of partitions to create
p	the percentage of data that goes to training
list	logical - should the results be in a list (TRUE) or a matrix with the number of rows equal to floor(p * length(y)) and times columns.
groups	for numeric y, the number of breaks in the quantiles (see below)
k	an integer for the number of folds.
returnTrain	a logical. When true, the values returned are the sample positions corresponding to the data used during training. This argument only works in conjunction with list = TRUE
initialWindow	The initial number of consecutive values in each training set sample
horizon	The number of consecutive values in test set sample
fixedWindow	A logical: if FALSE, the training set always start at the first sample.

Details

For bootstrap samples, simple random sampling is used.

For other data splitting, the random sampling is done within the levels of y when y is a factor in an attempt to balance the class distributions within the splits.

For numeric y, the sample is split into groups sections based on percentiles and sampling is done within these subgroups. For createDataPartition, the number of percentiles is set via the groups argument. For createFolds and createMultiFolds, the number of groups is set dynamically based on the sample size and k. For smaller samples sizes, these two functions may not do stratified splitting and, at most, will split the data into quartiles.

Also, for createDataPartition, very small class sizes (<= 3) the classes may not show up in both the training and test data

For multiple k-fold cross-validation, completely independent folds are created. The names of the list objects will denote the fold membership using the pattern "Foldi.Repj" meaning the ith section (of k) of the jth cross-validation set (of times). Note that this function calls createFolds with list = TRUE and returnTrain = TRUE.

Hyndman and Athanasopoulos (2013)) discuss rolling forecasting origin< techniques that move the training and test sets in time. `createTimeSlices` can create the indices for this type of splitting.

Value

A list or matrix of row position integers corresponding to the training data

Author(s)

Max Kuhn, `createTimeSlices` by Tony Cooper

References

http://topepo.github.io/caret/splitting.html

Hyndman and Athanasopoulos (2013), Forecasting: principles and practice. https://www.otexts.org/fpp

Examples

```
data(oil)
createDataPartition(oilType, 2)

x <- rgamma(50, 3, .5)
inA <- createDataPartition(x, list = FALSE)

plot(density(x[inA]))
rug(x[inA])

points(density(x[-inA]), type = "l", col = 4)
rug(x[-inA], col = 4)

createResample(oilType, 2)

createFolds(oilType, 10)
createFolds(oilType, 5, FALSE)

createFolds(rnorm(21))

createTimeSlices(1:9, 5, 1, fixedWindow = FALSE)
createTimeSlices(1:9, 5, 1, fixedWindow = TRUE)
createTimeSlices(1:9, 5, 3, fixedWindow = TRUE)
createTimeSlices(1:9, 5, 3, fixedWindow = FALSE)
```

---

dhfr *Dihydrofolate Reductase Inhibitors Data*

Description

Sutherland and Weaver (2004) discuss QSAR models for dihydrofolate reductase (DHFR) inhibition. This data set contains values for 325 compounds. For each compound, 228 molecular descriptors have been calculated. Additionally, each samples is designated as "active" or "inactive".

The data frame `dhfr` contains a column called `Y` with the outcome classification. The remainder of the columns are molecular descriptor values.

Usage

```
data(dhfr)
```

Value

`dhfr`	data frame of chemical descriptors and the activity values

Source

Sutherland, J.J. and Weaver, D.F. (2004). Three-dimensional quantitative structure-activity and structure-selectivity relationships of dihydrofolate reductase inhibitors, *Journal of Computer-Aided Molecular Design*, Vol. 18, pg. 309–331.

`diff.resamples` *Inferential Assessments About Model Performance*

Description

Methods for making inferences about differences between models

Usage

```
## S3 method for class 'resamples'
diff(x, models = x$models, metric = x$metrics,
     test = t.test,
     confLevel = 0.95, adjustment = "bonferroni",
     ...)

## S3 method for class 'diff.resamples'
summary(object, digits = max(3, getOption("digits") - 3), ...)

compare_models(a, b, metric = a$metric[1])
```

Arguments

x	an object generated by resamples
models	a character string for which models to compare
metric	a character string for which metrics to compare
test	a function to compute differences. The output of this function should have scalar outputs called estimate and p.value
object	a object generated by diff.resamples
adjustment	any p-value adjustment method to pass to p.adjust.
confLevel	confidence level to use for dotplot.diff.resamples. See Details below.
digits	the number of significant differences to display when printing
a, b	two objects of class train, sbf or rfe with a common set of resampling indices in the control object.
...	further arguments to pass to test

Details

The ideas and methods here are based on Hothorn et al. (2005) and Eugster et al. (2008).

For each metric, all pair-wise differences are computed and tested to assess if the difference is equal to zero.

When a Bonferroni correction is used, the confidence level is changed from confLevel to 1-((1-confLevel)/p) here p is the number of pair-wise comparisons are being made. For other correction methods, no such change is used.

compare_models is a shorthand function to compare two models using a single metric. It returns the results of t.test on the differences.

Value

An object of class "diff.resamples" with elements:

call	the call
difs	a list for each metric being compared. Each list contains a matrix with differences in columns and resamples in rows
statistics	a list of results generated by test
adjustment	the p-value adjustment used
models	a character string for which models were compared.
metrics	a character string of performance metrics that were used

or...

An object of class "summary.diff.resamples" with elements:

call	the call
table	a list of tables that show the differences and p-values

...or (for compare_models) an object of class htest resulting from t.test.

Author(s)

Max Kuhn

References

Hothorn et al. The design and analysis of benchmark experiments. Journal of Computational and Graphical Statistics (2005) vol. 14 (3) pp. 675-699

Eugster et al. Exploratory and inferential analysis of benchmark experiments. Ludwigs-Maximilians-Universitat Munchen, Department of Statistics, Tech. Rep (2008) vol. 30

See Also

resamples, dotplot.diff.resamples, densityplot.diff.resamples, bwplot.diff.resamples, levelplot.diff.resamples

Examples

```
## Not run:
#load(url("http://topepo.github.io/caret/exampleModels.RData"))

resamps <- resamples(list(CART = rpartFit,
                          CondInfTree = ctreeFit,
                          MARS = earthFit))

difs <- diff(resamps)

difs

summary(difs)

compare_models(rpartFit, ctreeFit)

## End(Not run)
```

---

dotPlot *Create a dotplot of variable importance values*

Description

A lattice dotplot is created from an object of class varImp.train.

Usage

```
dotPlot(x, top = min(20, dim(x$importance)[1]), ...)
```

Arguments

x	an object of class varImp.train
top	the number of predictors to plot
...	options passed to dotplot

Value

an object of class trellis.

Author(s)

Max Kuhn

See Also

varImp, dotplot

Examples

```
data(iris)
TrainData <- iris[,1:4]
TrainClasses <- iris[,5]

knnFit <- train(TrainData, TrainClasses, "knn")

knnImp <- varImp(knnFit)

dotPlot(knnImp)
```

---

dotplot.diff.resamples

Lattice Functions for Visualizing Resampling Differences

Description

Lattice functions for visualizing resampling result differences between models

Usage

```
## S3 method for class 'diff.resamples'
densityplot(x, data, metric = x$metric, ...)

## S3 method for class 'diff.resamples'
bwplot(x, data, metric = x$metric, ...)
```

```
## S3 method for class 'diff.resamples'
levelplot(x, data = NULL, metric = x$metric[1], what = "pvalues", ...)

## S3 method for class 'diff.resamples'
dotplot(x, data = NULL, metric = x$metric[1], ...)
```

Arguments

x	an object generated by diff.resamples
data	Not used
what	levelplot only: display either the "pvalues" or "differences"
metric	a character string for which metrics to plot. Note: dotplot and levelplot require exactly two models whereas the other methods can plot more than two.
...	further arguments to pass to either densityplot, dotplot or levelplot

Details

densityplot and bwplot display univariate visualizations of the resampling distributions. levelplot displays the matrix of pair-wide comparisons. dotplot shows the differences along with their associated confidence intervals.

Value

a lattice object

Author(s)

Max Kuhn

See Also

resamples, diff.resamples, bwplot, densityplot, xyplot, splom

Examples

```
## Not run:
#load(url("http://topepo.github.io/caret/exampleModels.RData"))

resamps <- resamples(list(CART = rpartFit,
                          CondInfTree = ctreeFit,
                          MARS = earthFit))
difs <- diff(resamps)

dotplot(difs)

densityplot(difs,
            metric = "RMSE",
            auto.key = TRUE,
            pch = "|")
```

```
bwplot(difs,
       metric = "RMSE")

levelplot(difs, what = "differences")


## End(Not run)
```

---

downSample *Down- and Up-Sampling Imbalanced Data*

Description

downSample will randomly sample a data set so that all classes have the same frequency as the minority class. upSample samples with replacement to make the class distributions equal

Usage

```
downSample(x, y, list = FALSE, yname = "Class")

upSample(x, y, list = FALSE, yname = "Class")
```

Arguments

x	a matrix or data frame of predictor variables
y	a factor variable with the class memberships
list	should the function return list(x, y) or bind x and y together? If TRUE, the output will be coerced to a data frame.
yname	if list = FALSE, a label for the class column

Details

Simple random sampling is used to down-sample for the majority class(es). Note that the minority class data are left intact and that the samples will be re-ordered in the down-sampled version.

For up-sampling, all the original data are left intact and additional samples are added to the minority classes with replacement.

Value

Either a data frame or a list with elements x and y.

Author(s)

Max Kuhn

Examples

```
## A ridiculous example...
data(oil)
table(oilType)
downSample(fattyAcids, oilType)

upSample(fattyAcids, oilType)
```

---

dummyVars *Create A Full Set of Dummy Variables*

Description

dummyVars creates a full set of dummy variables (i.e. less than full rank parameterization)

Usage

```
dummyVars(formula, ...)

## Default S3 method:
dummyVars(formula, data, sep = ".", levelsOnly = FALSE,
          fullRank = FALSE, ...)

## S3 method for class 'dummyVars'
predict(object, newdata, na.action = na.pass, ...)

contr.dummy(n, ...) ## DEPRECATED

contr.ltfr(n, contrasts = TRUE, sparse = FALSE)
```

Arguments

formula	An appropriate R model formula, see References
data	A data frame with the predictors of interest
sep	An optional separator between factor variable names and their levels. Use sep = NULL for no separator (i.e. normal behavior of model.matrix as shown in the Details section)
levelsOnly	A logical; TRUE means to completely remove the variable names from the column names
fullRank	A logical; should a full rank or less than full rank parameterization be used? If TRUE, factors are encoded to be consistent with model.matrix and the resulting there are no linear dependencies induced between the columns.
object	An object of class dummyVars
newdata	A data frame with the required columns

na.action	A function determining what should be done with missing values in newdata. The default is to predict NA.
n	A vector of levels for a factor, or the number of levels.
contrasts	A logical indicating whether contrasts should be computed.
sparse	A logical indicating if the result should be sparse.
...	additional arguments to be passed to other methods

Details

Most of the contrasts functions in R produce full rank parameterizations of the predictor data. For example, contr.treatment creates a reference cell in the data and defines dummy variables for all factor levels except those in the reference cell. For example, if a factor with 5 levels is used in a model formula alone, contr.treatment creates columns for the intercept and all the factor levels except the first level of the factor. For the data in the Example section below, this would produce:

```
  (Intercept) dayTue dayWed dayThu dayFri daySat daySun
1           1      1      0      0      0      0      0
2           1      1      0      0      0      0      0
3           1      1      0      0      0      0      0
4           1      0      0      1      0      0      0
5           1      0      0      1      0      0      0
6           1      0      0      0      0      0      0
7           1      0      1      0      0      0      0
8           1      0      1      0      0      0      0
9           1      0      0      0      0      0      0
```

In some situations, there may be a need for dummy variables for all the levels of the factor. For the same example:

```
  dayMon dayTue dayWed dayThu dayFri daySat daySun
1      0      1      0      0      0      0      0
2      0      1      0      0      0      0      0
3      0      1      0      0      0      0      0
4      0      0      0      1      0      0      0
5      0      0      0      1      0      0      0
6      1      0      0      0      0      0      0
7      0      0      1      0      0      0      0
8      0      0      1      0      0      0      0
9      1      0      0      0      0      0      0
```

Given a formula and initial data set, the class dummyVars gathers all the information needed to produce a full set of dummy variables for any data set. It uses contr.ltfr as the base function to do this.

Value

The output of dummyVars is a list of class 'dummyVars' with elements

call	the function call

form	the model formula
vars	names of all the variables in the model
facVars	names of all the factor variables in the model
lvls	levels of any factor variables
sep	NULL or a character separator
terms	the terms.formula object
levelsOnly	a logical

The predict function produces a data frame.

contr.ltfr generates a design matrix.

Author(s)

contr.ltfr is a small modification of contr.treatment by Max Kuhn

References

http://cran.r-project.org/doc/manuals/R-intro.html#Formulae-for-statistical-models

See Also

model.matrix, contrasts, formula

Examples

```
when <- data.frame(time = c("afternoon", "night", "afternoon",
                            "morning", "morning", "morning",
                            "morning", "afternoon", "afternoon"),
                   day = c("Mon", "Mon", "Mon",
                           "Wed", "Wed", "Fri",
                           "Sat", "Sat", "Fri"))

levels(when$time) <- c("morning", "afternoon", "night")
levels(when$day) <- c("Mon", "Tue", "Wed", "Thu", "Fri", "Sat", "Sun")

## Default behavior:
model.matrix(~day, when)

mainEffects <- dummyVars(~ day + time, data = when)
mainEffects
predict(mainEffects, when[1:3,])

when2 <- when
when2[1, 1] <- NA
predict(mainEffects, when2[1:3,])
predict(mainEffects, when2[1:3,], na.action = na.omit)


interactionModel <- dummyVars(~ day + time + day:time,
```

```
                              data = when,
                              sep = ".")
predict(interactionModel, when[1:3,])

noNames <- dummyVars(~ day + time + day:time,
                     data = when,
                     levelsOnly = TRUE)
predict(noNames, when)
```

`featurePlot` *Wrapper for Lattice Plotting of Predictor Variables*

Description

A shortcut to produce lattice graphs

Usage

```
featurePlot(x, y,
            plot = if(is.factor(y)) "strip" else "scatter",
            labels = c("Feature", ""),
            ...)
```

Arguments

`x`	a matrix or data frame of continuous feature/probe/spectra data.
`y`	a factor indicating class membership.
`plot`	the type of plot. For classification: `box`, `strip`, `density`, `pairs` or `ellipse`. For regression, `pairs` or `scatter`
`labels`	a bad attempt at pre-defined axis labels
`...`	options passed to lattice calls.

Details

This function "stacks" data to get it into a form compatible with lattice and creates the plots

Value

An object of class "trellis". The 'update' method can be used to update components of the object and the 'print' method (usually called by default) will plot it on an appropriate plotting device.

Author(s)

Max Kuhn

Examples

```
x <- matrix(rnorm(50*5),ncol=5)
y <- factor(rep(c("A", "B"),  25))

trellis.par.set(theme = col.whitebg(), warn = FALSE)
featurePlot(x, y, "ellipse")
featurePlot(x, y, "strip", jitter = TRUE)
featurePlot(x, y, "box")
featurePlot(x, y, "pairs")
```

`filterVarImp` *Calculation of filter-based variable importance*

Description

Specific engines for variable importance on a model by model basis.

Usage

```
filterVarImp(x, y, nonpara = FALSE, ...)
```

Arguments

`x`	A matrix or data frame of predictor data
`y`	A vector (numeric or factor) of outcomes)
`nonpara`	should nonparametric methods be used to assess the relationship between the features and response
`...`	options to pass to either `lm` or `loess`

Details

The importance of each predictor is evaluated individually using a "filter" approach.

For classification, ROC curve analysis is conducted on each predictor. For two class problems, a series of cutoffs is applied to the predictor data to predict the class. The sensitivity and specificity are computed for each cutoff and the ROC curve is computed. The trapezoidal rule is used to compute the area under the ROC curve. This area is used as the measure of variable importance. For multi–class outcomes, the problem is decomposed into all pair-wise problems and the area under the curve is calculated for each class pair (i.e class 1 vs. class 2, class 2 vs. class 3 etc.). For a specific class, the maximum area under the curve across the relevant pair–wise AUC's is used as the variable importance measure.

For regression, the relationship between each predictor and the outcome is evaluated. An argument, `nonpara`, is used to pick the model fitting technique. When `nonpara = FALSE`, a linear model is fit and the absolute value of the t–value for the slope of the predictor is used. Otherwise, a loess smoother is fit between the outcome and the predictor. The R^2 statistic is calculated for this model against the intercept only null model.

Value

A data frame with variable importances. Column names depend on the problem type. For regression, the data frame contains one column: "Overall" for the importance values.

Author(s)

Max Kuhn

Examples

```
data(mdrr)
filterVarImp(mdrrDescr[, 1:5], mdrrClass)

data(BloodBrain)

filterVarImp(bbbDescr[, 1:5], logBBB, nonpara = FALSE)
apply(bbbDescr[, 1:5],
      2,
      function(x, y) summary(lm(y~x))$coefficients[2,3],
      y = logBBB)

filterVarImp(bbbDescr[, 1:5], logBBB, nonpara = TRUE)
```

---

findCorrelation *Determine highly correlated variables*

Description

This function searches through a correlation matrix and returns a vector of integers corresponding to columns to remove to reduce pair-wise correlations.

Usage

```
findCorrelation(x, cutoff = .90, verbose = FALSE)
```

Arguments

x	A correlation matrix
cutoff	A numeric value for the pair-wise absolute correlation cutoff
verbose	A boolean for printing the details

Details

The absolute values of pair-wise correlations are considered. If two variables have a high correlation, the function looks at the mean absolute correlation of each variable and removes the variable with the largest mean absolute correlation.

There are several function in the **subselect** package (leaps, genetic, anneal) that can also be used to accomplish the same goal.

Value

A vector of indices denoting the columns to remove. If no correlations meet the criteria, `numeric(0)` is returned.

Author(s)

Original R code by Dong Li, modified by Max Kuhn

See Also

`leaps`, `genetic`, `anneal`, `findLinearCombos`

Examples

```
corrMatrix <- diag(rep(1, 5))
corrMatrix[2, 3] <- corrMatrix[3, 2] <- .7
corrMatrix[5, 3] <- corrMatrix[3, 5] <- -.7
corrMatrix[4, 1] <- corrMatrix[1, 4] <- -.67

corrDF <- expand.grid(row = 1:5, col = 1:5)
corrDF$correlation <- as.vector(corrMatrix)
levelplot(correlation ~ row+ col, corrDF)

findCorrelation(corrMatrix, cutoff = .65, verbose = TRUE)

findCorrelation(corrMatrix, cutoff = .99, verbose = TRUE)
```

---

findLinearCombos *Determine linear combinations in a matrix*

Description

Enumerate and resolve the linear combinations in a numeric matrix

Usage

```
findLinearCombos(x)
```

Arguments

x	a numeric matrix

Details

The QR decomposition is used to determine if the matrix is full rank and then identify the sets of columns that are involved in the dependencies.

To "resolve" them, columns are iteratively removed and the matrix rank is rechecked.

The `trim.matrix` function in the **subselect** package can also be used to accomplish the same goal.

Value

a list with elements:

linearCombos	If there are linear combinations, this will be a list with elements for each dependency that contains vectors of column numbers.
remove	a list of column numbers that can be removed to counter the linear combinations

Author(s)

Kirk Mettler and Jed Wing (enumLC) and Max Kuhn (findLinearCombos)

See Also

trim.matrix

Examples

```
testData1 <- matrix(0, nrow=20, ncol=8)
testData1[,1] <- 1
testData1[,2] <- round(rnorm(20), 1)
testData1[,3] <- round(rnorm(20), 1)
testData1[,4] <- round(rnorm(20), 1)
testData1[,5] <- 0.5 * testData1[,2] - 0.25 * testData1[,3] - 0.25 * testData1[,4]
testData1[1:4,6] <- 1
testData1[5:10,7] <- 1
testData1[11:20,8] <- 1

findLinearCombos(testData1)

testData2 <- matrix(0, nrow=6, ncol=6)
testData2[,1] <- c(1, 1, 1, 1, 1, 1)
testData2[,2] <- c(1, 1, 1, 0, 0, 0)
testData2[,3] <- c(0, 0, 0, 1, 1, 1)
testData2[,4] <- c(1, 0, 0, 1, 0, 0)
testData2[,5] <- c(0, 1, 0, 0, 1, 0)
testData2[,6] <- c(0, 0, 1, 0, 0, 1)

findLinearCombos(testData2)
```

---

format.bagEarth *Format 'bagEarth' objects*

Description

Return a string representing the 'bagEarth' expression.

Usage

```
## S3 method for class 'bagEarth'
format(x, file = "", cat = TRUE, ...)
```

Arguments

x	An bagEarth object. This is the only required argument.
file	A connection, or a character string naming the file to print to. If "" (the default), the output prints to the standard output connection. See cat.
cat	a logical; should the equation be printed?
...	Arguments to format.earth.

Value

A character representation of the bagged earth object.

See Also

earth

Examples

```
a <- bagEarth(Volume ~ ., data = trees, B= 3)
format(a)

# yields:
# (
#   31.61075
#   +  6.587273 * pmax(0,  Girth -   14.2)
#   -  3.229363 * pmax(0,   14.2 -  Girth)
#   - 0.3167140 * pmax(0,     79 - Height)
#   +
#    22.80225
#   +  5.309866 * pmax(0,  Girth -     12)
#   -  2.378658 * pmax(0,     12 -  Girth)
#   +  0.793045 * pmax(0, Height -     80)
#   - 0.3411915 * pmax(0,     80 - Height)
#   +
#    31.39772
#   +   6.18193 * pmax(0,  Girth -   14.2)
#   -  3.660456 * pmax(0,   14.2 -  Girth)
#   + 0.6489774 * pmax(0, Height -     80)
# )/3
```

---

gafs.default *Genetic algorithm feature selection*

Description

Supervised feature selection using genetic algorithms

Usage

```
gafs(x, ...)

## Default S3 method:
gafs(x, y,
     iters = 10,
     popSize = 50,
     pcrossover = 0.8,
     pmutation = 0.1,
     elite = 0,
     suggestions = NULL,
     differences = TRUE,
     gafsControl = gafsControl(),
     ...)
```

Arguments

x	an object where samples are in rows and features are in columns. This could be a simple matrix, data frame or other type (e.g. sparse matrix). See Details below
y	a numeric or factor vector containing the outcome for each sample
iters	number of search iterations
popSize	number of subsets evaluated at each iteration
pcrossover	the crossover probability
pmutation	the mutation probability
elite	the number of best subsets to survive at each generation
suggestions	a binary matrix of subsets strings to be included in the initial population. If provided the number of columns must match the number of columns in x
differences	a logical: should the difference in fitness values with and without each predictor be calculated?
gafsControl	a list of values that define how this function acts. See gafsControl and URL.
...	arguments passed to the classification or regression routine specified in the function gafsControl$functions$fit

Details

gafs conducts a supervised binary search of the predictor space using a genetic algorithm. See XXX and Scrucca (2012) for more details on genetic algorithms.

This function conducts the search of the feature space repeatedly within resampling iterations. First, the training data are split be whatever resampling method was specified in the control function. For example, if 10-fold cross-validation is selected, the entire genetic algorithm is conducted 10 separate times. For the first fold, nine tenths of the data are used in the search while the remaining tenth is used to estimate the external performance since these data points were not used in the search.

During the genetic algorithm, a measure of fitness is needed to guide the search. This is the internal measure of performance. During the search, the data that are available are the instances selected by the top-level resampling (e.g. the nine tenths mentioned above). A common approach is to conduct

another resampling procedure. Another option is to use a holdout set of samples to determine the internal estimate of performance (see the holdout argument of the control function). While this is faster, it is more likely to cause overfitting of the features and should only be used when a large amount of training data are available. Yet another idea is to use a penalized metric (such as the AIC statistic) but this may not exist for some metrics (e.g. the area under the ROC curve).

The internal estimates of performance will eventually overfit the subsets to the data. However, since the external estimate is not used by the search, it is able to make better assessments of overfitting. After resampling, this function determines the optimal number of generations for the GA.

Finally, the entire data set is used in the last execution of the genetic algorithm search and the final model is built on the predictor subset that is associated with the optimal number of generations determined by resampling (although the update function can be used to manually set the number of generations).

This is an example of the output produced when `gafsControl(verbose = TRUE)` is used:

```
Fold2  1 0.715 (13)
Fold2  2 0.715->0.737 (13->17, 30.4%) *
Fold2  3 0.737->0.732 (17->14, 24.0%)
Fold2  4 0.737->0.769 (17->23, 25.0%) *
```

For the second resample (e.g. fold 2), the best subset across all individuals tested in the first generation contained 13 predictors and was associated with a fitness value of 0.715. The second generation produced a better subset containing 17 samples with an associated fitness values of 0.737 (and improvement is symbolized by the `*`. The percentage listed is the Jaccard similarity between the previous best individual (with 13 predictors) and the new best. The third generation did not produce a better fitness value but the fourth generation did.

The search algorithm can be parallelized in several places:

1. each externally resampled GA can be run independently (controlled by the `allowParallel` option of `gafsControl`)
2. within a GA, the fitness calculations at a particular generation can be run in parallel over the current set of individuals (see the `genParallel` option in `gafsControl`)
3. if inner resampling is used, these can be run in parallel (controls depend on the function used. See, for example, `trainControl`)
4. any parallelization of the individual model fits. This is also specific to the modeling function.

It is probably best to pick one of these areas for parallelization and the first is likely to produces the largest decrease in run-time since it is the least likely to incur multiple re-starting of the worker processes. Keep in mind that if multiple levels of parallelization occur, this can effect the number of workers and the amount of memory required exponentially.

Value

an object of class `gafs`

Author(s)

Max Kuhn, Luca Scrucca (for GA internals)

References

Kuhn M and Johnson K (2013), Applied Predictive Modeling, Springer, Chapter 19 http://appliedpredictivemodeling.com

Scrucca L (2012). GA: A Package for Genetic Algorithms in R. Journal of Statistical Software, 53(4), 1-37. www.jstatsoft.org/v53/i04

http://en.wikipedia.org/wiki/Jaccard_index

See Also

gafsControl, predict.gafs, caretGA, rfGA treebagGA

Examples

```
## Not run:
set.seed(1)
train_data <- twoClassSim(100, noiseVars = 10)
test_data  <- twoClassSim(10,  noiseVars = 10)

## A short example
ctrl <- gafsControl(functions = rfGA,
                    method = "cv",
                    number = 3)

rf_search <- gafs(x = train_data[, -ncol(train_data)],
                  y = train_data$Class,
                  iters = 3,
                  gafsControl = ctrl)

rf_search

## End(Not run)
```

---

gafs_initial *Ancillary genetic algorithm functions*

Description

Built-in functions related to genetic algorithms

Usage

```
gafs_initial(vars, popSize, ...)


gafs_lrSelection(population, fitness,
                 r = NULL,
                 q = NULL, ...)
```

```
gafs_rwSelection(population, fitness, ...)

gafs_tourSelection(population, fitness, k = 3, ...)


gafs_spCrossover(population, fitness, parents, ...)

gafs_uCrossover(population, parents, ...)


gafs_raMutation(population, parent, ...)


caretGA
rfGA
treebagGA
```

Arguments

vars	number of possible predictors
popSize	the population size passed into gafs
population	a binary matrix of the current subsets with predictors in columns and individuals in rows
fitness	a vector of fitness values
parent, parents	integer(s) for which chromosomes are altered
r, q, k	tuning parameters for the specific selection operator
...	not currently used

Details

These functions are used with the functions argument of the gafsControl function. More information on the details of these functions are at http://topepo.github.io/caret/GA.html.

Most of the gafs_* functions are based on those from the GA package by Luca Scrucca. These functions here are small re-writes to work outside of the GA package.

The objects caretGA, rfGA and treebagGA are example lists that can be used with the functions argument of gafsControl.

In the case of caretGA, the ... structure of gafs passes through to the model fitting routine. As a consequence, the train function can easily be accessed by passing important arguments belonging to train to gafs. See the examples below. By default, using caretGA will used the resampled performance estimates produced by train as the internal estimate of fitness.

For rfGA and treebagGA, the randomForest and bagging functions are used directly (i.e. train is not used). Arguments to either of these functions can also be passed to them though the gafs call (see examples below). For these two functions, the internal fitness is estimated using the out-of-bag estimates naturally produced by those functions. While faster, this limits the user to accuracy or Kappa (for classification) and RMSE and R-squared (for regression).

Value

The return value depends on the function.

Author(s)

Luca Scrucca, `gafs_initial`, `caretGA`, `rfGA` and `treebagGA` by Max Kuhn

References

Scrucca L (2012). GA: A Package for Genetic Algorithms in R. Journal of Statistical Software, 53(4), 1-37.

cran.r-project.org/web/packages/GA/

http://topepo.github.io/caret/GA.html

See Also

`gafs`, `gafsControl`

Examples

```
pop <- gafs_initial(vars = 10, popSize = 10)
pop

gafs_lrSelection(population = pop, fitness = 1:10)

gafs_spCrossover(population = pop, fitness = 1:10, parents = 1:2)


## Not run:
## Hypothetical examples
lda_ga <- gafs(x = predictors,
               y = classes,
               gafsControl = gafsControl(functions = caretGA),
               ## now pass arguments to `train`
               method = "lda",
               metric = "Accuracy"
               trControl = trainControl(method = "cv", classProbs = TRUE))

rf_ga <- gafs(x = predictors,
              y = classes,
              gafsControl = gafsControl(functions = rfGA),
              ## these are arguments to `randomForest`
              ntree = 1000,
              importance = TRUE)

## End(Not run)
```

GermanCredit *German Credit Data*

Description

Data from Dr. Hans Hofmann of the University of Hamburg.

These data have two classes for the credit worthiness: good or bad. There are predictors related to attributes, such as: checking account status, duration, credit history, purpose of the loan, amount of the loan, savings accounts or bonds, employment duration, Installment rate in percentage of disposable income, personal information, other debtors/guarantors, residence duration, property, age, other installment plans, housing, number of existing credits, job information, Number of people being liable to provide maintenance for, telephone, and foreign worker status.

Many of these predictors are discrete and have been expanded into several 0/1 indicator variables

Usage

```
data(GermanCredit)
```

Source

UCI Machine Learning Repository

histogram.train *Lattice functions for plotting resampling results*

Description

A set of lattice functions are provided to plot the resampled performance estimates (e.g. classification accuracy, RMSE) over tuning parameters (if any).

Usage

```
## S3 method for class 'train'
histogram(x, data = NULL, metric = x$metric, ...)

## S3 method for class 'train'
densityplot(x, data = NULL, metric = x$metric, ...)

## S3 method for class 'train'
xyplot(x, data = NULL, metric = x$metric, ...)

## S3 method for class 'train'
stripplot(x, data = NULL, metric = x$metric, ...)
```

Arguments

x	An object produced by train
data	This argument is not used
metric	A character string specifying the single performance metric that will be plotted
...	arguments to pass to either histogram, densityplot, xyplot or stripplot

Details

By default, only the resampling results for the optimal model are saved in the train object. The function trainControl can be used to save all the results (see the example below).

If leave-one-out or out-of-bag resampling was specified, plots cannot be produced (see the method argument of trainControl)

For xyplot and stripplot, the tuning parameter with the most unique values will be plotted on the x-axis. The remaining parameters (if any) will be used as conditioning variables. For densityplot and histogram, all tuning parameters are used for conditioning.

Using horizontal = FALSE in stripplot works.

Value

A lattice plot object

Author(s)

Max Kuhn

See Also

train, trainControl, histogram, densityplot, xyplot, stripplot

Examples

```
## Not run:

library(mlbench)
data(BostonHousing)

library(rpart)
rpartFit <- train(medv ~ .,
                  data = BostonHousing,
                  "rpart",
                  tuneLength = 9,
                  trControl = trainControl(
                    method = "boot",
                    returnResamp = "all"))

densityplot(rpartFit,
            adjust = 1.25)

xyplot(rpartFit,
```

```
        metric = "Rsquared",
        type = c("p", "a"))

stripplot(rpartFit,
          horizontal = FALSE,
          jitter = TRUE)


## End(Not run)
```

`icr.formula` *Independent Component Regression*

Description

Fit a linear regression model using independent components

Usage

```
## S3 method for class 'formula'
icr(formula, data, weights, ..., subset, na.action, contrasts = NULL)
## Default S3 method:
icr(x, y, ...)

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

Arguments

`formula`	A formula of the form `class ~ x1 + x2 + ...`
`data`	Data frame from which variables specified in `formula` are preferentially to be taken.
`weights`	(case) weights for each example – if missing defaults to 1.
`subset`	An index vector specifying the cases to be used in the training sample. (NOTE: If given, this argument must be named.)
`na.action`	A function to specify the action to be taken if `NA`s are found. The default action is for the procedure to fail. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable. (NOTE: If given, this argument must be named.)
`contrasts`	a list of contrasts to be used for some or all of the factors appearing as variables in the model formula.
`...`	arguments passed to `fastICA`
`x`	matrix or data frame of `x` values for examples.
`y`	matrix or data frame of target values for examples.
`object`	an object of class `icr` as returned by `icr`.
`newdata`	matrix or data frame of test examples.

Details

This produces a model analogous to Principal Components Regression (PCR) but uses Independent Component Analysis (ICA) to produce the scores. The user must specify a value of `n.comp` to pass to `fastICA`.

The function `preProcess` to produce the ICA scores for the original data and for `newdata`.

Value

For `icr`, a list with elements

`model`	the results of `lm` after the ICA transformation
`ica`	pre-processing information
`n.comp`	number of ICA components
`names`	column names of the original data

Author(s)

Max Kuhn

See Also

`fastICA`, `preProcess`, `lm`

Examples

```
data(BloodBrain)

icrFit <- icr(bbbDescr, logBBB, n.comp = 5)

icrFit

predict(icrFit, bbbDescr[1:5,])
```

`index2vec` *Convert indicies to a binary vector*

Description

The function performs the opposite of `which` converting a set of integers to a binary vector

Usage

```
index2vec(x, vars, sign = FALSE)
```

Arguments

x	a vector of integers
vars	the number of possible locations
sign	a lgical; when true the data are encoded as -1/+1, and 0/1 otherwise

Value

a numeric vector

Author(s)

Max Kuhn

Examples

```
index2vec(x = 1:2, vars = 5)
index2vec(x = 1:2, vars = 5, sign = TRUE)
```

---

knn3 *k-Nearest Neighbour Classification*

Description

k-nearest neighbour classification that can return class votes for all classes.

Usage

```
## S3 method for class 'formula'
knn3(formula, data, subset, na.action, k = 5, ...)

## S3 method for class 'matrix'
knn3(x, y, k = 5, ...)

## S3 method for class 'data.frame'
knn3(x, y, k = 5, ...)

knn3Train(train, test, cl, k=1, l=0, prob = TRUE, use.all=TRUE)
```

Arguments

formula	a formula of the form `lhs ~ rhs` where `lhs` is the response variable and `rhs` a set of predictors.
data	optional data frame containing the variables in the model formula.
subset	optional vector specifying a subset of observations to be used.
na.action	function which indicates what should happen when the data contain `NA`s.

k	number of neighbours considered.
x	a matrix of training set predictors
y	a factor vector of training set classes
...	additional parameters to pass to knn3Train. However, passing prob = FALSE will be over–ridden.
train	matrix or data frame of training set cases.
test	matrix or data frame of test set cases. A vector will be interpreted as a row vector for a single case.
cl	factor of true classifications of training set
l	minimum vote for definite decision, otherwise doubt. (More precisely, less than k-l dissenting votes are allowed, even if k is increased by ties.)
prob	If this is true, the proportion of the votes for each class are returned as attribute prob.
use.all	controls handling of ties. If true, all distances equal to the kth largest are included. If false, a random selection of distances equal to the kth is chosen to use exactly k neighbours.

Details

knn3 is essentially the same code as ipredknn and knn3Train is a copy of knn. The underlying C code from the class package has been modified to return the vote percentages for each class (previously the percentage for the winning class was returned).

Value

An object of class knn3. See predict.knn3.

Author(s)

knn by W. N. Venables and B. D. Ripley and ipredknn by Torsten.Hothorn <Torsten.Hothorn@rzmail.uni-erlangen.de>, modifications by Max Kuhn and Andre Williams

Examples

```
irisFit1 <- knn3(Species ~ ., iris)

irisFit2 <- knn3(as.matrix(iris[, -5]), iris[,5])

data(iris3)
train <- rbind(iris3[1:25,,1], iris3[1:25,,2], iris3[1:25,,3])
test <- rbind(iris3[26:50,,1], iris3[26:50,,2], iris3[26:50,,3])
cl <- factor(c(rep("s",25), rep("c",25), rep("v",25)))
knn3Train(train, test, cl, k = 5, prob = TRUE)
```

knnreg *k-Nearest Neighbour Regression*

Description

k-nearest neighbour regression that can return the average value for the neighbours.

Usage

```
## Default S3 method:
knnreg(x, ...)

## S3 method for class 'formula'
knnreg(formula, data, subset, na.action, k = 5, ...)

## S3 method for class 'matrix'
knnreg(x, y, k = 5, ...)

## S3 method for class 'data.frame'
knnreg(x, y, k = 5, ...)

knnregTrain(train, test, y, k = 5, use.all=TRUE)
```

Arguments

formula	a formula of the form `lhs ~ rhs` where `lhs` is the response variable and `rhs` a set of predictors.
data	optional data frame containing the variables in the model formula.
subset	optional vector specifying a subset of observations to be used.
na.action	function which indicates what should happen when the data contain `NA`s.
k	number of neighbours considered.
x	a matrix or data frame of training set predictors.
y	a numeric vector of outcomes.
...	additional parameters to pass to `knnregTrain`.
train	matrix or data frame of training set cases.
test	matrix or data frame of test set cases. A vector will be interpreted as a row vector for a single case.
use.all	controls handling of ties. If true, all distances equal to the `k`th largest are included. If false, a random selection of distances equal to the `k`th is chosen to use exactly `k` neighbours.

Details

knnreg is similar to ipredknn and knnregTrain is a modification of knn. The underlying C code from the class package has been modified to return average outcome.

Value

An object of class knnreg. See predict.knnreg.

Author(s)

knn by W. N. Venables and B. D. Ripley and ipredknn by Torsten.Hothorn <Torsten.Hothorn@rzmail.uni-erlangen.de>, modifications by Max Kuhn and Chris Keefer

Examples

```
data(BloodBrain)

inTrain <- createDataPartition(logBBB, p = .8)[[1]]

trainX <- bbbDescr[inTrain,]
trainY <- logBBB[inTrain]

testX <- bbbDescr[-inTrain,]
testY <- logBBB[-inTrain]

fit <- knnreg(trainX, trainY, k = 3)

plot(testY, predict(fit, testX))
```

---

lattice.rfe *Lattice functions for plotting resampling results of recursive feature selection*

Description

A set of lattice functions are provided to plot the resampled performance estimates (e.g. classification accuracy, RMSE) over different subset sizes.

Usage

```
## S3 method for class 'rfe'
histogram(x, data = NULL, metric = x$metric, ...)

## S3 method for class 'rfe'
densityplot(x, data = NULL, metric = x$metric, ...)

## S3 method for class 'rfe'
xyplot(x, data = NULL, metric = x$metric, ...)
```

```
## S3 method for class 'rfe'
stripplot(x, data = NULL, metric = x$metric, ...)
```

Arguments

x	An object produced by rfe
data	This argument is not used
metric	A character string specifying the single performance metric that will be plotted
...	arguments to pass to either histogram, densityplot, xyplot or stripplot

Details

By default, only the resampling results for the optimal model are saved in the rfe object. The function rfeControl can be used to save all the results using the returnResamp argument.

If leave-one-out or out-of-bag resampling was specified, plots cannot be produced (see the method argument of rfeControl)

Value

A lattice plot object

Author(s)

Max Kuhn

See Also

rfe, rfeControl, histogram, densityplot, xyplot, stripplot

Examples

```
## Not run:
library(mlbench)
n <- 100
p <- 40
sigma <- 1
set.seed(1)
sim <- mlbench.friedman1(n, sd = sigma)
x <- cbind(sim$x,  matrix(rnorm(n * p), nrow = n))
y <- sim$y
colnames(x) <- paste("var", 1:ncol(x), sep = "")

normalization <- preProcess(x)
x <- predict(normalization, x)
x <- as.data.frame(x)
subsets <- c(10, 15, 20, 25)

ctrl <- rfeControl(
                   functions = lmFuncs,
```

```
                    method = "cv",
                    verbose = FALSE,
                    returnResamp = "all")

lmProfile <- rfe(x, y,
                 sizes = subsets,
                 rfeControl = ctrl)
xyplot(lmProfile)
stripplot(lmProfile)

histogram(lmProfile)
densityplot(lmProfile)

## End(Not run)
```

`lift` *Lift Plot*

Description

For classification models, this function creates a 'lift plot' that describes how well a model ranks samples for one class

Usage

```
lift(x, ...)

## S3 method for class 'formula'
lift(x, data = NULL, class = NULL,
     subset = TRUE, lattice.options = NULL, labels = NULL,
     ...)

## S3 method for class 'lift'
xyplot(x, data, plot = "gain", values = NULL, ...)
```

Arguments

`x`	a `lattice` formula (see `xyplot` for syntax) where the left-hand side of the formula is a factor class variable of the observed outcome and the right-hand side specifies one or model columns corresponding to a numeric ranking variable for a model (e.g. class probabilities). The classification variable should have two levels.
`data`	For `lift.formula`, a data frame (or more precisely, anything that is a valid `envir` argument in `eval`, e.g., a list or an environment) containing values for any variables in the formula, as well as `groups` and `subset` if applicable. If not found in `data`, or if `data` is unspecified, the variables are looked for in the environment of the formula. This argument is not used for `xyplot.lift`.

`class`	a character string for the class of interest
`subset`	An expression that evaluates to a logical or integer indexing vector. It is evaluated in `data`. Only the resulting rows of `data` are used for the plot.
`lattice.options`	A list that could be supplied to `lattice.options`
`labels`	A named list of labels for keys. The list should have an element for each term on the right-hand side of the formula and the names should match the names of the models.
`plot`	Either "gain" (the default) or "lift". The former plots the number of samples called events versus the event rate while the latter shows the event cut-off versus the lift statistic.
`values`	A vector of numbers between 0 and 100 specifying reference values for the percentage of samples found (i.e. the y-axis). Corresponding points on the x-axis are found via interpolation and line segments are shown to indicate how many samples must be tested before these percentages are found. The lines use either the `plot.line` or `superpose.line` component of the current lattice theme to draw the lines (depending on whether groups were used. These values are only used when `type = "gain"`.
`...`	options to pass through to `xyplot` or the panel function (not used in `lift.formula`).

Details

`lift.formula` is used to process the data and `xyplot.lift` is used to create the plot.

To construct data for the the lift and gain plots, the following steps are used for each model:

1. The data are ordered by the numeric model prediction used on the right-hand side of the model formula
2. Each unique value of the score is treated as a cut point
3. The number of samples with true results equal to `class` are determined
4. The lift is calculated as the ratio of the percentage of samples in each split corresponding to `class` over the same percentage in the entire data set

`lift` with `plot = "gain"` produces a plot of the cumulative lift values by the percentage of samples evaluated while `plot = "lift"` shows the cut point value versus the lift statistic.

This implementation uses the **lattice** function `xyplot`, so plot elements can be changed via panel functions, `trellis.par.set` or other means. `lift` uses the panel function `panel.lift2` by default, but it can be changes using `update.trellis` (see the examples in `panel.lift2`).

The following elements are set by default in the plot but can be changed by passing new values into `xyplot.lift`: `xlab = "% Samples Tested"`, `ylab = "% Samples Found"`, `type = "S"`, `ylim = extendrange(c(0, 100))` and `xlim = extendrange(c(0, 100))`.

Value

`lift.formula` returns a list with elements:

`data`	the data used for plotting

cuts	the number of cuts
class	the event class
probNames	the names of the model probabilities
pct	the baseline event rate

xyplot.lift returns a **lattice** object

Author(s)

Max Kuhn, some **lattice** code and documentation by Deepayan Sarkar

See Also

xyplot, trellis.par.set

Examples

```
set.seed(1)
simulated <- data.frame(obs = factor(rep(letters[1:2], each = 100)),
                        perfect = sort(runif(200), decreasing = TRUE),
                        random = runif(200))

lift1 <- lift(obs ~ random, data = simulated)
lift1
xyplot(lift1)

lift2 <- lift(obs ~ random + perfect, data = simulated)
lift2
xyplot(lift2, auto.key = list(columns = 2))

xyplot(lift2, auto.key = list(columns = 2), value = c(10, 30))

xyplot(lift2, plot = "lift", auto.key = list(columns = 2))
```

---

maxDissim *Maximum Dissimilarity Sampling*

Description

Functions to create a sub-sample by maximizing the dissimilarity between new samples and the existing subset.

Usage

```
maxDissim(a, b, n = 2, obj = minDiss, useNames = FALSE,
          randomFrac = 1, verbose = FALSE, ...)
minDiss(u)
sumDiss(u)
```

Arguments

a	a matrix or data frame of samples to start
b	a matrix or data frame of samples to sample from
n	the size of the sub-sample
obj	an objective function to measure overall dissimilarity
useNames	a logical: should the function return the row names (as opposed ot the row index)
randomFrac	a number in (0, 1] that can be used to sub-sample from the remaining candidate values
verbose	a logical; should each step be printed?
...	optional arguments to pass to dist
u	a vector of dissimilarities

Details

Given an initial set of m samples and a larger pool of n samples, this function iteratively adds points to the smaller set by finding with of the n samples is most dissimilar to the initial set. The argument obj measures the overall dissimilarity between the initial set and a candidate point. For example, maximizing the minimum or the sum of the m dissimilarities are two common approaches.

This algorithm tends to select points on the edge of the data mainstream and will reliably select outliers. To select more samples towards the interior of the data set, set randomFrac to be small (see the examples below).

Value

a vector of integers or row names (depending on useNames) corresponding to the rows of b that comprise the sub-sample.

Author(s)

Max Kuhn <max.kuhn@pfizer.com>

References

Willett, P. (1999), "Dissimilarity-Based Algorithms for Selecting Structurally Diverse Sets of Compounds," *Journal of Computational Biology*, 6, 447-457.

See Also

dist

Examples

```
example <- function(pct = 1, obj = minDiss, ...)
{
  tmp <- matrix(rnorm(200 * 2), nrow = 200)
```

```
  ## start with 15 data points
  start <- sample(1:dim(tmp)[1], 15)
  base <- tmp[start,]
  pool <- tmp[-start,]

  ## select 9 for addition
  newSamp <- maxDissim(
                       base, pool,
                       n = 9,
                       randomFrac = pct, obj = obj, ...)

  allSamp <- c(start, newSamp)

  plot(
       tmp[-newSamp,],
       xlim = extendrange(tmp[,1]), ylim = extendrange(tmp[,2]),
       col = "darkgrey",
       xlab = "variable 1", ylab = "variable 2")
  points(base, pch = 16, cex = .7)

  for(i in seq(along = newSamp))
    points(
           pool[newSamp[i],1],
           pool[newSamp[i],2],
           pch = paste(i), col = "darkred")
}

par(mfrow=c(2,2))

set.seed(414)
example(1, minDiss)
title("No Random Sampling, Min Score")

set.seed(414)
example(.1, minDiss)
title("10 Pct Random Sampling, Min Score")

set.seed(414)
example(1, sumDiss)
title("No Random Sampling, Sum Score")

set.seed(414)
example(.1, sumDiss)
title("10 Pct Random Sampling, Sum Score")
```

---

mdrr *Multidrug Resistance Reversal (MDRR) Agent Data*

Description

Svetnik et al. (2003) describe these data: "Bakken and Jurs studied a set of compounds originally discussed by Klopman et al., who were interested in multidrug resistance reversal (MDRR) agents. The original response variable is a ratio measuring the ability of a compound to reverse a leukemia cell's resistance to adriamycin. However, the problem was treated as a classification problem, and compounds with the ratio >4.2 were considered active, and those with the ratio <= 2.0 were considered inactive. Compounds with the ratio between these two cutoffs were called moderate and removed from the data for twoclass classification, leaving a set of 528 compounds (298 actives and 230 inactives). (Various other arrangements of these data were examined by Bakken and Jurs, but we will focus on this particular one.) We did not have access to the original descriptors, but we generated a set of 342 descriptors of three different types that should be similar to the original descriptors, using the DRAGON software."

The data and R code are in the Supplemental Data file for the article.

Usage

```
data(mdrr)
```

Value

`mdrrDescr`	the descriptors
`mdrrClass`	the categorical outcome ("Active" or "Inactive")

Source

Svetnik, V., Liaw, A., Tong, C., Culberson, J. C., Sheridan, R. P. Feuston, B. P (2003). Random Forest: A Classification and Regression Tool for Compound Classification and QSAR Modeling, *Journal of Chemical Information and Computer Sciences*, Vol. 43, pg. 1947-1958.

`modelLookup` *Tools for Models Available in* `train`

Description

These function show information about models and packages that are accessible via `train`

Usage

```
modelLookup(model = NULL)

getModelInfo(model = NULL, regex = TRUE, ...)

checkInstall(pkg)
```

Arguments

model	a character string associated with the method argument of train. If no value is passed, all models are returned. For getModelInfo, regular expressions can be used.
regex	a logical: should a regular expressions be used? If FALSE, a simple match is conducted against the whole name of the model.
pkg	a character string of package names.
...	options to pass to grepl

Details

modelLookup is good for getting information related to the tuning parameters for a model. getModelInfo will return all the functions and metadata associated with a model. Both of these functions will only search within the models bundled in this package.

checkInstall will check to see if packages are installed. If they are not and the session is interactive, an option is given to install the packages using install.packages using that functions default arguments (the missing packages are listed if you would like to install them with other options). If the session is not interactive, an error is thrown.

Value

modelLookup produces a data frame with columns

model	a character string for the model code
parameter	the tuning parameter name
label	a tuning parameter label (used in plots)
forReg	a logical; can the model be used for regression?
forClass	a logical; can the model be used for classification?
probModel	a logical; does the model produce class probabilities?

getModelInfo returns a list containing one or more lists of the standard model information.

checkInstall returns not value.

Note

The column seq is no longer included in the output of modelLookup.

Author(s)

Max Kuhn

See Also

train, install.packages, grepl

Examples

```
modelLookup()
modelLookup("gbm")

getModelInfo("pls")
getModelInfo("^pls")
getModelInfo("pls", regex = FALSE)

## Not run:
checkInstall(getModelInfo("pls")$library)

## End(Not run)
```

---

nearZeroVar *Identification of near zero variance predictors*

Description

nearZeroVar diagnoses predictors that have one unique value (i.e. are zero variance predictors) or predictors that are have both of the following characteristics: they have very few unique values relative to the number of samples and the ratio of the frequency of the most common value to the frequency of the second most common value is large. checkConditionalX looks at the distribution of the columns of x conditioned on the levels of y and identifies columns of x that are sparse within groups of y.

Usage

```
nearZeroVar(x, freqCut = 95/5, uniqueCut = 10, saveMetrics = FALSE,
            foreach = FALSE, allowParallel = TRUE)
nzv(x, freqCut = 95/5, uniqueCut = 10, saveMetrics = FALSE)

checkConditionalX(x, y)
checkResamples(index, x, y)
```

Arguments

x	a numeric vector or matrix, or a data frame with all numeric data
freqCut	the cutoff for the ratio of the most common value to the second most common value
uniqueCut	the cutoff for the percentage of distinct values out of the number of total samples
saveMetrics	a logical. If false, the positions of the zero- or near-zero predictors is returned. If true, a data frame with predictor information is returned.
y	a factor vector with at least two levels
index	a list. Each element corresponds to the training set samples in x for a given resample

foreach	should the **foreach** package be used for the computations? If TRUE, less memory should be used.
allowParallel	should the parallel processing via the **foreach** package be used for the computations? If TRUE, more memory will be used but execution time should be shorter.

Details

For example, an example of near zero variance predictor is one that, for 1000 samples, has two distinct values and 999 of them are a single value.

To be flagged, first the frequency of the most prevalent value over the second most frequent value (called the "frequency ratio") must be above freqCut. Secondly, the "percent of unique values," the number of unique values divided by the total number of samples (times 100), must also be below uniqueCut.

In the above example, the frequency ratio is 999 and the unique value percentage is 0.0001.

Checking the conditional distribution of x may be needed for some models, such as naive Bayes where the conditional distributions should have at least one data point within a class.

nzv is the original version of the function.

Value

For nearZeroVar: if saveMetrics = FALSE, a vector of integers corresponding to the column positions of the problematic predictors. If saveMetrics = TRUE, a data frame with columns:

freqRatio	the ratio of frequencies for the most common value over the second most common value
percentUnique	the percentage of unique data points out of the total number of data points
zeroVar	a vector of logicals for whether the predictor has only one distinct value
nzv	a vector of logicals for whether the predictor is a near zero variance predictor

For checkResamples or checkConditionalX, a vector of column indicators for predictors with empty conditional distributions in at least one class of y.

Author(s)

Max Kuhn, with speed improvements to nearZeroVar by Allan Engelhardt

Examples

```
nearZeroVar(iris[, -5], saveMetrics = TRUE)

data(BloodBrain)
nearZeroVar(bbbDescr)


set.seed(1)
classes <- factor(rep(letters[1:3], each = 30))
x <- data.frame(x1 = rep(c(0, 1), 45),
                x2 = c(rep(0, 10), rep(1, 80)))
```

```
lapply(x, table, y = classes)
checkConditionalX(x, classes)

folds <- createFolds(classes, k = 3, returnTrain = TRUE)
x$x3 <- x$x1
x$x3[folds[[1]]] <- 0

checkResamples(folds, x, classes)
```

`nullModel` *Fit a simple, non-informative model*

Description

Fit a single mean or largest class model

Usage

```
nullModel(x, ...)

## Default S3 method:
nullModel(x = NULL, y, ...)

## S3 method for class 'nullModel'
predict(object, newdata = NULL, type = NULL, ...)
```

Arguments

`x`	An optional matrix or data frame of predictors. These values are not used in the model fit
`y`	A numeric vector (for regression) or factor (for classification) of outcomes
`...`	Optional arguments (not yet used)
`object`	An object of class `nullModel`
`newdata`	A matrix or data frame of predictors (only used to determine the number of predictions to return)
`type`	Either "raw" (for regression), "class" or "prob" (for classification)

Details

`nullModel` emulates other model building functions, but returns the simplest model possible given a training set: a single mean for numeric outcomes and the most prevalent class for factor outcomes. When class probabilities are requested, the percentage of the training set samples with the most prevalent class is returned.

Value

The output of `nullModel` is a list of class `nullModel` with elements

`call`	the function call
`value`	the mean of `y` or the most prevalent class
`levels`	when `y` is a factor, a vector of levels. `NULL` otherwise
`pct`	when `y` is a factor, a data frame with a column for each class (`NULL` otherwise). The column for the most prevalent class has the proportion of the training samples with that class (the other columns are zero).
`n`	the number of elements in `y`

`predict.nullModel` returns a either a factor or numeric vector depending on the class of `y`. All predictions are always the same.

Examples

```
outcome <- factor(sample(letters[1:2],
                         size = 100,
                         prob = c(.1, .9),
                         replace = TRUE))
useless <- nullModel(y = outcome)
useless
predict(useless, matrix(NA, nrow = 10))
```

---

oil *Fatty acid composition of commercial oils*

Description

Fatty acid concentrations of commercial oils were measured using gas chromatography. The data is used to predict the type of oil. Note that only the known oils are in the data set. Also, the authors state that there are 95 samples of known oils. However, we count 96 in Table 1 (pgs. 33-35).

Usage

```
data(oil)
```

Value

`fattyAcids`	data frame of fatty acid compositions: Palmitic, Stearic, Oleic, Linoleic, Linolenic, Eicosanoic and Eicosenoic. When values fell below the lower limit of the assay (denoted as <X in the paper), the limit was used.
`oilType`	factor of oil types: pumpkin (A), sunflower (B), peanut (C), olive (D), soybean (E), rapeseed (F) and corn (G).

Source

Brodnjak-Voncina et al. (2005). Multivariate data analysis in classification of vegetable oils characterized by the content of fatty acids, *Chemometrics and Intelligent Laboratory Systems*, Vol. 75:31-45.

---

oneSE *Selecting tuning Parameters*

Description

Various functions for setting tuning parameters

Usage

```
best(x, metric, maximize)
oneSE(x, metric, num, maximize)
tolerance(x, metric, tol = 1.5, maximize)
```

Arguments

x	a data frame of tuning parameters and model results, sorted from least complex models to the mst complex
metric	a string that specifies what summary metric will be used to select the optimal model. By default, possible values are "RMSE" and "Rsquared" for regression and "Accuracy" and "Kappa" for classification. If custom performance metrics are used (via the summaryFunction argument in trainControl, the value of metric should match one of the arguments. If it does not, a warning is issued and the first metric given by the summaryFunction is used.
maximize	a logical: should the metric be maximized or minimized?
num	the number of resamples (for oneSE only)
tol	the acceptable percent tolerance (for tolerance only)

Details

These functions can be used by train to select the "optimal" model form a series of models. Each requires the user to select a metric that will be used to judge performance. For regression models, values of "RMSE" and "Rsquared" are applicable. Classification models use either "Accuracy" or "Kappa" (for unbalanced class distributions.

More details on these functions can be found at http://topepo.github.io/caret/training.html#custom.

By default, train uses best.

best simply chooses the tuning parameter associated with the largest (or lowest for "RMSE") performance.

oneSE is a rule in the spirit of the "one standard error" rule of Breiman et al. (1984), who suggest that the tuning parameter associated with eh best performance may over fit. They suggest that the

simplest model within one standard error of the empirically optimal model is the better choice. This assumes that the models can be easily ordered from simplest to most complex (see the Details section below).

`tolerance` takes the simplest model that is within a percent tolerance of the empirically optimal model. For example, if the largest Kappa value is 0.5 and a simpler model within 3 percent is acceptable, we score the other models using `(x - 0.5)/0.5 * 100`. The simplest model whose score is not less than 3 is chosen (in this case, a model with a Kappa value of 0.35 is acceptable).

User–defined functions can also be used. The argument `selectionFunction` in `trainControl` can be used to pass the function directly or to pass the function by name.

Value

an row index

Note

In many cases, it is not very clear how to order the models on simplicity. For simple trees and other models (such as PLS), this is straightforward. However, for others it is not.

For example, many of the boosting models used by **caret** have parameters for the number of boosting iterations and the tree complexity (others may also have a learning rate parameter). In this implementation, we order models on number of iterations, then tree depth. Clearly, this is arguable (please email the author for suggestions though).

For MARS models, they are orders on the degree of the features, then the number of retained terms.

RBF SVM models are ordered first by the cost parameter, then by the kernel parameter while polynomial models are ordered first on polynomial degree, then cost and scale.

Neural networks are ordered by the number of hidden units and then the amount of weight decay.

k–nearest neighbor models are ordered from most neighbors to least (i.e. smoothest to model jagged decision boundaries).

Elastic net models are ordered first n the L1 penalty, then by the L2 penalty.

Author(s)

Max Kuhn

References

Breiman, Friedman, Olshen, and Stone. (1984) *Classification and Regression Trees*. Wadsworth.

See Also

`train`, `trainControl`

Examples

```
## Not run:
# simulate a PLS regression model
test <- data.frame(ncomp = 1:5,
                   RMSE = c(3, 1.1, 1.02, 1, 2),
                   RMSESD = .4)

best(test, "RMSE", maximize = FALSE)
oneSE(test, "RMSE", maximize = FALSE, num = 10)
tolerance(test, "RMSE", tol = 3, maximize = FALSE)

### usage example

data(BloodBrain)

marsGrid <- data.frame(degree = 1, nprune = (1:10) * 3)

set.seed(1)
marsFit <- train(bbbDescr, logBBB,
                 method = "earth",
                 tuneGrid = marsGrid,
                 trControl = trainControl(method = "cv",
                                          number = 10,
                                          selectionFunction = "tolerance"))

# around 18 terms should yield the smallest CV RMSE

## End(Not run)
```

---

panel.lift2 *Lattice Panel Functions for Lift Plots*

Description

Two panel functions that be used in conjunction with `lift`.

Usage

```
panel.lift(x, y, ...)

panel.lift2(x, y, pct = 0, values = NULL, ...)
```

Arguments

x	the percentage of searched to be plotted in the scatterplot
y	the percentage of events found to be plotted in the scatterplot
pct	the baseline percentage of true events in the data

values — A vector of numbers between 0 and 100 specifying reference values for the percentage of samples found (i.e. the y-axis). Corresponding points on the x-axis are found via interpolation and line segments are shown to indicate how many samples must be tested before these percentages are found. The lines use either the `plot.line` or `superpose.line` component of the current lattice theme to draw the lines (depending on whether groups were used

... — options to pass to `panel.xyplot`

Details

`panel.lift` plots the data with a simple (black) 45 degree reference line.

`panel.lift2` is the default for `lift` and plots the data points with a shaded region encompassing the space between to the random model and perfect model trajectories. The color of the region is determined by the lattice `reference.line` information (see example below).

Author(s)

Max Kuhn

See Also

`lift`, `panel.xyplot`, `xyplot`, trellis.par.set

Examples

```
set.seed(1)
simulated <- data.frame(obs = factor(rep(letters[1:2], each = 100)),
                        perfect = sort(runif(200), decreasing = TRUE),
                        random = runif(200))

regionInfo <- trellis.par.get("reference.line")
regionInfo$col <- "lightblue"
trellis.par.set("reference.line", regionInfo)

lift2 <- lift(obs ~ random + perfect, data = simulated)
lift2
xyplot(lift2, auto.key = list(columns = 2))

## use a different panel function
xyplot(lift2, panel = panel.lift)
```

---

panel.needle *Needle Plot Lattice Panel*

Description

A variation of `panel.dotplot` that plots horizontal lines from zero to the data point.

Usage

```
panel.needle(x, y, horizontal = TRUE,
             pch, col, lty, lwd,
             col.line, levels.fos,
             groups = NULL,
             ...)
```

Arguments

x,y	variables to be plotted in the panel. Typically y is the 'factor'
horizontal	logical. If FALSE, the plot is 'transposed' in the sense that the behaviours of x and y are switched. x is now the 'factor'. Interpretation of other arguments change accordingly. See documentation of bwplot for a fuller explanation.
pch, col, lty, lwd, col.line	graphical parameters
levels.fos	locations where reference lines will be drawn
groups	grouping variable (affects graphical parameters)
...	extra parameters, passed to panel.xyplot which is responsible for drawing the foreground points (panel.dotplot only draws the background reference lines).

Details

Creates (possibly grouped) needleplot of x against y or vice versa

Author(s)

Max Kuhn, based on panel.dotplot by Deepayan Sarkar

See Also

dotplot

---

pcaNNet.default *Neural Networks with a Principal Component Step*

Description

Run PCA on a dataset, then use it in a neural network model

Usage

```
## Default S3 method:
pcaNNet(x, y, thresh = 0.99, ...)
## S3 method for class 'formula'
pcaNNet(formula, data, weights, ...,
        thresh = .99, subset, na.action, contrasts = NULL)

## S3 method for class 'pcaNNet'
predict(object, newdata, type = c("raw", "class"), ...)
```

Arguments

formula	A formula of the form `class ~ x1 + x2 + ...`
x	matrix or data frame of `x` values for examples.
y	matrix or data frame of target values for examples.
weights	(case) weights for each example – if missing defaults to 1.
thresh	a threshold for the cumulative proportion of variance to capture from the PCA analysis. For example, to retain enough PCA components to capture 95 percent of variation, set `thresh = .95`
data	Data frame from which variables specified in `formula` are preferentially to be taken.
subset	An index vector specifying the cases to be used in the training sample. (NOTE: If given, this argument must be named.)
na.action	A function to specify the action to be taken if `NA`s are found. The default action is for the procedure to fail. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable. (NOTE: If given, this argument must be named.)
contrasts	a list of contrasts to be used for some or all of the factors appearing as variables in the model formula.
object	an object of class `pcaNNet` as returned by `pcaNNet`.
newdata	matrix or data frame of test examples. A vector is considered to be a row vector comprising a single case.
type	Type of output
...	arguments passed to `nnet`

Details

The function first will run principal component analysis on the data. The cumulative percentage of variance is computed for each principal component. The function uses the `thresh` argument to determine how many components must be retained to capture this amount of variance in the predictors.

The principal components are then used in a neural network model.

When predicting samples, the new data are similarly transformed using the information from the PCA analysis on the training data and then predicted.

Because the variance of each predictor is used in the PCA analysis, the code does a quick check to make sure that each predictor has at least two distinct values. If a predictor has one unique value, it is removed prior to the analysis.

Value

For pcaNNet, an object of "pcaNNet" or "pcaNNet.formula". Items of interest in the output are:

pc	the output from preProcess
model	the model generated from nnet
names	if any predictors had only one distinct value, this is a character string of the remaining columns. Otherwise a value of NULL

Author(s)

These are heavily based on the nnet code from Brian Ripley.

References

Ripley, B. D. (1996) *Pattern Recognition and Neural Networks.* Cambridge.

See Also

nnet, preProcess

Examples

```
data(BloodBrain)
modelFit <- pcaNNet(bbbDescr[, 1:10], logBBB, size = 5, linout = TRUE, trace = FALSE)
modelFit

predict(modelFit, bbbDescr[, 1:10])
```

---

plot.gafs *Plot Method for the gafs and safs Classes*

Description

Plot the performance values versus search iteration

Usage

```
## S3 method for class 'gafs'
plot(x, metric = x$control$metric["external"],
     estimate = c("internal", "external"), output = "ggplot", ...)

## S3 method for class 'safs'
plot(x, metric = x$control$metric["external"],
     estimate = c("internal", "external"), output = "ggplot", ...)
```

Arguments

x	an object of class gafs or safs
metric	the measure of performance to plot (e.g. RMSE, accuracy, etc)
estimate	the type of estimate: either "internal" or "external"
output	either "data", "ggplot" or "lattice"
...	options passed to xyplot

Details

The mean (averaged over the resamples) is plotted against the search iteration using a scatter plot.

When `output = "data"`, the unaveraged data are returned with columns for all the performance metrics and the resample indicator.

Value

Either a data frame, ggplot object or lattice object

Author(s)

Max Kuhn

See Also

gafs, safs, ggplot, xyplot

Examples

```
## Not run:
set.seed(1)
train_data <- twoClassSim(100, noiseVars = 10)
test_data  <- twoClassSim(10,  noiseVars = 10)

## A short example
ctrl <- safsControl(functions = rfSA,
                    method = "cv",
                    number = 3)

rf_search <- safs(x = train_data[, -ncol(train_data)],
                  y = train_data$Class,
                  iters = 50,
                  safsControl = ctrl)

plot(rf_search)
plot(rf_search,
 output = "lattice",
 auto.key = list(columns = 2))

plot_data <- plot(rf_search, output = "data")
summary(plot_data)
```

```
## End(Not run)
```

`plot.rfe` *Plot RFE Performance Profiles*

Description

These functions plot the resampling results for the candidate subset sizes evaluated during the recursive feature elimination (RFE) process

Usage

```
## S3 method for class 'rfe'
plot(x, metric = x$metric,  ...)

## S3 method for class 'rfe'
ggplot(data = NULL, metric = data$metric[1], output = "layered", ...)
```

Arguments

`x`	an object of class `rfe`.
`metric`	What measure of performance to plot. Examples of possible values are "RMSE", "Rsquared", "Accuracy" or "Kappa". Other values can be used depending on what metrics have been calculated.
`...`	`plot` only: specifications to be passed to `xyplot`. The function automatically sets some arguments (e.g. axis labels) but passing in values here will over-ride the defaults.
`data`	an object of class `rfe`.
`output`	either "data", "ggplot" or "layered". The first returns a data frame while the second returns a simple `ggplot` object with no layers. The third value returns a plot with a set of layers.

Details

These plots show the average performance versus the subset sizes.

Value

a lattice or ggplot object

Author(s)

Max Kuhn

References

Kuhn (2008), "Building Predictive Models in R Using the caret" (http://www.jstatsoft.org/v28/i05/)

See Also

rfe, xyplot, ggplot

Examples

```
## Not run:
data(BloodBrain)

x <- scale(bbbDescr[,-nearZeroVar(bbbDescr)])
x <- x[, -findCorrelation(cor(x), .8)]
x <- as.data.frame(x)

set.seed(1)
lmProfile <- rfe(x, logBBB,
                 sizes = c(2:25, 30, 35, 40, 45, 50, 55, 60, 65),
                 rfeControl = rfeControl(functions = lmFuncs,
                                         number = 200))
plot(lmProfile)
plot(lmProfile, metric = "Rsquared")
ggplot(lmProfile)

## End(Not run)
```

---

plot.train *Plot Method for the train Class*

Description

This function takes the output of a train object and creates a line or level plot using the **lattice** or **ggplot2** libraries.

Usage

```
## S3 method for class 'train'
plot(x,
     plotType = "scatter",
     metric = x$metric[1],
     digits = getOption("digits") - 3,
     xTrans = NULL,
     nameInStrip = FALSE,
     ...)

## S3 method for class 'train'
```

```
ggplot(data = NULL,
       metric = data$metric[1],
       plotType = "scatter",
       output = "layered",
       nameInStrip = FALSE,
       ...)
```

Arguments

x	an object of class train.
metric	What measure of performance to plot. Examples of possible values are "RMSE", "Rsquared", "Accuracy" or "Kappa". Other values can be used depending on what metrics have been calculated.
plotType	a string describing the type of plot ("scatter", "level" or "line" (plot only))
digits	an integer specifying the number of significant digits used to label the parameter value.
xTrans	a function that will be used to scale the x-axis in scatter plots.
data	an object of class train.
output	either "data", "ggplot" or "layered". The first returns a data frame while the second returns a simple ggplot object with no layers. The third value returns a plot with a set of layers.
nameInStrip	a logical: if there are more than 2 tuning parameters, should the name and value be included in the panel title?
...	plot only: specifications to be passed to levelplot, xyplot, stripplot (for line plots). The function automatically sets some arguments (e.g. axis labels) but passing in values here will over-ride the defaults

Details

If there are no tuning parameters, or none were varied, an error is produced.

If the model has one tuning parameter with multiple candidate values, a plot is produced showing the profile of the results over the parameter. Also, a plot can be produced if there are multiple tuning parameters but only one is varied.

If there are two tuning parameters with different values, a plot can be produced where a different line is shown for each value of of the other parameter. For three parameters, the same line plot is created within conditioning panels/facets of the other parameter.

Also, with two tuning parameters (with different values), a levelplot (i.e. un-clustered heatmap) can be created. For more than two parameters, this plot is created inside conditioning panels/facets.

Author(s)

Max Kuhn

References

Kuhn (2008), "Building Predictive Models in R Using the caret" (http://www.jstatsoft.org/v28/i05/)

See Also

train, levelplot, xyplot, stripplot, ggplot

Examples

```
## Not run:
library(klaR)
rdaFit <- train(Species ~ .,
                data = iris,
                method = "rda",
                control = trainControl(method = "cv"))
plot(rdaFit)
plot(rdaFit, plotType = "level")

ggplot(rdaFit) + theme_bw()


## End(Not run)
```

---

plot.varImp.train *Plotting variable importance measures*

Description

This function produces lattice plots of objects with class "varImp.train". More info will be forthcoming.

Usage

```
## S3 method for class 'varImp.train'
plot(x, top = dim(x$importance)[1],  ...)
```

Arguments

x	an object with class varImp.
top	a scalar numeric that specifies the number of variables to be displayed (in order of importance)
...	arguments to pass to the lattice plot function (dotplot and panel.needle)

Details

For models where there is only one importance value, such a regression models, a "Pareto-type" plot is produced where the variables are ranked by their importance and a needle-plot is used to show the top variables.

When there is more than one importance value per predictor, the same plot is produced within conditioning panels for each class. The top predictors are sorted by their average importance.

Value

a lattice plot object

Author(s)

Max Kuhn

---

plotClassProbs *Plot Predicted Probabilities in Classification Models*

Description

This function takes an object (preferably from the function `extractProb`) and creates a lattice plot.

If the call to `extractProb` included test data, these data are shown, but if unknowns were also included, these are not plotted

Usage

```
plotClassProbs(object,
               plotType = "histogram",
               useObjects = FALSE,
               ...)
```

Arguments

`object`	an object (preferably from the function `extractProb`. There should be columns for each level of the class factor and columns named `obs`, `pred`, `model` (e.g. "rpart", "nnet" etc), `dataType` (e.g. "Training", "Test" etc) and optionally `objects` (for giving names to objects with the same model type).
`plotType`	either "histogram" or "densityplot"
`useObjects`	a logical; should the object name (if any) be used as a conditioning variable?
`...`	parameters to pass to `histogram` or `densityplot`

Value

A lattice object. Note that the plot has to be printed to be displayed (especially in a loop).

Author(s)

Max Kuhn

Examples

```
## Not run:
data(mdrr)
set.seed(90)
inTrain <- createDataPartition(mdrrClass, p = .5)[[1]]

trainData <- mdrrDescr[inTrain,1:20]
testData <- mdrrDescr[-inTrain,1:20]

trainY <- mdrrClass[inTrain]
testY <- mdrrClass[-inTrain]

ctrl <- trainControl(method = "cv")

nbFit1 <- train(trainData, trainY, "nb",
                trControl = ctrl,
                tuneGrid = data.frame(usekernel = TRUE, fL = 0))

nbFit2 <- train(trainData, trainY, "nb",
                trControl = ctrl,
                tuneGrid = data.frame(usekernel = FALSE, fL = 0))


models <- list(para = nbFit2, nonpara = nbFit1)

predProbs <- extractProb(models, testX = testData,  testY = testY)

plotClassProbs(predProbs, useObjects = TRUE)
plotClassProbs(predProbs,
               subset = object == "para" & dataType == "Test")
plotClassProbs(predProbs,
               useObjects = TRUE,
               plotType = "densityplot",
               auto.key = list(columns = 2))

## End(Not run)
```

`plotObsVsPred` *Plot Observed versus Predicted Results in Regression and Classification Models*

Description

This function takes an object (preferably from the function extractPrediction) and creates a lattice plot. For numeric outcomes, the observed and predicted data are plotted with a 45 degree reference line and a smoothed fit. For factor outcomes, a dotplot plot is produced with the accuracies for the different models.

If the call to extractPrediction included test data, these data are shown, but if unknowns were also included, they are not plotted

Usage

```
plotObsVsPred(object, equalRanges = TRUE, ...)
```

Arguments

object	an object (preferably from the function extractPrediction. There should be columns named obs, pred, model (e.g. "rpart", "nnet" etc.) and dataType (e.g. "Training", "Test" etc)
equalRanges	a logical; should the x- and y-axis ranges be the same?
...	parameters to pass to xyplot or dotplot, such as auto.key

Value

A lattice object. Note that the plot has to be printed to be displayed (especially in a loop).

Author(s)

Max Kuhn

Examples

```
## Not run:
# regression example
data(BostonHousing)
rpartFit <- train(BostonHousing[1:100, -c(4, 14)],
                  BostonHousing$medv[1:100],
                  "rpart", tuneLength = 9)
plsFit <- train(BostonHousing[1:100, -c(4, 14)],
                BostonHousing$medv[1:100],
                "pls")

predVals <- extractPrediction(list(rpartFit, plsFit),
                              testX = BostonHousing[101:200, -c(4, 14)],
                              testY = BostonHousing$medv[101:200],
                              unkX = BostonHousing[201:300, -c(4, 14)])

plotObsVsPred(predVals)


#classification example
data(Satellite)
```

```
numSamples <- dim(Satellite)[1]
set.seed(716)

varIndex <- 1:numSamples

trainSamples <- sample(varIndex, 150)

varIndex <- (1:numSamples)[-trainSamples]
testSamples <- sample(varIndex, 100)

varIndex <- (1:numSamples)[-c(testSamples, trainSamples)]
unkSamples <- sample(varIndex, 50)

trainX <- Satellite[trainSamples, -37]
trainY <- Satellite[trainSamples, 37]

testX <- Satellite[testSamples, -37]
testY <- Satellite[testSamples, 37]

unkX <- Satellite[unkSamples, -37]

knnFit  <- train(trainX, trainY, "knn")
rpartFit <- train(trainX, trainY, "rpart")

predTargets <- extractPrediction(list(knnFit, rpartFit),
                                 testX = testX,
                                 testY = testY,
                                 unkX = unkX)

plotObsVsPred(predTargets)

## End(Not run)
```

---

plsda *Partial Least Squares and Sparse Partial Least Squares Discriminant Analysis*

Description

plsda is used to fit standard PLS models for classification while splsda performs sparse PLS that embeds feature selection and regularization for the same purpose.

Usage

```
plsda(x, ...)

## Default S3 method:
plsda(x,  y, ncomp = 2, probMethod = "softmax", prior = NULL, ...)

## S3 method for class 'plsda'
```

```
predict(object, newdata = NULL, ncomp = NULL, type = "class", ...)

splsda(x, ...)

## Default S3 method:
splsda(x, y, probMethod = "softmax", prior = NULL, ...)

## S3 method for class 'splsda'
predict(object, newdata = NULL, type = "class", ...)
```

Arguments

x	a matrix or data frame of predictors
y	a factor or indicator matrix for the discrete outcome. If a matrix, the entries must be either 0 or 1 and rows must sum to one
ncomp	the number of components to include in the model. Predictions can be made for models with values less than ncomp.
probMethod	either "softmax" or "Bayes" (see Details)
prior	a vector or prior probabilities for the classes (only used for probeMethod = "Bayes")
...	arguments to pass to plsr or spls. For splsda, this is the method for passing tuning parameters specifications (e.g. K, eta or kappa)
object	an object produced by plsda
newdata	a matrix or data frame of predictors
type	either "class", "prob" or "raw" to produce the predicted class, class probabilities or the raw model scores, respectively.

Details

If a factor is supplied, the appropriate indicator matrix is created.

A multivariate PLS model is fit to the indicator matrix using the plsr or spls function.

Two prediction methods can be used.

The **softmax function** transforms the model predictions to "probability-like" values (e.g. on [0, 1] and sum to 1). The class with the largest class probability is the predicted class.

Also, **Bayes rule** can be applied to the model predictions to form posterior probabilities. Here, the model predictions for the training set are used along with the training set outcomes to create conditional distributions for each class. When new samples are predicted, the raw model predictions are run through these conditional distributions to produce a posterior probability for each class (along with the prior). This process is repeated ncomp times for every possible PLS model. The NaiveBayes function is used with usekernel = TRUE for the posterior probability calculations.

Value

For plsda, an object of class "plsda" and "mvr". For splsda, an object of class splsda.

The predict methods produce either a vector, matrix or three-dimensional array, depending on the values of type of ncomp. For example, specifying more than one value of ncomp with type = "class" with produce a three dimensional array but the default specification would produce a factor vector.

See Also

plsr, spls

Examples

```
## Not run:
data(mdrr)
set.seed(1)
inTrain <- sample(seq(along = mdrrClass), 450)

nzv <- nearZeroVar(mdrrDescr)
filteredDescr <- mdrrDescr[, -nzv]

training <- filteredDescr[inTrain,]
test <- filteredDescr[-inTrain,]
trainMDRR <- mdrrClass[inTrain]
testMDRR <- mdrrClass[-inTrain]

preProcValues <- preProcess(training)

trainDescr <- predict(preProcValues, training)
testDescr <- predict(preProcValues, test)

useBayes   <- plsda(trainDescr, trainMDRR, ncomp = 5,
                    probMethod = "Bayes")
useSoftmax <- plsda(trainDescr, trainMDRR, ncomp = 5)

confusionMatrix(predict(useBayes, testDescr),
                testMDRR)

confusionMatrix(predict(useSoftmax, testDescr),
                testMDRR)

histogram(~predict(useBayes, testDescr, type = "prob")[,"Active",]
          | testMDRR, xlab = "Active Prob", xlim = c(-.1,1.1))
histogram(~predict(useSoftmax, testDescr, type = "prob")[,"Active",]
          | testMDRR, xlab = "Active Prob", xlim = c(-.1,1.1))


## different sized objects are returned
length(predict(useBayes, testDescr))
dim(predict(useBayes, testDescr, ncomp = 1:3))
dim(predict(useBayes, testDescr, type = "prob"))
dim(predict(useBayes, testDescr, type = "prob", ncomp = 1:3))

## Using spls:
## (As of 11/09, the spls package now has a similar function with
## the same mane. To avoid conflicts, use caret:::splsda to
## get this version)

splsFit <- caret:::splsda(trainDescr, trainMDRR,
                          K = 5, eta = .9,
```

```
                          probMethod = "Bayes")

confusionMatrix(caret:::predict.splsda(splsFit, testDescr),
                testMDRR)

## End(Not run)
```

---

postResample *Calculates performance across resamples*

Description

Given two numeric vectors of data, the mean squared error and R-squared are calculated. For two factors, the overall agreement rate and Kappa are determined.

Usage

```
postResample(pred, obs)
defaultSummary(data, lev = NULL, model = NULL)

twoClassSummary(data, lev = NULL, model = NULL)

R2(pred, obs, formula = "corr", na.rm = FALSE)
RMSE(pred, obs, na.rm = FALSE)

getTrainPerf(x)
```

Arguments

pred	A vector of numeric data (could be a factor)
obs	A vector of numeric data (could be a factor)
data	a data frame or matrix with columns obs and pred for the observed and predicted outcomes. For twoClassSummary, columns should also include predicted probabilities for each class. See the classProbs argument to trainControl
lev	a character vector of factors levels for the response. In regression cases, this would be NULL.
model	a character string for the model name (as taken form the method argument of train.
formula	which R^2 formula should be used? Either "corr" or "traditional". See Kvalseth (1985) for a summary of the different equations.
na.rm	a logical value indicating whether NA values should be stripped before the computation proceeds.
x	an object of class train.

Details

postResample is meant to be used with apply across a matrix. For numeric data the code checks to see if the standard deviation of either vector is zero. If so, the correlation between those samples is assigned a value of zero. NA values are ignored everywhere.

Note that many models have more predictors (or parameters) than data points, so the typical mean squared error denominator (n - p) does not apply. Root mean squared error is calculated using sqrt(mean((pred - obs)^2. Also, R^2 is calculated wither using as the square of the correlation between the observed and predicted outcomes when form = "corr". when form = "traditional",

$$R^2 = 1 - \frac{\sum(y_i - \hat{y}_i)^2}{\sum(y_i - \bar{y}_i)^2}$$

For defaultSummary is the default function to compute performance metrics in train. It is a wrapper around postResample.

twoClassSummary computes sensitivity, specificity and the area under the ROC curve. To use this function, the classProbs argument of trainControl should be TRUE.

Other functions can be used via the summaryFunction argument of trainControl. Custom functions must have the same arguments asdefaultSummary.

The function getTrainPerf returns a one row data frame with the resampling results for the chosen model. The statistics will have the prefix "Train" (i.e. "TrainROC"). There is also a column called "method" that echoes the argument of the call to trainControl of the same name.

Value

A vector of performance estimates.

Author(s)

Max Kuhn

References

Kvalseth. Cautionary note about R^2. American Statistician (1985) vol. 39 (4) pp. 279-285

See Also

trainControl

Examples

```
predicted <-  matrix(rnorm(50), ncol = 5)
observed <- rnorm(10)
apply(predicted, 2, postResample, obs = observed)
```

pottery *Pottery from Pre-Classical Sites in Italy*

Description

Measurements of 58 pottery samples.

Usage

```
data(pottery)
```

Value

`pottery`	11 elemental composition measurements
`potteryClass`	factor of pottery type: black carbon containing bulks (A) and clayey (B)

Source

R. G. Brereton (2003). *Chemometrics: Data Analysis for the Laboratory and Chemical Plant*, pg. 261.

prcomp.resamples *Principal Components Analysis of Resampling Results*

Description

Performs a principal components analysis on an object of class `resamples` and returns the results as an object with classes `prcomp.resamples` and `prcomp`.

Usage

```
## S3 method for class 'resamples'
prcomp(x, metric = x$metrics[1], ...)

cluster(x, ...)
## S3 method for class 'resamples'
cluster(x, metric = x$metrics[1], ...)

## S3 method for class 'prcomp.resamples'
plot(x, what = "scree", dims = max(2, ncol(x$rotation)), ...)
```

Arguments

x	For prcomp, an object of class resamples and for plot.prcomp.resamples, an object of class plot.prcomp.resamples
metric	a performance metric that was estimated for every resample
what	the type of plot: "scree" produces a bar chart of standard deviations, "cumulative" produces a bar chart of the cumulative percent of variance, "loadings" produces a scatterplot matrix of the loading values and "components" produces a scatterplot matrix of the PCA components
dims	The number of dimensions to plot when what = "loadings" or what = "components"
...	For prcomp.resamples, options to pass to prcomp, for plot.prcomp.resamples, options to pass to Lattice objects (see Details below) and, for cluster.resamples, options to pass to hclust.

Details

The principal components analysis treats the models as variables and the resamples are realizations of the variables. In this way, we can use PCA to "cluster" the assays and look for similarities. Most of the methods for prcomp can be used, although custom print and plot methods are used.

The plot method uses lattice graphics. When what = "scree" or what = "cumulative", barchart is used. When what = "loadings" or what = "components", either xyplot or splom are used (the latter when dims > 2). Options can be passed to these methods using ....

When what = "loadings" or what = "components", the plots are put on a common scale so that later components are less likely to be over-interpreted. See Geladi et al. (2003) for examples of why this can be important.

For clustering, hclust is used to determine clusters of models based on the resampled performance values.

Value

For prcomp.resamples, an object with classes prcomp.resamples and prcomp. This object is the same as the object produced by prcomp, but with additional elements:

metric	the value for the metric argument
call	the call

For plot.prcomp.resamples, a Lattice object (see Details above)

Author(s)

Max Kuhn

References

Geladi, P.; Manley, M.; and Lestander, T. (2003), "Scatter plotting in multivariate data analysis," J. Chemometrics, 17: 503-511

See Also

resamples, barchart, xyplot, splom, hclust

Examples

```
## Not run:
#load(url("http://topepo.github.io/caret/exampleModels.RData"))

resamps <- resamples(list(CART = rpartFit,
                          CondInfTree = ctreeFit,
                          MARS = earthFit))
resampPCA <- prcomp(resamps)

resampPCA

plot(resampPCA, what = "scree")

plot(resampPCA, what = "components")

plot(resampPCA, what = "components", dims = 2, auto.key = list(columns = 3))

clustered <- cluster(resamps)
plot(clustered)


## End(Not run)
```

---

predict.bagEarth *Predicted values based on bagged Earth and FDA models*

Description

Predicted values based on bagged Earth and FDA models

Usage

```
## S3 method for class 'bagEarth'
predict(object, newdata = NULL, type = "response", ...)
## S3 method for class 'bagFDA'
predict(object, newdata = NULL, type = "class", ...)
```

Arguments

object	Object of class inheriting from bagEarth
newdata	An optional data frame or matrix in which to look for variables with which to predict. If omitted, the fitted values are used (see note below).

type	The type of prediction. For bagged earth regression model, type = "response" will produce a numeric vector of the usual model predictions. earth also allows the user to fit generalized linear models. In this case, type = "response" produces the inverse link results as a vector. In the case of a binomial generalized linear model, type = "response" produces a vector of probabilities, type = "class" generates a factor vector and type = "prob" produces a two-column matrix with probabilities for both classes (averaged across the individual models). Similarly, for bagged fda models, type = "class" generates a factor vector and type = "probs" outputs a matrix of class probabilities.
...	not used

Value

a vector of predictions

Note

If the predictions for the original training set are needed, there are two ways to calculate them. First, the original data set can be predicted by each bagged earth model. Secondly, the predictions from each bootstrap sample could be used (but are more likely to overfit). If the original call to bagEarth or bagFDA had keepX = TRUE, the first method is used, otherwise the values are calculated via the second method.

Author(s)

Max Kuhn

See Also

bagEarth

Examples

```
## Not run:
data(trees)
## out of bag predictions vs just re-predicting the training set
fit1 <- bagEarth(Volume ~ ., data = trees, keepX = TRUE)
fit2 <- bagEarth(Volume ~ ., data = trees, keepX = FALSE)
hist(predict(fit1) - predict(fit2))

## End(Not run)
```

predict.gafs *Predict new samples*

Description

Predict new samples using safs and gafs objects.

Usage

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

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

Arguments

object	an object of class safs or gafs
newdata	a data frame or matrix of predictors.
...	not currently used

Details

Only the predictors listed in object$optVariables are required.

Value

The type of result depends on what was specified in object$control$functions$predict.

Author(s)

Max Kuhn

See Also

safs, gafs

Examples

```
## Not run:

set.seed(1)
train_data <- twoClassSim(100, noiseVars = 10)
test_data  <- twoClassSim(10,  noiseVars = 10)

## A short example
ctrl <- safsControl(functions = rfSA,
                    method = "cv",
```

```
                    number = 3)

rf_search <- safs(x = train_data[, -ncol(train_data)],
                  y = train_data$Class,
                  iters = 3,
                  safsControl = ctrl)

rf_search

predict(rf_search, train_data)

## End(Not run)
```

`predict.knn3` *Predictions from k-Nearest Neighbors*

Description

Predict the class of a new observation based on k-NN.

Usage

```
## S3 method for class 'knn3'
predict(object, newdata, type=c("prob", "class"), ...)
```

Arguments

`object`	object of class `knn3`.
`newdata`	a data frame of new observations.
`type`	return either the predicted class or the proportion of the votes for the winning class.
`...`	additional arguments.

Details

This function is a method for the generic function `predict` for class `knn3`. For the details see `knn3`. This is essentially a copy of `predict.ipredknn`.

Value

Either the predicted class or the proportion of the votes for each class.

Author(s)

`predict.ipredknn` by Torsten.Hothorn <Torsten.Hothorn@rzmail.uni-erlangen.de>

predict.knnreg *Predictions from k-Nearest Neighbors Regression Model*

Description

Predict the outcome of a new observation based on k-NN.

Usage

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

Arguments

object	object of class knnreg.
newdata	a data frame or matrix of new observations.
...	additional arguments.

Details

This function is a method for the generic function predict for class knnreg. For the details see knnreg. This is essentially a copy of predict.ipredknn.

Value

a numeric vector

Author(s)

Max Kuhn, Chris Keefer, adapted from knn and predict.ipredknn

predict.train *Extract predictions and class probabilities from train objects*

Description

These functions can be used for a single train object or to loop through a number of train objects to calculate the training and test data predictions and class probabilities.

Usage

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

## S3 method for class 'train'
predict(object, newdata = NULL, type = "raw", na.action = na.omit, ...)

extractPrediction(models,
                  testX = NULL, testY = NULL,
                  unkX = NULL,
                  unkOnly = !is.null(unkX) & is.null(testX),
                  verbose = FALSE)

extractProb(models,
            testX = NULL,  testY = NULL,
            unkX = NULL,
            unkOnly = !is.null(unkX) & is.null(testX),
            verbose = FALSE)
```

Arguments

object	For predict.train, an object of class train. For predict.list, a list of objects of class train.
newdata	an optional set of data to predict on. If NULL, then the original training data are used
type	either "raw" or "prob", for the number/class predictions or class probabilities, respectively. Class probabilities are not available for all classification models
models	a list of objects of the class train. The objects must have been generated with fitBest = FALSE and returnData = TRUE.
na.action	the method for handling missing data
testX	an optional set of data to predict
testY	an optional outcome corresponding to the data given in testX
unkX	another optional set of data to predict without known outcomes
unkOnly	a logical to bypass training and test set predictions. This is useful if speed is needed for unknown samples.
verbose	a logical for printing messages
...	additional arguments to be passed to other methods

Details

These functions are wrappers for the specific prediction functions in each modeling package. In each case, the optimal tuning values given in the tuneValue slot of the finalModel object are used to predict.

To get simple predictions for a new data set, the `predict` function can be used. Limits can be imposed on the range of predictions. See `trainControl` for more information.

To get predictions for a series of models at once, a list of `train` objects can be passes to the `predict` function and a list of model predictions will be returned.

The two extraction functions can be used to get the predictions and observed outcomes at once for the training, test and/or unknown samples at once in a single data frame (instead of a list of just the predictions). These objects can then be passes to `plotObsVsPred` or `plotClassProbs`.

Value

For `predict.train`, a vector of predictions if `type = "raw"` or a data frame of class probabilities for `type = "probs"`. In the latter case, there are columns for each class.

For `predict.list`, a list results. Each element is produced by `predict.train`.

For `extractPrediction`, a data frame with columns:

`obs`	the observed training and test data
`pred`	predicted values
`model`	the type of model used to predict
`object`	the names of the objects within `models`. If `models` is an un-named list, the values of `object` will be "Object1", "Object2" and so on
`dataType`	"Training", "Test" or "Unknown" depending on what was specified

For `extractProb`, a data frame. There is a column for each class containing the probabilities. The remaining columns are the same as above (although the `pred` column is the predicted class)

Author(s)

Max Kuhn

References

Kuhn (2008), "Building Predictive Models in R Using the caret" (http://www.jstatsoft.org/v28/i05/)

See Also

`plotObsVsPred`, `plotClassProbs`, `trainControl`

Examples

```
   ## Not run:

knnFit <- train(Species ~ ., data = iris, method = "knn",
                trControl = trainControl(method = "cv"))

rdaFit <- train(Species ~ ., data = iris, method = "rda",
                trControl = trainControl(method = "cv"))
```

```
predict(knnFit)
predict(knnFit, type = "prob")

bothModels <- list(knn = knnFit,
                   tree = rdaFit)

predict(bothModels)

extractPrediction(bothModels, testX = iris[1:10, -5])
extractProb(bothModels, testX = iris[1:10, -5])

## End(Not run)
```

`predictors` *List predictors used in the model*

Description

This class uses a model fit to determine which predictors were used in the final model.

Usage

```
predictors(x, ...)

## Default S3 method:
predictors(x,  ...)

## S3 method for class 'formula'
predictors(x,  ...)

## S3 method for class 'list'
predictors(x,  ...)

## S3 method for class 'rfe'
predictors(x,  ...)

## S3 method for class 'sbf'
predictors(x,  ...)

## S3 method for class 'terms'
predictors(x,  ...)

## S3 method for class 'train'
predictors(x,  ...)
```

Arguments

`x`	a model object, list or terms
`...`	not currently used

Details

For randomForest, cforest, ctree, rpart, ipredbagg, bagging, earth, fda, pamr.train, superpc.train, bagEarth and bagFDA, an attempt was made to report the predictors that were actually used in the final model.

The predictors function can be called on the model object (as opposed to the train) object) and the package will try to find the appropriate coed (if it exists).

In cases where the predictors cannot be determined, NA is returned. For example, nnet may return missing values from predictors.

Value

a character string of predictors or NA.

---

preProcess *Pre-Processing of Predictors*

Description

Pre-processing transformation (centering, scaling etc.) can be estimated from the training data and applied to any data set with the same variables.

Usage

```
preProcess(x, ...)

## Default S3 method:
preProcess(x,
           method = c("center", "scale"),
           thresh = 0.95,
           pcaComp = NULL,
           na.remove = TRUE,
           k = 5,
           knnSummary = mean,
           outcome = NULL,
           fudge = .2,
           numUnique = 3,
           verbose = FALSE,
           ...)

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

Arguments

x	a matrix or data frame. All variables must be numeric.
method	a character vector specifying the type of processing. Possible values are "BoxCox", "YeoJohnson", "expoTrans", "center", "scale", "range", "knnImpute", "bagImpute", "medianImpute", pca", "ica" and "spatialSign" (see Details below)
thresh	a cutoff for the cumulative percent of variance to be retained by PCA
pcaComp	the specific number of PCA components to keep. If specified, this over-rides thresh
na.remove	a logical; should missing values be removed from the calculations?
object	an object of class preProcess
newdata	a matrix or data frame of new data to be pre-processed
k	the number of nearest neighbors from the training set to use for imputation
knnSummary	function to average the neighbor values per column during imputation
outcome	a numeric or factor vector for the training set outcomes. This can be used to help estimate the Box-Cox transformation of the predictor variables (see Details below)
fudge	a tolerance value: Box-Cox transformation lambda values within +/-fudge will be coerced to 0 and within 1+/-fudge will be coerced to 1
numUnique	how many unique values should y have to estimate the Box-Cox transformation?
verbose	a logical: prints a log as the computations proceed
...	additional arguments to pass to fastICA, such as n.comp

Details

The Box-Cox, Yeo-Johnson and exponential transformations have been "repurposed" here: they are being used to transform the predictor variables. The Box-Cox transformation was developed for transforming the response variable while another method, the Box-Tidwell transformation, was created to estimate transformations of predictor data. However, the Box-Cox method is simpler, more computationally efficient and is equally effective for estimating power transformations. The Yeo-Johnson transformation is similar to the Box-Cox model but can accommodate predictors with zero and/or negative values (while the predictors values for the Box-Cox transformation must be strictly positive.) The exponential transformation of Manly (1976) can also be used for positive or negative data.

The "range" transformation scales the data to be within [0, 1]. If new samples have values larger or smaller than those in the training set, values will be outside of this range.

The operations are applied in this order: Box-Cox/Yeo-Johnson transformation, centering, scaling, range, imputation, PCA, ICA then spatial sign. This is a departure from versions of **caret** prior to version 4.76 (where imputation was done first) and is not backwards compatible if bagging was used for imputation.

If PCA is requested but centering and scaling are not, the values will still be centered and scaled. Similarly, when ICA is requested, the data are automatically centered and scaled.

k-nearest neighbor imputation is carried out by finding the k closest samples (Euclidian distance) in the training set. Imputation via bagging fits a bagged tree model for each predictor (as a function of

all the others). This method is simple, accurate and accepts missing values, but it has much higher computational cost. Imputation via medians takes the median of each predictor in the training set, and uses them to fill missing values. This method is simple, fast, and accepts missing values, but treats each predictor independently, and may be inaccurate.

A warning is thrown if both PCA and ICA are requested. ICA, as implemented by the fastICA package automatically does a PCA decomposition prior to finding the ICA scores.

The function will throw an error of any variables in x has less than two unique values.

Value

preProcess results in a list with elements

call	the function call
dim	the dimensions of x
bc	Box-Cox transformation values, see BoxCoxTrans
mean	a vector of means (if centering was requested)
std	a vector of standard deviations (if scaling or PCA was requested)
rotation	a matrix of eigenvectors if PCA was requested
method	the value ofmethod
thresh	the value ofthresh
ranges	a matrix of min and max values for each predictor when method includes "range" (and NULL otherwise)
numComp	the number of principal components required of capture the specified amount of variance
ica	contains values for the W and K matrix of the decomposition
median	a vector of medians (if median imputation was requested)

Author(s)

Max Kuhn, median imputation by Zachary Mayer

References

http://topepo.github.io/caret/preprocess.html

Kuhn and Johnson (2013), Applied Predictive Modeling, Springer, New York (chapter 4)

Kuhn (2008), Building predictive models in R using the caret (http://www.jstatsoft.org/v28/i05/)

Box, G. E. P. and Cox, D. R. (1964) An analysis of transformations (with discussion). Journal of the Royal Statistical Society B, 26, 211-252.

Box, G. E. P. and Tidwell, P. W. (1962) Transformation of the independent variables. Technometrics 4, 531-550.

Manly, B. L. (1976) Exponential data transformations. The Statistician, 25, 37 - 42.

Yeo, I-K. and Johnson, R. (2000). A new family of power transformations to improve normality or symmetry. Biometrika, 87, 954-959.

See Also

BoxCoxTrans, expoTrans boxcox, prcomp, fastICA, spatialSign

Examples

```
data(BloodBrain)
# one variable has one unique value
## Not run:
preProc <- preProcess(bbbDescr)

preProc  <- preProcess(bbbDescr[1:100,-3])
training <- predict(preProc, bbbDescr[1:100,-3])
test     <- predict(preProc, bbbDescr[101:208,-3])

## End(Not run)
```

---

print.confusionMatrix *Print method for confusionMatrix*

Description

a print method for confusionMatrix

Usage

```
## S3 method for class 'confusionMatrix'
print(x, digits = max(3, getOption("digits") - 3),
      printStats = TRUE, ...)
```

Arguments

x	an object of class confusionMatrix
digits	number of significant digits when printed
printStats	a logical: if TRUE then table statistics are also printed
...	optional arguments to pass to print.table

Value

x is invisibly returned

Author(s)

Max Kuhn

See Also

confusionMatrix

print.train *Print Method for the train Class*

Description

Print the results of a train object.

Usage

```
## S3 method for class 'train'
print(x,
      printCall = FALSE,
      details = FALSE,
      selectCol = FALSE,
      ...)
```

Arguments

x	an object of class train.
printCall	a logical to print the call at the top of the output
details	a logical to show print or summary methods for the final model. In some cases (such as gbm, knn, lvq, naive Bayes and bagged tree models), no information will be printed even if details = TRUE
selectCol	a logical whether to add a column with a star next to the selected parameters
...	options passed to format

Details

The table of complexity parameters used, their resampled performance and a flag for which rows are optimal.

Value

A matrix with the complexity parameters and performance (invisibly).

Author(s)

Max Kuhn

See Also

train

Examples

```
## Not run:
data(iris)
TrainData <- iris[,1:4]
TrainClasses <- iris[,5]

library(klaR)
rdaFit <- train(TrainData, TrainClasses, method = "rda",
                control = trainControl(method = "cv"))
print(rdaFit)

## End(Not run)
```

`resampleHist` *Plot the resampling distribution of the model statistics*

Description

Create a lattice histogram or densityplot from the resampled outcomes from a `train` object.

Usage

```
resampleHist(object, type = "density", ...)
```

Arguments

`object`	an object resulting form a call to `train`
`type`	a character string. Either "hist" or "density"
`...`	options to pass to histogram or densityplot

Details

All the metrics from the object are plotted, but only for the final model. For more comprehensive plots functions, see `histogram.train`, `densityplot.train`, `xyplot.train`, `stripplot.train`.

For the plot to be made, the `returnResamp` argument in `trainControl` should be either "final" or "all".

Value

a object of class `trellis`

Author(s)

Max Kuhn

See Also

`train`, `histogram`, `densityplot`, `histogram.train`, `densityplot.train`, `xyplot.train`, `stripplot.train`

Examples

```
## Not run:
data(iris)
TrainData <- iris[,1:4]
TrainClasses <- iris[,5]

knnFit <- train(TrainData, TrainClasses, "knn")

resampleHist(knnFit)

## End(Not run)
```

---

resamples *Collation and Visualization of Resampling Results*

Description

These functions provide methods for collection, analyzing and visualizing a set of resampling results from a common data set.

Usage

```
resamples(x, ...)

## Default S3 method:
resamples(x, modelNames = names(x), ...)

## S3 method for class 'resamples'
summary(object, metric = object$metrics, ...)

## S3 method for class 'resamples'
sort(x, decreasing = FALSE, metric = x$metric[1], FUN = mean, ...)

modelCor(x, metric = x$metric[1], ...)
```

Arguments

x	a list of two or more objects of class train, sbf or rfe with a common set of resampling indices in the control object. For sort.resamples, it is an object generated by resamples.
modelNames	an optional set of names to give to the resampling results
object	an object generated by resamples
metric	a character string for the performance measure used to sort or computing the between-model correlations
decreasing	logical. Should the sort be increasing or decreasing?

FUN	a function whose first argument is a vector and returns a scalar, to be applied to each model's performance measure.
...	only used for sort and modelCor and captures arguments to pass to sort or FUN.

Details

The ideas and methods here are based on Hothorn et al. (2005) and Eugster et al. (2008).

The results from train can have more than one performance metric per resample. Each metric in the input object is saved.

resamples checks that the resampling results match; that is, the indices in the object trainObject$control$index are the same. Also, the argument trainControl returnResamp should have a value of "final" for each model.

The summary function computes summary statistics across each model/metric combination.

Value

For resamples: an object with class "resamples" with elements

call	the call
values	a data frame of results where rows correspond to resampled data sets and columns indicate the model and metric
models	a character string of model labels
metrics	a character string of performance metrics
methods	a character string of the train method argument values for each model

For sort.resamples a character string in the sorted order is generated. modelCor returns a correlation matrix.

Author(s)

Max Kuhn

References

Hothorn et al. The design and analysis of benchmark experiments. Journal of Computational and Graphical Statistics (2005) vol. 14 (3) pp. 675-699

Eugster et al. Exploratory and inferential analysis of benchmark experiments. Ludwigs-Maximilians-Universitat Munchen, Department of Statistics, Tech. Rep (2008) vol. 30

See Also

train, trainControl, diff.resamples, xyplot.resamples, densityplot.resamples, bwplot.resamples, splom.resamples

Examples

```
data(BloodBrain)
set.seed(1)

## tmp <- createDataPartition(logBBB,
##                            p = .8,
##                            times = 100)

## rpartFit <- train(bbbDescr, logBBB,
##                   "rpart",
##                   tuneLength = 16,
##                   trControl = trainControl(
##                     method = "LGOCV", index = tmp))

## ctreeFit <- train(bbbDescr, logBBB,
##                   "ctree",
##                   trControl = trainControl(
##                     method = "LGOCV", index = tmp))

## earthFit <- train(bbbDescr, logBBB,
##                   "earth",
##                   tuneLength = 20,
##                   trControl = trainControl(
##                     method = "LGOCV", index = tmp))

## or load pre-calculated results using:
## load(url("http://caret.r-forge.r-project.org/exampleModels.RData"))

## resamps <- resamples(list(CART = rpartFit,
##                           CondInfTree = ctreeFit,
##                           MARS = earthFit))

## resamps
## summary(resamps)
```

`resampleSummary` *Summary of resampled performance estimates*

Description

This function uses the out-of-bag predictions to calculate overall performance metrics and returns the observed and predicted data.

Usage

```
resampleSummary(obs, resampled, index = NULL, keepData = TRUE)
```

Arguments

obs	A vector (numeric or factor) of the outcome data
resampled	For bootstrapping, this is either a matrix (for numeric outcomes) or a data frame (for factors). For cross-validation, a vector is produced.
index	The list to index of samples in each cross–validation fold (only used for cross-validation).
keepData	A logical for returning the observed and predicted data.

Details

The mean and standard deviation of the values produced by `postResample` are calculated.

Value

A list with:

metrics	A vector of values describing the bootstrap distribution.
data	A data frame or NULL. Columns include obs, pred and group (for tracking cross-validation folds or bootstrap samples)

Author(s)

Max Kuhn

See Also

`postResample`

Examples

```
resampleSummary(rnorm(10), matrix(rnorm(50), ncol = 5))
```

---

rfe *Backwards Feature Selection*

Description

A simple backwards selection, a.k.a. recursive feature selection (RFE), algorithm

Usage

```
rfe(x, ...)

## Default S3 method:
rfe(x, y,
    sizes = 2^(2:4),
    metric = ifelse(is.factor(y), "Accuracy", "RMSE"),
    maximize = ifelse(metric == "RMSE", FALSE, TRUE),
    rfeControl = rfeControl(),
    ...)

rfeIter(x, y,
        testX, testY,
        sizes,
        rfeControl = rfeControl(),
        label = "",
        seeds = NA,
        ...)

## S3 method for class 'rfe'
update(object, x, y, size, ...)

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

Arguments

x	a matrix or data frame of predictors for model training. This object must have unique column names.
y	a vector of training set outcomes (either numeric or factor)
testX	a matrix or data frame of test set predictors. This must have the same column names as x
testY	a vector of test set outcomes
sizes	a numeric vector of integers corresponding to the number of features that should be retained
metric	a string that specifies what summary metric will be used to select the optimal model. By default, possible values are "RMSE" and "Rsquared" for regression and "Accuracy" and "Kappa" for classification. If custom performance metrics are used (via the functions argument in rfeControl, the value of metric should match one of the arguments.
maximize	a logical: should the metric be maximized or minimized?
rfeControl	a list of options, including functions for fitting and prediction. The web page http://topepo.github.io/caret/featureselection.html#rfe has more details and examples related to this function.
object	an object of class rfe

size	a single integers corresponding to the number of features that should be retained in the updated model
newdata	a matrix or data frame of new samples for prediction
label	an optional character string to be printed when in verbose mode.
seeds	an optional vector of integers for the size. The vector should have length of length(sizes)+1
...	options to pass to the model fitting function (ignored in predict.rfe)

Details

More details on this function can be found at http://topepo.github.io/caret/featureselection.html.

This function implements backwards selection of predictors based on predictor importance ranking. The predictors are ranked and the less important ones are sequentially eliminated prior to modeling. The goal is to find a subset of predictors that can be used to produce an accurate model. The web page http://topepo.github.io/caret/featureselection.html#rfe has more details and examples related to this function.

rfe can be used with "explicit parallelism", where different resamples (e.g. cross-validation group) can be split up and run on multiple machines or processors. By default, rfe will use a single processor on the host machine. As of version 4.99 of this package, the framework used for parallel processing uses the **foreach** package. To run the resamples in parallel, the code for rfe does not change; prior to the call to rfe, a parallel backend is registered with **foreach** (see the examples below).

rfeIter is the basic algorithm while rfe wraps these operations inside of resampling. To avoid selection bias, it is better to use the function rfe than rfeIter.

When updating a model, if the entire set of resamples were not saved using rfeControl(returnResamp = "final"), the existing resamples are removed with a warning.

Value

A list with elements

finalVariables	a list of size length(sizes) + 1 containing the column names of the "surviving" predictors at each stage of selection. The first element corresponds to all the predictors (i.e. size = ncol(x))
pred	a data frame with columns for the test set outcome, the predicted outcome and the subset size.

Author(s)

Max Kuhn

See Also

rfeControl

Examples

```
## Not run:
data(BloodBrain)

x <- scale(bbbDescr[,-nearZeroVar(bbbDescr)])
x <- x[, -findCorrelation(cor(x), .8)]
x <- as.data.frame(x)

set.seed(1)
lmProfile <- rfe(x, logBBB,
                 sizes = c(2:25, 30, 35, 40, 45, 50, 55, 60, 65),
                 rfeControl = rfeControl(functions = lmFuncs,
                                         number = 200))
set.seed(1)
lmProfile2 <- rfe(x, logBBB,
                 sizes = c(2:25, 30, 35, 40, 45, 50, 55, 60, 65),
                 rfeControl = rfeControl(functions = lmFuncs,
                                         rerank = TRUE,
                                         number = 200))

xyplot(lmProfile$results$RMSE + lmProfile2$results$RMSE  ~
       lmProfile$results$Variables,
       type = c("g", "p", "l"),
       auto.key = TRUE)

rfProfile <- rfe(x, logBBB,
                 sizes = c(2, 5, 10, 20),
                 rfeControl = rfeControl(functions = rfFuncs))

bagProfile <- rfe(x, logBBB,
                  sizes = c(2, 5, 10, 20),
                  rfeControl = rfeControl(functions = treebagFuncs))

set.seed(1)
svmProfile <- rfe(x, logBBB,
                  sizes = c(2, 5, 10, 20),
                  rfeControl = rfeControl(functions = caretFuncs,
                                          number = 200),
                  ## pass options to train()
                  method = "svmRadial")

## classification

data(mdrr)
mdrrDescr <- mdrrDescr[,-nearZeroVar(mdrrDescr)]
mdrrDescr <- mdrrDescr[, -findCorrelation(cor(mdrrDescr), .8)]

set.seed(1)
inTrain <- createDataPartition(mdrrClass, p = .75, list = FALSE)[,1]

train <- mdrrDescr[ inTrain, ]
test  <- mdrrDescr[-inTrain, ]
```

```
trainClass <- mdrrClass[ inTrain]
testClass  <- mdrrClass[-inTrain]

set.seed(2)
ldaProfile <- rfe(train, trainClass,
                  sizes = c(1:10, 15, 30),
                  rfeControl = rfeControl(functions = ldaFuncs, method = "cv"))
plot(ldaProfile, type = c("o", "g"))

postResample(predict(ldaProfile, test), testClass)


## End(Not run)

########################################
## Parallel Processing Example via multicore

## Not run:
library(doMC)

## Note: if the underlying model also uses foreach, the
## number of cores specified above will double (along with
## the memory requirements)
registerDoMC(cores = 2)

set.seed(1)
lmProfile <- rfe(x, logBBB,
                 sizes = c(2:25, 30, 35, 40, 45, 50, 55, 60, 65),
                 rfeControl = rfeControl(functions = lmFuncs,
                                         number = 200))



## End(Not run)
```

`rfeControl` *Controlling the Feature Selection Algorithms*

Description

This function generates a control object that can be used to specify the details of the feature selection algorithms used in this package.

Usage

```
rfeControl(functions = NULL,
           rerank = FALSE,
           method = "boot",
           saveDetails = FALSE,
```

```
            number = ifelse(method %in% c("cv", "repeatedcv"), 10, 25),
            repeats = ifelse(method %in% c("cv", "repeatedcv"), 1, number),
            verbose = FALSE,
            returnResamp = "final",
            p = .75,
            index = NULL,
            indexOut = NULL,
            timingSamps = 0,
            seeds = NA,
            allowParallel = TRUE)
```

Arguments

functions	a list of functions for model fitting, prediction and variable importance (see Details below)
rerank	a logical: should variable importance be re-calculated each time features are removed?
method	The external resampling method: boot, cv, LOOCV or LGOCV (for repeated training/test splits
number	Either the number of folds or number of resampling iterations
repeats	For repeated k-fold cross-validation only: the number of complete sets of folds to compute
saveDetails	a logical to save the predictions and variable importances from the selection process
verbose	a logical to print a log for each external resampling iteration
returnResamp	A character string indicating how much of the resampled summary metrics should be saved. Values can be "final", "all" or "none"
p	For leave-group out cross-validation: the training percentage
index	a list with elements for each external resampling iteration. Each list element is the sample rows used for training at that iteration.
indexOut	a list (the same length as index) that dictates which sample are held-out for each resample. If NULL, then the unique set of samples not contained in index is used.
timingSamps	the number of training set samples that will be used to measure the time for predicting samples (zero indicates that the prediction time should not be estimated).
seeds	an optional set of integers that will be used to set the seed at each resampling iteration. This is useful when the models are run in parallel. A value of NA will stop the seed from being set within the worker processes while a value of NULL will set the seeds using a random set of integers. Alternatively, a list can be used. The list should have B+1 elements where B is the number of resamples. The first B elements of the list should be vectors of integers of length P where P is the number of subsets being evaluated (including the full set). The last element of the list only needs to be a single integer (for the final model). See the Examples section below.
allowParallel	if a parallel backend is loaded and available, should the function use it?

Details

More details on this function can be found at http://topepo.github.io/caret/featureselection.html#rfe.

Backwards selection requires function to be specified for some operations.

The `fit` function builds the model based on the current data set. The arguments for the function must be:

- `x` the current training set of predictor data with the appropriate subset of variables
- `y` the current outcome data (either a numeric or factor vector)
- `first` a single logical value for whether the current predictor set has all possible variables
- `last` similar to `first`, but `TRUE` when the last model is fit with the final subset size and predictors.
- `...` optional arguments to pass to the fit function in the call to `rfe`

The function should return a model object that can be used to generate predictions.

The `pred` function returns a vector of predictions (numeric or factors) from the current model. The arguments are:

- `object` the model generated by the `fit` function
- `x` the current set of predictor set for the held-back samples

The `rank` function is used to return the predictors in the order of the most important to the least important. Inputs are:

- `object` the model generated by the `fit` function
- `x` the current set of predictor set for the training samples
- `y` the current training outcomes

The function should return a data frame with a column called `var` that has the current variable names. The first row should be the most important predictor etc. Other columns can be included in the output and will be returned in the final `rfe` object.

The `selectSize` function determines the optimal number of predictors based on the resampling output. Inputs for the function are:

- `x` a matrix with columns for the performance metrics and the number of variables, called `"Variables"`
- `metric` a character string of the performance measure to optimize (e.g. "RMSE", "Rsquared", "Accuracy" or "Kappa")
- `maximize` a single logical for whether the metric should be maximized

This function should return an integer corresponding to the optimal subset size. **caret** comes with two examples functions for this purpose: `pickSizeBest` and `pickSizeTolerance`.

After the optimal subset size is determined, the `selectVar` function will be used to calculate the best rankings for each variable across all the resampling iterations. Inputs for the function are:

- y a list of variables importance for each resampling iteration and each subset size (generated by the user–defined rank function). In the example, each each of the cross–validation groups the output of the rank function is saved for each of the subset sizes (including the original subset). If the rankings are not recomputed at each iteration, the values will be the same within each cross-validation iteration.
- size the integer returned by the selectSize function

This function should return a character string of predictor names (of length size) in the order of most important to least important

Examples of these functions are included in the package: lmFuncs, rfFuncs, treebagFuncs and nbFuncs.

Model details about these functions, including examples, are at http://topepo.github.io/caret/featureselection.html. .

Value

A list

Author(s)

Max Kuhn

See Also

rfe, lmFuncs, rfFuncs, treebagFuncs, nbFuncs, pickSizeBest, pickSizeTolerance

Examples

```
  ## Not run:
subsetSizes <- c(2, 4, 6, 8)
set.seed(123)
seeds <- vector(mode = "list", length = 51)
for(i in 1:50) seeds[[i]] <- sample.int(1000, length(subsetSizes) + 1)
seeds[[51]] <- sample.int(1000, 1)

set.seed(1)
rfMod <- rfe(bbbDescr, logBBB,
             sizes = subsetSizes,
             rfeControl = rfeControl(functions = rfFuncs,
                                     seeds = seeds,
                                     number = 50))

## End(Not run)
```

safs.default *Simulated annealing feature selection*

Description

Supervised feature selection using simulated annealing

Usage

```
safs(x, ...)

## Default S3 method:
safs(x, y, iters = 10, differences = TRUE, safsControl = safsControl(), ...)
```

Arguments

x	an object where samples are in rows and features are in columns. This could be a simple matrix, data frame or other type (e.g. sparse matrix). See Details below.
y	a numeric or factor vector containing the outcome for each sample.
iters	number of search iterations
differences	a logical: should the difference in fitness values with and without each predictor be calculated
safsControl	a list of values that define how this function acts. See safsControl and URL.
...	arguments passed to the classification or regression routine specified in the function safsControl$functions$fit

Details

safs conducts a supervised binary search of the predictor space using simulated annealing (SA). See XXX for more information on this search algorithm.

This function conducts the search of the feature space repeatedly within resampling iterations. First, the training data are split be whatever resampling method was specified in the control function. For example, if 10-fold cross-validation is selected, the entire simulated annealing search is conducted 10 separate times. For the first fold, nine tenths of the data are used in the search while the remaining tenth is used to estimate the external performance since these data points were not used in the search.

During the search, a measure of fitness (i.e. SA energy value) is needed to guide the search. This is the internal measure of performance. During the search, the data that are available are the instances selected by the top-level resampling (e.g. the nine tenths mentioned above). A common approach is to conduct another resampling procedure. Another option is to use a holdout set of samples to determine the internal estimate of performance (see the holdout argument of the control function). While this is faster, it is more likely to cause overfitting of the features and should only be used when a large amount of training data are available. Yet another idea is to use a penalized metric (such as the AIC statistic) but this may not exist for some metrics (e.g. the area under the ROC curve).

The internal estimates of performance will eventually overfit the subsets to the data. However, since the external estimate is not used by the search, it is able to make better assessments of overfitting. After resampling, this function determines the optimal number of iterations for the SA.

Finally, the entire data set is used in the last execution of the simulated annealing algorithm search and the final model is built on the predictor subset that is associated with the optimal number of iterations determined by resampling (although the update function can be used to manually set the number of iterations).

This is an example of the output produced when `safsControl(verbose = TRUE)` is used:

```
Fold03 1 0.401 (11)
Fold03 2 0.401->0.410 (11+1, 91.7%) *
Fold03 3 0.410->0.396 (12+1, 92.3%)  0.969  A
Fold03 4 0.410->0.370 (12+2, 85.7%)  0.881
Fold03 5 0.410->0.399 (12+2, 85.7%)  0.954  A
Fold03 6 0.410->0.399 (12+1, 78.6%)  0.940  A
Fold03 7 0.410->0.428 (12+2, 73.3%) *
```

The text "Fold03" indicates that this search is for the third cross-validation fold. The initial subset of 11 predictors had a fitness value of 0.401. The next iteration added a single feature the the existing best subset of 11 (as indicated by "11+1") that increased the fitness value to 0.410. This new solution, which has a Jaccard similarity value of 91.7% to the current best solution, is automatically accepted. The third iteration adds another feature to the current set of 12 but does not improve the fitness. The acceptance probability for this difference is shown to be 95.6% and the "A" indicates that this new sub-optimal subset is accepted. The fourth iteration does not show an increase and is not accepted. Note that the Jaccard similarity value of 85.7% is the similarity to the current best solution (from iteration 2) and the "12+2" indicates that there are two additional features added from the current best that contains 12 predictors.

The search algorithm can be parallelized in several places:

1. each externally resampled SA can be run independently (controlled by the `allowParallel` option of `safsControl`)
2. if inner resampling is used, these can be run in parallel (controls depend on the function used. See, for example, `trainControl`)
3. any parallelization of the individual model fits. This is also specific to the modeling function.

It is probably best to pick one of these areas for parallelization and the first is likely to produces the largest decrease in run-time since it is the least likely to incur multiple re-starting of the worker processes. Keep in mind that if multiple levels of parallelization occur, this can effect the number of workers and the amount of memory required exponentially.

Value

an object of class `safs`

Author(s)

Max Kuhn

References

http://topepo.github.io/caret/GA.html

http://topepo.github.io/caret/SA.html

Kuhn and Johnson (2013), Applied Predictive Modeling, Springer

See Also

safsControl, predict.safs

Examples

```
## Not run:

set.seed(1)
train_data <- twoClassSim(100, noiseVars = 10)
test_data  <- twoClassSim(10,  noiseVars = 10)

## A short example
ctrl <- safsControl(functions = rfSA,
                    method = "cv",
                    number = 3)

rf_search <- safs(x = train_data[, -ncol(train_data)],
                  y = train_data$Class,
                  iters = 3,
                  safsControl = ctrl)

rf_search

## End(Not run)
```

---

safsControl *Control parameters for GA and SA feature selection*

Description

Control the computational nuances of the gafs and safs functions

Usage

```
gafsControl(functions = NULL,
            method = "repeatedcv",
            metric = NULL,
            maximize = NULL,
            number = ifelse(grepl("cv", method), 10, 25),
            repeats = ifelse(grepl("cv", method), 1, 5),
            verbose = FALSE,
            returnResamp = "final",
```

```
            p = 0.75,
            index = NULL,
            indexOut = NULL,
            seeds = NULL,
            holdout = 0,
            genParallel = FALSE,
            allowParallel = TRUE)

safsControl(functions = NULL,
            method = "repeatedcv",
            metric = NULL,
            maximize = NULL,
            number = ifelse(grepl("cv", method), 10, 25),
            repeats = ifelse(grepl("cv", method), 1, 5),
            verbose = FALSE,
            returnResamp = "final",
            p = 0.75,
            index = NULL,
            indexOut = NULL,
            seeds = NULL,
            holdout = 0,
            improve = Inf,
            allowParallel = TRUE)
```

Arguments

functions	a list of functions for model fitting, prediction etc (see Details below)
method	The resampling method: boot, boot632, cv, repeatedcv, LOOCV, LGOCV (for repeated training/test splits)
metric	a two-element string that specifies what summary metric will be used to select the optimal number of iterations from the external fitness value and which metric should guide subset selection. If specified, this vector should have names "internal" and "external". See gafs and/or safs for explanations of the difference.
maximize	a two-element logical: should the metrics be maximized or minimized? Like the metric argument, this this vector should have names "internal" and "external".
number	Either the number of folds or number of resampling iterations
repeats	For repeated k-fold cross-validation only: the number of complete sets of folds to compute
verbose	a logical for printing results
returnResamp	A character string indicating how much of the resampled summary metrics should be saved. Values can be "all" or "none"
p	For leave-group out cross-validation: the training percentage
index	a list with elements for each resampling iteration. Each list element is the sample rows used for training at that iteration.

indexOut	a list (the same length as index) that dictates which sample are held-out for each resample. If NULL, then the unique set of samples not contained in index is used.
seeds	a vector or integers that can be used to set the seed during each search. The number of seeds must be equal to the number of resamples plus one.
holdout	the proportion of data in [0, 1) to be held-back from x and y to calculate the internal fitness values
improve	the number of iterations without improvement before safs reverts back to the previous optimal subset
genParallel	if a parallel backend is loaded and available, should gafs use it tp parallelize the fitness calculations within a generation within a resample?
allowParallel	if a parallel backend is loaded and available, should the function use it?

Details

Many of these options are the same as those described for trainControl. More extensive documentation and examples can be found on the **caret** website at http://topepo.github.io/caret/GA.html#syntax and http://topepo.github.io/caret/SA.html#syntax.

The functions component contains the information about how the model should be fit and summarized. It also contains the elements needed for the GA and SA modules (e.g. cross-over, etc).

The elements of functions that are the same for GAs and SAs are:

- fit, with arguments x, y, lev, last, and ..., is used to fit the classification or regression model
- pred, with arguments object and x, predicts new samples
- fitness_intern, with arguments object, x, y, maximize, and p, summarizes performance for the internal estimates of fitness
- fitness_extern, with arguments data, lev, and model, summarizes performance using the externally held-out samples
- selectIter, with arguments x, metric, and maximize, determines the best search iteration for feature selection.

The elements of functions specific to genetic algorithms are:

- initial, with arguments vars, popSize and ..., creates an initial population.
- selection, with arguments population, fitness, r, q, and ..., conducts selection of individuals.
- crossover, with arguments population, fitness, parents and ..., control genetic reproduction.
- mutation, with arguments population, parent and ..., adds mutations.

The elements of functions specific to simulated annealing are:

- initial, with arguments vars, prob, and ..., creates the initial subset.
- perturb, with arguments x, vars, and number, makes incremental changes to the subsets.
- prob, with arguments old, new, and iteration, computes the acceptance probabilities

The pages http://topepo.github.io/caret/GA.html#custom and http://topepo.github.io/caret/SA.html#custom have more details about each of these functions.

holdout can be used to hold out samples for computing the internal fitness value. Note that this is independent of the external resampling step. Suppose 10-fold CV is being used. Within a resampling iteration, holdout can be used to sample an additional proportion of the 90% resampled data to use for estimating fitness. This may not be a good idea unless you have a very large training set and want to avoid an internal resampling procedure to estimate fitness.

The search algorithms can be parallelized in several places:

1. each externally resampled GA or SA can be run independently (controlled by the allowParallel options)
2. within a GA, the fitness calculations at a particular generation can be run in parallel over the current set of individuals (see the genParallel)
3. if inner resampling is used, these can be run in parallel (controls depend on the function used. See, for example, trainControl)
4. any parallelization of the individual model fits. This is also specific to the modeling function.

It is probably best to pick one of these areas for parallelization and the first is likely to produces the largest decrease in run-time since it is the least likely to incur multiple re-starting of the worker processes. Keep in mind that if multiple levels of parallelization occur, this can effect the number of workers and the amount of memory required exponentially.

Value

An echo of the parameters specified

Author(s)

Max Kuhn

References

http://topepo.github.io/caret/GA.html, http://topepo.github.io/caret/SA.html

See Also

safs, safs, , caretGA, rfGA, treebagGA, caretSA, rfSA, treebagSA

---

safs_initial *Ancillary simulated annealing functions*

Description

Built-in functions related to simulated annealing

Usage

```
safs_initial(vars, prob = 0.2, ...)
safs_perturb(x, vars, number = floor(vars*.01) + 1)
safs_prob(old, new, iteration = 1)

caretSA
rfSA
treebagSA
```

Arguments

vars	the total number of possible predictor variables
prob	The probability that an individual predictor is included in the initial predictor set
x	the integer index vector for the current subset
old, new	fitness values associated with the current and new subset
iteration	the number of iterations overall or the number of iterations since restart (if improve is used in safsControl)
number	the number of predictor variables to perturb
...	not currently used

Details

These functions are used with the functions argument of the safsControl function. More information on the details of these functions are at http://topepo.github.io/caret/SA.html.

The initial function is used to create the first predictor subset. The function safs_initial randomly selects 20% of the predictors. Note that, instead of a function, safs can also accept a vector of column numbers as the initial subset.

safs_perturb is an example of the operation that changes the subset configuration at the start of each new iteration. By default, it will change roughly 1% of the variables in the current subset.

The prob function defines the acceptance probability at each iteration, given the old and new fitness (i.e. energy values). It assumes that smaller values are better. The default probability function computed the percentage difference between the current and new fitness value and using an exponential function to compute a probability:

```
prob = exp[(current-new)/current*iteration]
```

Value

The return value depends on the function. Note that the SA code encodes the subsets as a vector of integers that are included in the subset (which is different than the encoding used for GAs).

The objects caretSA, rfSA and treebagSA are example lists that can be used with the functions argument of safsControl.

In the case of caretSA, the ... structure of safs passes through to the model fitting routine. As a consequence, the train function can easily be accessed by passing important arguments belonging

to train to safs. See the examples below. By default, using caretSA will used the resampled performance estimates produced by train as the internal estimate of fitness.

For rfSA and treebagSA, the randomForest and bagging functions are used directly (i.e. train is not used). Arguments to either of these functions can also be passed to them though the safs call (see examples below). For these two functions, the internal fitness is estimated using the out-of-bag estimates naturally produced by those functions. While faster, this limits the user to accuracy or Kappa (for classification) and RMSE and R-squared (for regression).

Author(s)

Max Kuhn

References

http://topepo.github.io/caret/SA.html

See Also

safs, safsControl

Examples

```
selected_vars <- safs_initial(vars = 10 , prob = 0.2)
selected_vars

###

safs_perturb(selected_vars, vars = 10, number = 1)

###

safs_prob(old = .8, new = .9, iteration = 1)
safs_prob(old = .5, new = .6, iteration = 1)

grid <- expand.grid(old = c(4, 3.5),
                    new = c(4.5, 4, 3.5) + 1,
                    iter = 1:40)
grid <- subset(grid, old < new)

grid$prob <- apply(grid, 1,
                   function(x)
                     safs_prob(new = x["new"],
                               old= x["old"],
                               iteration = x["iter"]))

grid$Difference <- factor(grid$new - grid$old)
grid$Group <- factor(paste("Current Value", grid$old))

ggplot(grid, aes(x = iter, y = prob, color = Difference)) +
  geom_line() + facet_wrap(~Group) + theme_bw() +
  ylab("Probability") + xlab("Iteration")
```

```
## Not run:
###
## Hypothetical examples
lda_sa <- safs(x = predictors,
               y = classes,
               safsControl = safsControl(functions = caretSA),
               ## now pass arguments to `train`
               method = "lda",
               metric = "Accuracy"
               trControl = trainControl(method = "cv", classProbs = TRUE))

rf_sa <- safs(x = predictors,
              y = classes,
              safsControl = safsControl(functions = rfSA),
              ## these are arguments to `randomForest`
              ntree = 1000,
              importance = TRUE)

## End(Not run)
```

---

sbf *Selection By Filtering (SBF)*

Description

Model fitting after applying univariate filters

Usage

```
sbf(x, ...)

## Default S3 method:
sbf(x, y, sbfControl = sbfControl(), ...)

## S3 method for class 'formula'
sbf(form, data, ..., subset, na.action, contrasts = NULL)

## S3 method for class 'sbf'
predict(object, newdata = NULL, ...)
```

Arguments

x	a data frame containing training data where samples are in rows and features are in columns.
y	a numeric or factor vector containing the outcome for each sample.

form	A formula of the form y ~ x1 + x2 + ...
data	Data frame from which variables specified in formula are preferentially to be taken.
subset	An index vector specifying the cases to be used in the training sample. (NOTE: If given, this argument must be named.)
na.action	A function to specify the action to be taken if NAs are found. The default action is for the procedure to fail. An alternative is na.omit, which leads to rejection of cases with missing values on any required variable. (NOTE: If given, this argument must be named.)
contrasts	a list of contrasts to be used for some or all the factors appearing as variables in the model formula.
sbfControl	a list of values that define how this function acts. See sbfControl. (NOTE: If given, this argument must be named.)
object	an object of class sbf
newdata	a matrix or data frame of predictors. The object must have non-null column names
...	for sbf: arguments passed to the classification or regression routine (such as randomForest). For predict.sbf: augments cannot be passed to the prediction function using predict.sbf as it uses the function originally specified for prediction.

Details

More details on this function can be found at http://topepo.github.io/caret/featureselection.html#filter.

This function can be used to get resampling estimates for models when simple, filter-based feature selection is applied to the training data.

For each iteration of resampling, the predictor variables are univariately filtered prior to modeling. Performance of this approach is estimated using resampling. The same filter and model are then applied to the entire training set and the final model (and final features) are saved.

sbf can be used with "explicit parallelism", where different resamples (e.g. cross-validation group) can be split up and run on multiple machines or processors. By default, sbf will use a single processor on the host machine. As of version 4.99 of this package, the framework used for parallel processing uses the **foreach** package. To run the resamples in parallel, the code for sbf does not change; prior to the call to sbf, a parallel backend is registered with **foreach** (see the examples below).

The modeling and filtering techniques are specified in sbfControl. Example functions are given in lmSBF.

Value

for sbf, an object of class sbf with elements:

pred	if sbfControl$saveDetails is TRUE, this is a list of predictions for the hold-out samples at each resampling iteration. Otherwise it is NULL

variables	a list of variable names that survived the filter at each resampling iteration
results	a data frame of results aggregated over the resamples
fit	the final model fit with only the filtered variables
optVariables	the names of the variables that survived the filter using the training set
call	the function call
control	the control object
resample	if sbfControl$returnResamp is "all", a data frame of the resampled performance measures. Otherwise, NULL
metrics	a character vector of names of the performance measures
dots	a list of optional arguments that were passed in

For predict.sbf, a vector of predictions.

Author(s)

Max Kuhn

See Also

sbfControl

Examples

```
## Not run:
data(BloodBrain)

## Use a GAM is the filter, then fit a random forest model
RFwithGAM <- sbf(bbbDescr, logBBB,
                 sbfControl = sbfControl(functions = rfSBF,
                                         verbose = FALSE,
                                         method = "cv"))
RFwithGAM

predict(RFwithGAM, bbbDescr[1:10,])

## classification example with parallel processing

## library(doMC)

## Note: if the underlying model also uses foreach, the
## number of cores specified above will double (along with
## the memory requirements)
## registerDoMC(cores = 2)

data(mdrr)
mdrrDescr <- mdrrDescr[,-nearZeroVar(mdrrDescr)]
mdrrDescr <- mdrrDescr[, -findCorrelation(cor(mdrrDescr), .8)]

set.seed(1)
```

```
filteredNB <- sbf(mdrrDescr, mdrrClass,
                  sbfControl = sbfControl(functions = nbSBF,
                                          verbose = FALSE,
                                          method = "repeatedcv",
                                          repeats = 5))
confusionMatrix(filteredNB)

## End(Not run)
```

---

sbfControl *Control Object for Selection By Filtering (SBF)*

Description

Controls the execution of models with simple filters for feature selection

Usage

```
sbfControl(functions = NULL,
           method = "boot",
           saveDetails = FALSE,
           number = ifelse(method %in% c("cv", "repeatedcv"), 10, 25),
           repeats = ifelse(method %in% c("cv", "repeatedcv"), 1, number),
           verbose = FALSE,
           returnResamp = "final",
           p = 0.75,
           index = NULL,
           indexOut = NULL,
           timingSamps = 0,
           seeds = NA,
           allowParallel = TRUE,
           multivariate = FALSE)
```

Arguments

functions	a list of functions for model fitting, prediction and variable filtering (see Details below)
method	The external resampling method: boot, cv, LOOCV or LGOCV (for repeated training/test splits
number	Either the number of folds or number of resampling iterations
repeats	For repeated k-fold cross-validation only: the number of complete sets of folds to compute
saveDetails	a logical to save the predictions and variable importances from the selection process
verbose	a logical to print a log for each external resampling iteration

returnResamp	A character string indicating how much of the resampled summary metrics should be saved. Values can be "final" or "none"
p	For leave-group out cross-validation: the training percentage
index	a list with elements for each external resampling iteration. Each list element is the sample rows used for training at that iteration.
indexOut	a list (the same length as index) that dictates which sample are held-out for each resample. If NULL, then the unique set of samples not contained in index is used.
timingSamps	the number of training set samples that will be used to measure the time for predicting samples (zero indicates that the prediction time should not be estimated).
seeds	an optional set of integers that will be used to set the seed at each resampling iteration. This is useful when the models are run in parallel. A value of NA will stop the seed from being set within the worker processes while a value of NULL will set the seeds using a random set of integers. Alternatively, a vector of integers can be used. The vector should have B+1 elements where B is the number of resamples. See the Examples section below.
allowParallel	if a parallel backend is loaded and available, should the function use it?
multivariate	a logical; should all the columns of x be exposed to the score function at once?

Details

More details on this function can be found at http://topepo.github.io/caret/featureselection.html#filter.

Simple filter-based feature selection requires function to be specified for some operations.

The fit function builds the model based on the current data set. The arguments for the function must be:

- x the current training set of predictor data with the appropriate subset of variables (i.e. after filtering)
- y the current outcome data (either a numeric or factor vector)
- ... optional arguments to pass to the fit function in the call to sbf

The function should return a model object that can be used to generate predictions.

The pred function returns a vector of predictions (numeric or factors) from the current model. The arguments are:

- object the model generated by the fit function
- x the current set of predictor set for the held-back samples

The score function is used to return scores with names for each predictor (such as a p-value). Inputs are:

- x the predictors for the training samples. If sbfControl()$multivariate is TRUE, this will be the full predictor matrix. Otherwise it is a vector for a specific predictor.
- y the current training outcomes

When `sbfControl()$multivariate` is `TRUE`, the `score` function should return a named vector where `length(scores) == ncol(x)`. Otherwise, the function's output should be a single value. Univariate examples are give by `anovaScores` for classification and `gamScores` for regression and the example below.

The `filter` function is used to return a logical vector with names for each predictor (`TRUE` indicates that the prediction should be retained). Inputs are:

- `score` the output of the `score` function
- `x` the predictors for the training samples
- `y` the current training outcomes

The function should return a named logical vector.

Examples of these functions are included in the package: `caretSBF`, `lmSBF`, `rfSBF`, `treebagSBF`, `ldaSBF` and `nbSBF`.

The web page http://topepo.github.io/caret/ has more details and examples related to this function.

Value

a list that echos the specified arguments

Author(s)

Max Kuhn

See Also

`sbf`, `caretSBF`, `lmSBF`, `rfSBF`, `treebagSBF`, `ldaSBF` and `nbSBF`

Examples

```
## Not run:
data(BloodBrain)

## Use a GAM is the filter, then fit a random forest model
set.seed(1)
RFwithGAM <- sbf(bbbDescr, logBBB,
                 sbfControl = sbfControl(functions = rfSBF,
                                         verbose = FALSE,
                                         seeds = sample.int(100000, 11),
                                         method = "cv"))
RFwithGAM


## A simple example for multivariate scoring
rfSBF2 <- rfSBF
rfSBF2$score <- function(x, y) apply(x, 2, rfSBF$score, y = y)

set.seed(1)
RFwithGAM2 <- sbf(bbbDescr, logBBB,
```

```
                    sbfControl = sbfControl(functions = rfSBF2,
                                            verbose = FALSE,
                                            seeds = sample.int(100000, 11),
                                            method = "cv",
                                            multivariate = TRUE))
RFwithGAM2


## End(Not run)
```

---

segmentationData *Cell Body Segmentation*

Description

Hill, LaPan, Li and Haney (2007) develop models to predict which cells in a high content screen were well segmented. The data consists of 119 imaging measurements on 2019. The original analysis used 1009 for training and 1010 as a test set (see the column called `Case`).

The outcome class is contained in a factor variable called `Class` with levels "PS" for poorly segmented and "WS" for well segmented.

The raw data used in the paper can be found at the Biomedcentral website. Versions of caret < 4.98 contained the original data. The version now contained in `segmentationData` is modified. First, several discrete versions of some of the predictors (with the suffix "Status") were removed. Second, there are several skewed predictors with minimum values of zero (that would benefit from some transformation, such as the log). A constant value of 1 was added to these fields: `AvgIntenCh2`, `FiberAlign2Ch3`, `FiberAlign2Ch4`, `SpotFiberCountCh4` and `TotalIntenCh2`.

A binary version of the original data is at http://topepo.github.io/caret/segmentationOriginal.RData.

Usage

```
data(segmentationData)
```

Value

`segmentationData`
: data frame of cells

Source

Hill, LaPan, Li and Haney (2007). Impact of image segmentation on high-content screening data quality for SK-BR-3 cells, *BMC Bioinformatics*, Vol. 8, pg. 340, http://www.biomedcentral.com/1471-2105/8/340.

sensitivity *Calculate sensitivity, specificity and predictive values*

Description

These functions calculate the sensitivity, specificity or predictive values of a measurement system compared to a reference results (the truth or a gold standard). The measurement and "truth" data must have the same two possible outcomes and one of the outcomes must be thought of as a "positive" results.

The sensitivity is defined as the proportion of positive results out of the number of samples which were actually positive. When there are no positive results, sensitivity is not defined and a value of NA is returned. Similarly, when there are no negative results, specificity is not defined and a value of NA is returned. Similar statements are true for predictive values.

The positive predictive value is defined as the percent of predicted positives that are actually positive while the negative predictive value is defined as the percent of negative positives that are actually negative.

Usage

```
sensitivity(data, ...)
## Default S3 method:
sensitivity(data, reference, positive = levels(reference)[1], na.rm = TRUE, ...)
## S3 method for class 'table'
sensitivity(data, positive = rownames(data)[1], ...)
## S3 method for class 'matrix'
sensitivity(data, positive = rownames(data)[1], ...)

specificity(data, ...)
## Default S3 method:
specificity(data, reference, negative = levels(reference)[-1], na.rm = TRUE, ...)
## S3 method for class 'table'
specificity(data, negative = rownames(data)[-1], ...)
## S3 method for class 'matrix'
specificity(data, negative = rownames(data)[-1], ...)

posPredValue(data, ...)
## Default S3 method:
posPredValue(data, reference, positive = levels(reference)[1],
             prevalence = NULL, ...)
## S3 method for class 'table'
posPredValue(data, positive = rownames(data)[1], prevalence = NULL, ...)
## S3 method for class 'matrix'
posPredValue(data, positive = rownames(data)[1], prevalence = NULL, ...)

negPredValue(data, ...)
## Default S3 method:
```

```
negPredValue(data, reference, negative = levels(reference)[2],
             prevalence = NULL, ...)
## S3 method for class 'table'
negPredValue(data, negative = rownames(data)[-1], prevalence = NULL, ...)
## S3 method for class 'matrix'
negPredValue(data, negative = rownames(data)[-1], prevalence = NULL, ...)
```

Arguments

data	for the default functions, a factor containing the discrete measurements. For the table or matrix functions, a table or matric object, respectively.
reference	a factor containing the reference values
positive	a character string that defines the factor level corresponding to the "positive" results
negative	a character string that defines the factor level corresponding to the "negative" results
prevalence	a numeric value for the rate of the "positive" class of the data
na.rm	a logical value indicating whether NA values should be stripped before the computation proceeds
...	not currently used

Details

Suppose a 2x2 table with notation

	Reference	
Predicted	Event	No Event
Event	A	B
No Event	C	D

The formulas used here are:

$$Sensitivity = A/(A+C)$$

$$Specificity = D/(B+D)$$

$$Prevalence = (A+C)/(A+B+C+D)$$

$PPV = (sensitivity*Prevalence)/((sensitivity*Prevalence)+((1-specificity)*(1-Prevalence)))$

$NPV = (specificity*(1-Prevalence))/(((1-sensitivity)*Prevalence)+((specificity)*(1-Prevalence)))$

See the references for discussions of the statistics.

Value

A number between 0 and 1 (or NA).

Author(s)

Max Kuhn

References

Kuhn, M. (2008), "Building predictive models in R using the caret package, " *Journal of Statistical Software*, (http://www.jstatsoft.org/v28/i05/).

Altman, D.G., Bland, J.M. (1994) "Diagnostic tests 1: sensitivity and specificity," *British Medical Journal*, vol 308, 1552.

Altman, D.G., Bland, J.M. (1994) "Diagnostic tests 2: predictive values," *British Medical Journal*, vol 309, 102.

See Also

confusionMatrix

Examples

```
## Not run:
###################
## 2 class example

lvs <- c("normal", "abnormal")
truth <- factor(rep(lvs, times = c(86, 258)),
                levels = rev(lvs))
pred <- factor(
               c(
                 rep(lvs, times = c(54, 32)),
                 rep(lvs, times = c(27, 231))),
               levels = rev(lvs))

xtab <- table(pred, truth)

sensitivity(pred, truth)
sensitivity(xtab)
posPredValue(pred, truth)
posPredValue(pred, truth, prevalence = 0.25)

specificity(pred, truth)
negPredValue(pred, truth)
negPredValue(xtab)
negPredValue(pred, truth, prevalence = 0.25)


prev <- seq(0.001, .99, length = 20)
npvVals <- ppvVals <- prev  * NA
for(i in seq(along = prev))
  {
    ppvVals[i] <- posPredValue(pred, truth, prevalence = prev[i])
    npvVals[i] <- negPredValue(pred, truth, prevalence = prev[i])
  }
```

```
plot(prev, ppvVals,
     ylim = c(0, 1),
     type = "l",
     ylab = "",
     xlab = "Prevalence (i.e. prior)")
points(prev, npvVals, type = "l", col = "red")
abline(h=sensitivity(pred, truth), lty = 2)
abline(h=specificity(pred, truth), lty = 2, col = "red")
legend(.5, .5,
       c("ppv", "npv", "sens", "spec"),
       col = c("black", "red", "black", "red"),
       lty = c(1, 1, 2, 2))

###################
## 3 class example

library(MASS)

fit <- lda(Species ~ ., data = iris)
model <- predict(fit)$class

irisTabs <- table(model, iris$Species)

## When passing factors, an error occurs with more
## than two levels
sensitivity(model, iris$Species)

## When passing a table, more than two levels can
## be used
sensitivity(irisTabs, "versicolor")
specificity(irisTabs, c("setosa", "virginica"))

## End(Not run)
```

`spatialSign` *Compute the multivariate spatial sign*

Description

Compute the spatial sign (a projection of a data vector to a unit length circle). The spatial sign of a vector `w` is `w /norm(w)`.

Usage

```
## Default S3 method:
spatialSign(x)
## S3 method for class 'matrix'
spatialSign(x)
## S3 method for class 'data.frame'
spatialSign(x)
```

Arguments

x	an object full of numeric data (which should probably be scaled). Factors are not allowed. This could be a vector, matrix or data frame.

Value

A vector, matrix or data frame with the same dim names of the original data.

Author(s)

Max Kuhn

References

Serneels et al. Spatial sign preprocessing: a simple way to impart moderate robustness to multivariate estimators. J. Chem. Inf. Model (2006) vol. 46 (3) pp. 1402-1409

Examples

```
spatialSign(rnorm(5))

spatialSign(matrix(rnorm(12), ncol = 3))

# should fail since the fifth column is a factor
try(spatialSign(iris), silent = TRUE)

spatialSign(iris[,-5])

trellis.par.set(caretTheme())
featurePlot(iris[,-5], iris[,5], "pairs")
featurePlot(spatialSign(scale(iris[,-5])), iris[,5], "pairs")
```

---

summary.bagEarth *Summarize a bagged earth or FDA fit*

Description

The function shows a summary of the results from a bagged earth model

Usage

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

Arguments

object	an object of class "bagEarth" or "bagFDA"
...	optional arguments (not used)

Details

The out-of-bag statistics are summarized, as well as the distribution of the number of model terms and number of variables used across all the bootstrap samples.

Value

a list with elements

modelInfo	a matrix with the number of model terms and variables used
oobStat	a summary of the out-of-bag statistics
bmarsCall	the original call to bagEarth

Author(s)

Max Kuhn

Examples

```
## Not run:
data(trees)
fit <- bagEarth(trees[,-3], trees[3])
summary(fit)

## End(Not run)
```

---

tecator *Fat, Water and Protein Content of Meat Samples*

Description

"These data are recorded on a Tecator Infratec Food and Feed Analyzer working in the wavelength range 850 - 1050 nm by the Near Infrared Transmission (NIT) principle. Each sample contains finely chopped pure meat with different moisture, fat and protein contents.

If results from these data are used in a publication we want you to mention the instrument and company name (Tecator) in the publication. In addition, please send a preprint of your article to

Karin Thente, Tecator AB, Box 70, S-263 21 Hoganas, Sweden

The data are available in the public domain with no responsibility from the original data source. The data can be redistributed as long as this permission note is attached."

"For each meat sample the data consists of a 100 channel spectrum of absorbances and the contents of moisture (water), fat and protein. The absorbance is -log10 of the transmittance measured by the spectrometer. The three contents, measured in percent, are determined by analytic chemistry."

Included here are the traning, monitoring and test sets.

Usage

```
data(tecator)
```

Value

absorp	absorbance data for 215 samples. The first 129 were originally used as a training set
endpoints	the percentages of water, fat and protein

Examples

```
data(tecator)

splom(~endpoints)

# plot 10 random spectra
set.seed(1)
inSubset <- sample(1:dim(endpoints)[1], 10)

absorpSubset <- absorp[inSubset,]
endpointSubset <- endpoints[inSubset, 3]

newOrder <- order(absorpSubset[,1])
absorpSubset <- absorpSubset[newOrder,]
endpointSubset <- endpointSubset[newOrder]

plotColors <- rainbow(10)

plot(absorpSubset[1,],
     type = "n",
     ylim = range(absorpSubset),
     xlim = c(0, 105),
     xlab = "Wavelength Index",
     ylab = "Absorption")

for(i in 1:10)
{
   points(absorpSubset[i,], type = "l", col = plotColors[i], lwd = 2)
   text(105, absorpSubset[i,100], endpointSubset[i], col = plotColors[i])
}
title("Predictor Profiles for 10 Random Samples")
```

---

train *Fit Predictive Models over Different Tuning Parameters*

Description

This function sets up a grid of tuning parameters for a number of classification and regression routines, fits each model and calculates a resampling based performance measure.

Usage

```
train(x, ...)

## Default S3 method:
train(x, y,
      method = "rf",
      preProcess = NULL,
      ...,
      weights = NULL,
      metric = ifelse(is.factor(y), "Accuracy", "RMSE"),
      maximize = ifelse(metric == "RMSE", FALSE, TRUE),
      trControl = trainControl(),
      tuneGrid = NULL,
      tuneLength = 3)

## S3 method for class 'formula'
train(form, data, ..., weights, subset, na.action, contrasts = NULL)
```

Arguments

x	an object where samples are in rows and features are in columns. This could be a simple matrix, data frame or other type (e.g. sparse matrix). See Details below.
y	a numeric or factor vector containing the outcome for each sample.
form	A formula of the form `y ~ x1 + x2 + ...`
data	Data frame from which variables specified in `formula` are preferentially to be taken.
weights	a numeric vector of case weights. This argument will only affect models that allow case weights.
subset	An index vector specifying the cases to be used in the training sample. (NOTE: If given, this argument must be named.)
na.action	A function to specify the action to be taken if NAs are found. The default action is for the procedure to fail. An alternative is `na.omit`, which leads to rejection of cases with missing values on any required variable. (NOTE: If given, this argument must be named.)
contrasts	a list of contrasts to be used for some or all the factors appearing as variables in the model formula.
method	a string specifying which classification or regression model to use. Possible values are found using `names(getModelInfo())`. See http://topepo.github.io/caret/bytag.html. A list of functions can also be passed for a custom model function. See http://topepo.github.io/caret/custom_models.html for details.
...	arguments passed to the classification or regression routine (such as randomForest). Errors will occur if values for tuning parameters are passed here.

preProcess	a string vector that defines a pre-processing of the predictor data. Current possibilities are "BoxCox", "YeoJohnson", "expoTrans", "center", "scale", "range", "knnImpute", "bagImpute", "medianImpute", "pca", "ica" and "spatialSign". The default is no pre-processing. See preProcess and trainControl on the procedures and how to adjust them. Pre-processing code is only designed to work when x is a simple matrix or data frame.
metric	a string that specifies what summary metric will be used to select the optimal model. By default, possible values are "RMSE" and "Rsquared" for regression and "Accuracy" and "Kappa" for classification. If custom performance metrics are used (via the summaryFunction argument in trainControl, the value of metric should match one of the arguments. If it does not, a warning is issued and the first metric given by the summaryFunction is used. (NOTE: If given, this argument must be named.)
maximize	a logical: should the metric be maximized or minimized?
trControl	a list of values that define how this function acts. See trainControl and http://topepo.github.io/caret/training.html#custom. (NOTE: If given, this argument must be named.)
tuneGrid	a data frame with possible tuning values. The columns are named the same as the tuning parameters. Use getModelInfo to get a list of tuning parameters for each model or see http://topepo.github.io/caret/modelList.html. (NOTE: If given, this argument must be named.)
tuneLength	an integer denoting the number of levels for each tuning parameters that should be generated by train. (NOTE: If given, this argument must be named.)

Details

train can be used to tune models by picking the complexity parameters that are associated with the optimal resampling statistics. For particular model, a grid of parameters (if any) is created and the model is trained on slightly different data for each candidate combination of tuning parameters. Across each data set, the performance of held-out samples is calculated and the mean and standard deviation is summarized for each combination. The combination with the optimal resampling statistic is chosen as the final model and the entire training set is used to fit a final model.

The predictors in x can be most any object as long as the underlying model fit function can deal with the object class. The function was designed to work with simple matrices and data frame inputs, so some functionality may not work (e.g. pre-processing). When using string kernels, the vector of character strings should be converted to a matrix with a single column.

More details on this function can be found at http://topepo.github.io/caret/training.html.

A variety of models are currently available and are enumerated by tag (i.e. their model characteristics) at http://topepo.github.io/caret/bytag.html.

Value

A list is returned of class train containing:

method	the chosen model.
modelType	an identifier of the model type.

results	a data frame the training error rate and values of the tuning parameters.
bestTune	a data frame with the final parameters.
call	the (matched) function call with dots expanded
dots	a list containing any ... values passed to the original call
metric	a string that specifies what summary metric will be used to select the optimal model.
control	the list of control parameters.
preProcess	either NULL or an object of class preProcess
finalModel	an fit object using the best parameters
trainingData	a data frame
resample	A data frame with columns for each performance metric. Each row corresponds to each resample. If leave-one-out cross-validation or out-of-bag estimation methods are requested, this will be NULL. The returnResamp argument of trainControl controls how much of the resampled results are saved.
perfNames	a character vector of performance metrics that are produced by the summary function
maximize	a logical recycled from the function arguments.
yLimits	the range of the training set outcomes.
times	a list of execution times: everything is for the entire call to train, final for the final model fit and, optionally, prediction for the time to predict new samples (see trainControl)

Author(s)

Max Kuhn (the guts of train.formula were based on Ripley's nnet.formula)

References

http://topepo.github.io/caret/training.html

Kuhn (2008), "Building Predictive Models in R Using the caret" (http://www.jstatsoft.org/v28/i05/)

See Also

models, trainControl, update.train, modelLookup, createFolds

Examples

```
## Not run:

#######################################
## Classification Example

data(iris)
TrainData <- iris[,1:4]
TrainClasses <- iris[,5]
```

```
knnFit1 <- train(TrainData, TrainClasses,
                 method = "knn",
                 preProcess = c("center", "scale"),
                 tuneLength = 10,
                 trControl = trainControl(method = "cv"))

knnFit2 <- train(TrainData, TrainClasses,
                 method = "knn",
                 preProcess = c("center", "scale"),
                 tuneLength = 10,
                 trControl = trainControl(method = "boot"))


library(MASS)
nnetFit <- train(TrainData, TrainClasses,
                 method = "nnet",
                 preProcess = "range",
                 tuneLength = 2,
                 trace = FALSE,
                 maxit = 100)

########################################
## Regression Example

library(mlbench)
data(BostonHousing)

lmFit <- train(medv ~ . + rm:lstat,
               data = BostonHousing,
               method = "lm")

library(rpart)
rpartFit <- train(medv ~ .,
                  data = BostonHousing,
                  method = "rpart",
                  tuneLength = 9)

########################################
## Example with a custom metric

madSummary <- function (data,
                        lev = NULL,
                        model = NULL) {
  out <- mad(data$obs - data$pred,
             na.rm = TRUE)
  names(out) <- "MAD"
  out
}

robustControl <- trainControl(summaryFunction = madSummary)
marsGrid <- expand.grid(degree = 1, nprune = (1:10) * 2)
```

```
earthFit <- train(medv ~ .,
                  data = BostonHousing,
                  method = "earth",
                  tuneGrid = marsGrid,
                  metric = "MAD",
                  maximize = FALSE,
                  trControl = robustControl)

#######################################
## Parallel Processing Example via multicore package

## library(doMC)
## registerDoMC(2)

## NOTE: don't run models form RWeka when using
### multicore. The session will crash.

## The code for train() does not change:
set.seed(1)
usingMC <-  train(medv ~ .,
                  data = BostonHousing,
                  method = "glmboost")

## or use:
## library(doMPI) or
## library(doParallel) or
## library(doSMP) and so on


## End(Not run)
```

`trainControl` *Control parameters for train*

Description

Control the computational nuances of the `train` function

Usage

```
trainControl(method = "boot",
             number = ifelse(grepl("cv", method), 10, 25),
             repeats = ifelse(grepl("cv", method), 1, number),
             p = 0.75,
             initialWindow = NULL,
             horizon = 1,
             fixedWindow = TRUE,
             verboseIter = FALSE,
```

```
                returnData = TRUE,
                returnResamp = "final",
                savePredictions = FALSE,
                classProbs = FALSE,
                summaryFunction = defaultSummary,
                selectionFunction = "best",
                preProcOptions = list(thresh = 0.95, ICAcomp = 3, k = 5),
                index = NULL,
                indexOut = NULL,
                timingSamps = 0,
                predictionBounds = rep(FALSE, 2),
                seeds = NA,
                adaptive = list(min = 5, alpha = 0.05,
                                method = "gls", complete = TRUE),
                allowParallel = TRUE)
```

Arguments

method	The resampling method: boot, boot632, cv, repeatedcv, LOOCV, LGOCV (for repeated training/test splits), none (only fits one model to the entire training set), oob (only for random forest, bagged trees, bagged earth, bagged flexible discriminant analysis, or conditional tree forest models), "adaptive_cv", "adaptive_boot" or "adaptive_LGOCV"
number	Either the number of folds or number of resampling iterations
repeats	For repeated k-fold cross-validation only: the number of complete sets of folds to compute
verboseIter	A logical for printing a training log.
returnData	A logical for saving the data
returnResamp	A character string indicating how much of the resampled summary metrics should be saved. Values can be "final", "all" or "none"
savePredictions	a logical to save the hold-out predictions for each resample
p	For leave-group out cross-validation: the training percentage
initialWindow, horizon, fixedWindow	possible arguments to createTimeSlices
classProbs	a logical; should class probabilities be computed for classification models (along with predicted values) in each resample?
summaryFunction	a function to compute performance metrics across resamples. The arguments to the function should be the same as those in defaultSummary.
selectionFunction	the function used to select the optimal tuning parameter. This can be a name of the function or the function itself. See best for details and other options.
preProcOptions	A list of options to pass to preProcess. The type of pre-processing (e.g. center, scaling etc) is passed in via the preProc option in train.

index	a list with elements for each resampling iteration. Each list element is the sample rows used for training at that iteration.
indexOut	a list (the same length as index) that dictates which sample are held-out for each resample. If NULL, then the unique set of samples not contained in index is used.
timingSamps	the number of training set samples that will be used to measure the time for predicting samples (zero indicates that the prediction time should not be estimated.
predictionBounds	a logical or numeric vector of length 2 (regression only). If logical, the predictions can be constrained to be within the limit of the training set outcomes. For example, a value of c(TRUE, FALSE) would only constrain the lower end of predictions. If numeric, specific bounds can be used. For example, if c(10, NA), values below 10 would be predicted as 10 (with no constraint in the upper side).
seeds	an optional set of integers that will be used to set the seed at each resampling iteration. This is useful when the models are run in parallel. A value of NA will stop the seed from being set within the worker processes while a value of NULL will set the seeds using a random set of integers. Alternatively, a list can be used. The list should have B+1 elements where B is the number of resamples. The first B elements of the list should be vectors of integers of length M where M is the number of models being evaluated. The last element of the list only needs to be a single integer (for the final model). See the Examples section below and the Details section.
adaptive	a list used when method is "adaptive_cv", "adaptive_boot" or "adaptive_LGOCV". See Details below.
allowParallel	if a parallel backend is loaded and available, should the function use it?

Details

When setting the seeds manually, the number of models being evaluated is required. This may not be obvious as train does some optimizations for certain models. For example, when tuning over PLS model, the only model that is fit is the one with the largest number of components. So if the model is being tuned over comp in 1:10, the only model fit is ncomp = 10. However, if the vector of integers used in the seeds arguments is longer than actually needed, no error is thrown.

Using method = "none" and specifying model than one model in train's tuneGrid or tuneLength arguments will result in an error.

Using adaptive resampling when method is either "adaptive_cv", "adaptive_boot" or "adaptive_LGOCV", the full set of resamples is not run for each model. As resampling continues, a futility analysis is conducted and models with a low probability of being optimal are removed. These features are experimental. See Kuhn (2014) for more details. The options for this procedure are:

- min: the minimum number of resamples used before models are removed
- alpha: the confidence level of the one-sided intervals used to measure futility
- method: either generalized least squares (method = "gls") or a Bradley-Terry model (method = "BT")
- complete: if a single parameter value is found before the end of resampling, should the full set of resamples be computed for that parameter.)

Value

An echo of the parameters specified

Author(s)

Max Kuhn

References

Kuhn (2014), "Futility Analysis in the Cross-Validation of Machine Learning Models" http://arxiv.org/abs/1405.6974

Examples

```
## Not run:

## Do 5 repeats of 10-Fold CV for the iris data. We will fit
## a KNN model that evaluates 12 values of k and set the seed
## at each iteration.

set.seed(123)
seeds <- vector(mode = "list", length = 51)
for(i in 1:50) seeds[[i]] <- sample.int(1000, 22)

## For the last model:
seeds[[51]] <- sample.int(1000, 1)

ctrl <- trainControl(method = "repeatedcv",
                     repeats = 5,
                     seeds = seeds)

set.seed(1)
mod <- train(Species ~ ., data = iris,
             method = "knn",
             tuneLength = 12,
             trControl = ctrl)


ctrl2 <- trainControl(method = "adaptive_cv",
                      repeats = 5,
                      verboseIter = TRUE,
                      seeds = seeds)

set.seed(1)
mod2 <- train(Species ~ ., data = iris,
              method = "knn",
              tuneLength = 12,
              trControl = ctrl2)


## End(Not run)
```

`train_model_list` *A List of Available Models in train*

Description

These models are included in the package via wrappers for `train`. Custom models can also be created. See the URL below.

AdaBoost.M1 (`method = 'AdaBoost.M1'`)

For classification using package **adabag** with tuning parameters:

- Number of Trees (`mfinal`, numeric)
- Max Tree Depth (`maxdepth`, numeric)
- Coefficient Type (`coeflearn`, character)

Adaptive Mixture Discriminant Analysis (`method = 'amdai'`)

For classification using package **adaptDA** with tuning parameters:

- Model Type (`model`, character)

Adaptive-Network-Based Fuzzy Inference System (`method = 'ANFIS'`)

For regression using package **frbs** with tuning parameters:

- Number of Fuzzy Terms (`num.labels`, numeric)
- Max. Iterations (`max.iter`, numeric)

Bagged AdaBoost (`method = 'AdaBag'`)

For classification using package **adabag** with tuning parameters:

- Number of Trees (`mfinal`, numeric)
- Max Tree Depth (`maxdepth`, numeric)

Bagged CART (`method = 'treebag'`)

For classification and regression using packages **ipred** and **plyr** with no tuning parameters

Bagged FDA using gCV Pruning (`method = 'bagFDAGCV'`)

For classification using package **earth** with tuning parameters:

- Product Degree (`degree`, numeric)

Bagged Flexible Discriminant Analysis (`method = 'bagFDA'`)

For classification using packages **earth** and **mda** with tuning parameters:

- Product Degree (`degree`, numeric)
- Number of Terms (`nprune`, numeric)

Bagged Logic Regression (`method = 'logicBag'`)

For classification and regression using package **logicFS** with tuning parameters:

- Maximum Number of Leaves (nleaves, numeric)
- Number of Trees (ntrees, numeric)

Bagged MARS (method = 'bagEarth')

For classification and regression using package **earth** with tuning parameters:

- Number of Terms (nprune, numeric)
- Product Degree (degree, numeric)

Bagged MARS using gCV Pruning (method = 'bagEarthGCV')

For classification and regression using package **earth** with tuning parameters:

- Product Degree (degree, numeric)

Bagged Model (method = 'bag')

For classification and regression using package **caret** with tuning parameters:

- Number of Randomly Selected Predictors (vars, numeric)

Bayesian Generalized Linear Model (method = 'bayesglm')

For classification and regression using package **arm** with no tuning parameters

Bayesian Regularized Neural Networks (method = 'brnn')

For regression using package **brnn** with tuning parameters:

- Number of Neurons (neurons, numeric)

Binary Discriminant Analysis (method = 'binda')

For classification using package **binda** with tuning parameters:

- Shrinkage Intensity (lambda.freqs, numeric)

Boosted Classification Trees (method = 'ada')

For classification using package **ada** with tuning parameters:

- Number of Trees (iter, numeric)
- Max Tree Depth (maxdepth, numeric)
- Learning Rate (nu, numeric)

Boosted Generalized Additive Model (method = 'gamboost')

For classification and regression using package **mboost** with tuning parameters:

- Number of Boosting Iterations (mstop, numeric)
- AIC Prune? (prune, character)

Boosted Generalized Linear Model (method = 'glmboost')

For classification and regression using package **mboost** with tuning parameters:

- Number of Boosting Iterations (mstop, numeric)
- AIC Prune? (prune, character)

Boosted Linear Model (`method = 'bstLs'`)

For classification and regression using packages **bst** and **plyr** with tuning parameters:

- Number of Boosting Iterations (`mstop`, numeric)
- Shrinkage (`nu`, numeric)

Boosted Logistic Regression (`method = 'LogitBoost'`)

For classification using package **caTools** with tuning parameters:

- Number of Boosting Iterations (`nIter`, numeric)

Boosted Smoothing Spline (`method = 'bstSm'`)

For classification and regression using packages **bst** and **plyr** with tuning parameters:

- Number of Boosting Iterations (`mstop`, numeric)
- Shrinkage (`nu`, numeric)

Boosted Tree (`method = 'blackboost'`)

For classification and regression using packages **party**, **mboost** and **plyr** with tuning parameters:

- Number of Trees (`mstop`, numeric)
- Max Tree Depth (`maxdepth`, numeric)

Boosted Tree (`method = 'bstTree'`)

For classification and regression using packages **bst** and **plyr** with tuning parameters:

- Number of Boosting Iterations (`mstop`, numeric)
- Max Tree Depth (`maxdepth`, numeric)
- Shrinkage (`nu`, numeric)

C4.5-like Trees (`method = 'J48'`)

For classification using package **RWeka** with tuning parameters:

- Confidence Threshold (`C`, numeric)

C5.0 (`method = 'C5.0'`)

For classification using packages **C50** and **plyr** with tuning parameters:

- Number of Boosting Iterations (`trials`, numeric)
- Model Type (`model`, character)
- Winnow (`winnow`, logical)

CART (`method = 'rpart'`)

For classification and regression using package **rpart** with tuning parameters:

- Complexity Parameter (`cp`, numeric)

CART (`method = 'rpart2'`)

For classification and regression using package **rpart** with tuning parameters:

- Max Tree Depth (maxdepth, numeric)

Conditional Inference Random Forest (method = 'cforest')

For classification and regression using package **party** with tuning parameters:

- Number of Randomly Selected Predictors (mtry, numeric)

Conditional Inference Tree (method = 'ctree')

For classification and regression using package **party** with tuning parameters:

- 1 - P-Value Threshold (mincriterion, numeric)

Conditional Inference Tree (method = 'ctree2')

For classification and regression using package **party** with tuning parameters:

- Max Tree Depth (maxdepth, numeric)

Cost-Sensitive C5.0 (method = 'C5.0Cost')

For classification using packages **C50** and **plyr** with tuning parameters:

- Number of Boosting Iterations (trials, numeric)
- Model Type (model, character)
- Winnow (winnow, logical)
- Cost (cost, numeric)

Cost-Sensitive CART (method = 'rpartCost')

For classification using package **rpart** with tuning parameters:

- Complexity Parameter (cp, numeric)
- Cost (Cost, numeric)

Cubist (method = 'cubist')

For regression using package **Cubist** with tuning parameters:

- Number of Committees (committees, numeric)
- Number of Instances (neighbors, numeric)

Dynamic Evolving Neural-Fuzzy Inference System (method = 'DENFIS')

For regression using package **frbs** with tuning parameters:

- Threshold (Dthr, numeric)
- Max. Iterations (max.iter, numeric)

Elasticnet (method = 'enet')

For regression using package **elasticnet** with tuning parameters:

- Fraction of Full Solution (fraction, numeric)
- Weight Decay (lambda, numeric)

Ensemble Partial Least Squares Regression (`method = 'enpls'`)

For regression using package **enpls** with tuning parameters:

- Max. Number of Components (`maxcomp`, numeric)

Ensemble Partial Least Squares Regression with Feature Selection (`method = 'enpls.fs'`)

For regression using package **enpls** with tuning parameters:

- Max. Number of Components (`maxcomp`, numeric)
- Importance Cutoff (`threshold`, numeric)

Extreme Learning Machine (`method = 'elm'`)

For classification and regression using package **elmNN** with tuning parameters:

- Number of Hidden Units (`nhid`, numeric)
- Activation Function (`actfun`, character)

Factor-Based Linear Discriminant Analysis (`method = 'RFlda'`)

For classification using package **HiDimDA** with tuning parameters:

- Number of Factors (`q`, numeric)

Flexible Discriminant Analysis (`method = 'fda'`)

For classification using packages **earth** and **mda** with tuning parameters:

- Product Degree (`degree`, numeric)
- Number of Terms (`nprune`, numeric)

Fuzzy Inference Rules by Descent Method (`method = 'FIR.DM'`)

For regression using package **frbs** with tuning parameters:

- Number of Fuzzy Terms (`num.labels`, numeric)
- Max. Iterations (`max.iter`, numeric)

Fuzzy Rules Using Chi's Method (`method = 'FRBCS.CHI'`)

For classification using package **frbs** with tuning parameters:

- Number of Fuzzy Terms (`num.labels`, numeric)
- Membership Function (`type.mf`, character)

Fuzzy Rules Using Genetic Cooperative-Competitive Learning (`method = 'GFS.GCCL'`)

For classification using package **frbs** with tuning parameters:

- Number of Fuzzy Terms (`num.labels`, numeric)
- Population Size (`popu.size`, numeric)
- Max. Generations (`max.gen`, numeric)

Fuzzy Rules Using Genetic Cooperative-Competitive Learning and Pittsburgh (`method = 'FH.GBML'`)

For classification using package **frbs** with tuning parameters:

- Max. Number of Rules (max.num.rule, numeric)
- Population Size (popu.size, numeric)
- Max. Generations (max.gen, numeric)

Fuzzy Rules Using the Structural Learning Algorithm on Vague Environment (method = 'SLAVE')

For classification using package **frbs** with tuning parameters:

- Number of Fuzzy Terms (num.labels, numeric)
- Max. Iterations (max.iter, numeric)
- Max. Generations (max.gen, numeric)

Fuzzy Rules via MOGUL (method = 'GFS.FR.MOGAL')

For regression using package **frbs** with tuning parameters:

- Max. Generations (max.gen, numeric)
- Max. Iterations (max.iter, numeric)
- Max. Tuning Iterations (max.tune, numeric)

Fuzzy Rules via Thrift (method = 'GFS.THRIFT')

For regression using package **frbs** with tuning parameters:

- Population Size (popu.size, numeric)
- Number of Fuzzy Labels (num.labels, numeric)
- Max. Generations (max.gen, numeric)

Fuzzy Rules with Weight Factor (method = 'FRBCS.W')

For classification using package **frbs** with tuning parameters:

- Number of Fuzzy Terms (num.labels, numeric)
- Membership Function (type.mf, character)

Gaussian Process (method = 'gaussprLinear')

For classification and regression using package **kernlab** with no tuning parameters

Gaussian Process with Polynomial Kernel (method = 'gaussprPoly')

For classification and regression using package **kernlab** with tuning parameters:

- Polynomial Degree (degree, numeric)
- Scale (scale, numeric)

Gaussian Process with Radial Basis Function Kernel (method = 'gaussprRadial')

For classification and regression using package **kernlab** with tuning parameters:

- Sigma (sigma, numeric)

Generalized Additive Model using LOESS (method = 'gamLoess')

For classification and regression using package **gam** with tuning parameters:

- Span (span, numeric)
- Degree (degree, numeric)

Generalized Additive Model using Splines (method = 'gam')

For classification and regression using package **mgcv** with tuning parameters:

- Feature Selection (select, logical)
- Method (method, character)

Generalized Additive Model using Splines (method = 'gamSpline')

For classification and regression using package **gam** with tuning parameters:

- Degrees of Freedom (df, numeric)

Generalized Linear Model (method = 'glm')

For classification and regression with no tuning parameters

Generalized Linear Model with Stepwise Feature Selection (method = 'glmStepAIC')

For classification and regression using package **MASS** with no tuning parameters

Generalized Partial Least Squares (method = 'gpls')

For classification using package **gpls** with tuning parameters:

- Number of Components (K.prov, numeric)

Genetic Lateral Tuning and Rule Selection of Linguistic Fuzzy Systems (method = 'GFS.LT.RS')

For regression using package **frbs** with tuning parameters:

- Population Size (popu.size, numeric)
- Number of Fuzzy Labels (num.labels, numeric)
- Max. Generations (max.gen, numeric)

glmnet (method = 'glmnet')

For classification and regression using package **glmnet** with tuning parameters:

- Mixing Percentage (alpha, numeric)
- Regularization Parameter (lambda, numeric)

Greedy Prototype Selection (method = 'protoclass')

For classification using packages **proxy** and **protoclass** with tuning parameters:

- Ball Size (eps, numeric)
- Distance Order (Minkowski, numeric)

Heteroscedastic Discriminant Analysis (method = 'hda')

For classification using package **hda** with tuning parameters:

- Gamma (gamma, numeric)
- Lambda (lambda, numeric)

- Dimension of the Discriminative Subspace (`newdim`, numeric)

High Dimensional Discriminant Analysis (`method = 'hdda'`)

For classification using package **HDclassif** with tuning parameters:

- Threshold (`threshold`, character)
- Model Type (`model`, numeric)

Hybrid Neural Fuzzy Inference System (`method = 'HYFIS'`)

For regression using package **frbs** with tuning parameters:

- Number of Fuzzy Terms (`num.labels`, numeric)
- Max. Iterations (`max.iter`, numeric)

Independent Component Regression (`method = 'icr'`)

For regression using package **fastICA** with tuning parameters:

- Number of Components (`n.comp`, numeric)

k-Nearest Neighbors (`method = 'kknn'`)

For classification and regression using package **kknn** with tuning parameters:

- Max. Number of Neighbors (`kmax`, numeric)
- Distance (`distance`, numeric)
- Kernel (`kernel`, character)

k-Nearest Neighbors (`method = 'knn'`)

For classification and regression with tuning parameters:

- Number of Neighbors (`k`, numeric)

Learning Vector Quantization (`method = 'lvq'`)

For classification using package **class** with tuning parameters:

- Codebook Size (`size`, numeric)
- Number of Prototypes (`k`, numeric)

Least Angle Regression (`method = 'lars'`)

For regression using package **lars** with tuning parameters:

- Fraction (`fraction`, numeric)

Least Angle Regression (`method = 'lars2'`)

For regression using package **lars** with tuning parameters:

- Number of Steps (`step`, numeric)

Least Squares Support Vector Machine (`method = 'lssvmLinear'`)

For classification using package **kernlab** with no tuning parameters

Least Squares Support Vector Machine with Polynomial Kernel (`method = 'lssvmPoly'`)

For classification using package **kernlab** with tuning parameters:

- Polynomial Degree (degree, numeric)
- Scale (scale, numeric)

Least Squares Support Vector Machine with Radial Basis Function Kernel (method = 'lssvmRadial')
For classification using package **kernlab** with tuning parameters:

- Sigma (sigma, numeric)

Linear Discriminant Analysis (method = 'lda')
For classification using package **MASS** with no tuning parameters
Linear Discriminant Analysis (method = 'lda2')
For classification using package **MASS** with tuning parameters:

- Number of Discriminant Functions (dimen, numeric)

Linear Discriminant Analysis with Stepwise Feature Selection (method = 'stepLDA')
For classification using packages **klaR** and **MASS** with tuning parameters:

- Maximum Number of Variables (maxvar, numeric)
- Search Direction (direction, character)

Linear Regression (method = 'lm')
For regression with no tuning parameters
Linear Regression with Backwards Selection (method = 'leapBackward')
For regression using package **leaps** with tuning parameters:

- Maximum Number of Predictors (nvmax, numeric)

Linear Regression with Forward Selection (method = 'leapForward')
For regression using package **leaps** with tuning parameters:

- Maximum Number of Predictors (nvmax, numeric)

Linear Regression with Stepwise Selection (method = 'leapSeq')
For regression using package **leaps** with tuning parameters:

- Maximum Number of Predictors (nvmax, numeric)

Linear Regression with Stepwise Selection (method = 'lmStepAIC')
For regression using package **MASS** with no tuning parameters
Logic Regression (method = 'logreg')
For classification and regression using package **LogicReg** with tuning parameters:

- Maximum Number of Leaves (treesize, numeric)
- Number of Trees (ntrees, numeric)

Logistic Model Trees (method = 'LMT')
For classification using package **RWeka** with tuning parameters:

- Number of Iteratons (iter, numeric)

Maximum Uncertainty Linear Discriminant Analysis (method = 'Mlda')

For classification using package **HiDimDA** with no tuning parameters

Mixture Discriminant Analysis (method = 'mda')

For classification using package **mda** with tuning parameters:

- Number of Subclasses Per Class (subclasses, numeric)

Model Averaged Neural Network (method = 'avNNet')

For classification and regression using package **nnet** with tuning parameters:

- Number of Hidden Units (size, numeric)
- Weight Decay (decay, numeric)
- Bagging (bag, logical)

Model Rules (method = 'M5Rules')

For regression using package **RWeka** with tuning parameters:

- Pruned (pruned, character)
- Smoothed (smoothed, character)

Model Tree (method = 'M5')

For regression using package **RWeka** with tuning parameters:

- Pruned (pruned, character)
- Smoothed (smoothed, character)
- Rules (rules, character)

Multi-Layer Perceptron (method = 'mlp')

For classification and regression using package **RSNNS** with tuning parameters:

- Number of Hidden Units (size, numeric)

Multi-Layer Perceptron (method = 'mlpWeightDecay')

For classification and regression using package **RSNNS** with tuning parameters:

- Number of Hidden Units (size, numeric)
- Weight Decay (decay, numeric)

Multivariate Adaptive Regression Spline (method = 'earth')

For classification and regression using package **earth** with tuning parameters:

- Number of Terms (nprune, numeric)
- Product Degree (degree, numeric)

Multivariate Adaptive Regression Splines (method = 'gcvEarth')

For classification and regression using package **earth** with tuning parameters:

- Product Degree (degree, numeric)

Naive Bayes (method = 'nb')

For classification using package **klaR** with tuning parameters:

- Laplace Correction (fL, numeric)
- Distribution Type (usekernel, logical)

Nearest Shrunken Centroids (method = 'pam')

For classification using package **pamr** with tuning parameters:

- Shrinkage Threshold (threshold, numeric)

Neural Network (method = 'neuralnet')

For regression using package **neuralnet** with tuning parameters:

- Number of Hidden Units in Layer 1 (layer1, numeric)
- Number of Hidden Units in Layer 2 (layer2, numeric)
- Number of Hidden Units in Layer 3 (layer3, numeric)

Neural Network (method = 'nnet')

For classification and regression using package **nnet** with tuning parameters:

- Number of Hidden Units (size, numeric)
- Weight Decay (decay, numeric)

Neural Networks with Feature Extraction (method = 'pcaNNet')

For classification and regression using package **nnet** with tuning parameters:

- Number of Hidden Units (size, numeric)
- Weight Decay (decay, numeric)

Oblique Random Forest (method = 'ORFlog')

For classification using package **obliqueRF** with tuning parameters:

- Number of Randomly Selected Predictors (mtry, numeric)

Oblique Random Forest (method = 'ORFpls')

For classification using package **obliqueRF** with tuning parameters:

- Number of Randomly Selected Predictors (mtry, numeric)

Oblique Random Forest (method = 'ORFridge')

For classification using package **obliqueRF** with tuning parameters:

- Number of Randomly Selected Predictors (mtry, numeric)

Oblique Random Forest (method = 'ORFsvm')

For classification using package **obliqueRF** with tuning parameters:

- Number of Randomly Selected Predictors (`mtry`, numeric)

Oblique Trees (`method = 'oblique.tree'`)

For classification using package **oblique.tree** with tuning parameters:

- Oblique Splits (`oblique.splits`, character)
- Variable Selection Method (`variable.selection`, character)

Ordered Logistic or Probit Regression (`method = 'polr'`)

For classification using package **MASS** with no tuning parameters

Parallel Random Forest (`method = 'parRF'`)

For classification and regression using package **randomForest** with tuning parameters:

- Number of Randomly Selected Predictors (`mtry`, numeric)

partDSA (`method = 'partDSA'`)

For classification and regression using package **partDSA** with tuning parameters:

- Number of Terminal Partitions (`cut.off.growth`, numeric)
- Minimum Percent Difference (`MPD`, numeric)

Partial Least Squares (`method = 'kernelpls'`)

For classification and regression using package **pls** with tuning parameters:

- Number of Components (`ncomp`, numeric)

Partial Least Squares (`method = 'pls'`)

For classification and regression using package **pls** with tuning parameters:

- Number of Components (`ncomp`, numeric)

Partial Least Squares (`method = 'simpls'`)

For classification and regression using package **pls** with tuning parameters:

- Number of Components (`ncomp`, numeric)

Partial Least Squares (`method = 'widekernelpls'`)

For classification and regression using package **pls** with tuning parameters:

- Number of Components (`ncomp`, numeric)

Partial Least Squares Generalized Linear Models (`method = 'plsRglm'`)

For classification and regression using package **plsRglm** with tuning parameters:

- Number of PLS Components (`nt`, numeric)
- p-Value threshold (`alpha.pvals.expli`, numeric)

Penalized Discriminant Analysis (`method = 'pda'`)

For classification using package **mda** with tuning parameters:

- Shrinkage Penalty Coefficient (lambda, numeric)

Penalized Discriminant Analysis (method = 'pda2')

For classification using package **mda** with tuning parameters:

- Degrees of Freedom (df, numeric)

Penalized Linear Discriminant Analysis (method = 'PenalizedLDA')

For classification using packages **penalizedLDA** and **plyr** with tuning parameters:

- L1 Penalty (lambda, numeric)
- Number of Discriminant Functions (K, numeric)

Penalized Linear Regression (method = 'penalized')

For regression using package **penalized** with tuning parameters:

- L1 Penalty (lambda1, numeric)
- L2 Penalty (lambda2, numeric)

Penalized Logistic Regression (method = 'plr')

For classification using package **stepPlr** with tuning parameters:

- L2 Penalty (lambda, numeric)
- Complexity Parameter (cp, character)

Penalized Multinomial Regression (method = 'multinom')

For classification using package **nnet** with tuning parameters:

- Weight Decay (decay, numeric)

Polynomial Kernel Regularized Least Squares (method = 'krlsPoly')

For regression using package **KRLS** with tuning parameters:

- Regularization Parameter (lambda, numeric)
- Polynomial Degree (degree, numeric)

Principal Component Analysis (method = 'pcr')

For regression using package **pls** with tuning parameters:

- Number of Components (ncomp, numeric)

Projection Pursuit Regression (method = 'ppr')

For regression with tuning parameters:

- Number of Terms (nterms, numeric)

Quadratic Discriminant Analysis (method = 'qda')

For classification using package **MASS** with no tuning parameters

Quadratic Discriminant Analysis with Stepwise Feature Selection (method = 'stepQDA')

For classification using packages **klaR** and **MASS** with tuning parameters:

- Maximum Number of Variables (maxvar, numeric)
- Search Direction (direction, character)

Quantile Random Forest (method = 'qrf')

For regression using package **quantregForest** with tuning parameters:

- Number of Randomly Selected Predictors (mtry, numeric)

Quantile Regression Neural Network (method = 'qrnn')

For regression using package **qrnn** with tuning parameters:

- Number of Hidden Units (n.hidden, numeric)
- Weight Decay (penalty, numeric)
- Bagged Models? (bag, logical)

Radial Basis Function Kernel Regularized Least Squares (method = 'krlsRadial')

For regression using packages **KRLS** and **kernlab** with tuning parameters:

- Regularization Parameter (lambda, numeric)
- Sigma (sigma, numeric)

Radial Basis Function Network (method = 'rbf')

For classification using package **RSNNS** with tuning parameters:

- Number of Hidden Units (size, numeric)

Radial Basis Function Network (method = 'rbfDDA')

For classification and regression using package **RSNNS** with tuning parameters:

- Activation Limit for Conflicting Classes (negativeThreshold, numeric)

Random Ferns (method = 'rFerns')

For classification using package **rFerns** with tuning parameters:

- Fern Depth (depth, numeric)

Random Forest (method = 'rf')

For classification and regression using package **randomForest** with tuning parameters:

- Number of Randomly Selected Predictors (mtry, numeric)

Random Forest by Randomization (method = 'extraTrees')

For classification and regression using package **extraTrees** with tuning parameters:

- Number of Randomly Selected Predictors (mtry, numeric)
- Number of Random Cuts (numRandomCuts, numeric)

Random Forest with Additional Feature Selection (method = 'Boruta')

For classification and regression using packages **Boruta** and **randomForest** with tuning parameters:

- Number of Randomly Selected Predictors (`mtry`, numeric)

Random k-Nearest Neighbors (`method = 'rknn'`)

For classification and regression using package **rknn** with tuning parameters:

- Number of Neighbors (`k`, numeric)
- Number of Randomly Selected Predictors (`mtry`, numeric)

Random k-Nearest Neighbors with Feature Selection (`method = 'rknnBel'`)

For classification and regression using packages **rknn** and **plyr** with tuning parameters:

- Number of Neighbors (`k`, numeric)
- Number of Randomly Selected Predictors (`mtry`, numeric)
- Number of Features Dropped (`d`, numeric)

Regularized Discriminant Analysis (`method = 'rda'`)

For classification using package **klaR** with tuning parameters:

- Gamma (`gamma`, numeric)
- Lambda (`lambda`, numeric)

Regularized Random Forest (`method = 'RRF'`)

For classification and regression using packages **randomForest** and **RRF** with tuning parameters:

- Number of Randomly Selected Predictors (`mtry`, numeric)
- Regularization Value (`coefReg`, numeric)
- Importance Coefficient (`coefImp`, numeric)

Regularized Random Forest (`method = 'RRFglobal'`)

For classification and regression using package **RRF** with tuning parameters:

- Number of Randomly Selected Predictors (`mtry`, numeric)
- Regularization Value (`coefReg`, numeric)

Relaxed Lasso (`method = 'relaxo'`)

For regression using packages **relaxo** and **plyr** with tuning parameters:

- Penalty Parameter (`lambda`, numeric)
- Relaxation Parameter (`phi`, numeric)

Relevance Vector Machines with Linear Kernel (`method = 'rvmLinear'`)

For regression using package **kernlab** with no tuning parameters

Relevance Vector Machines with Polynomial Kernel (`method = 'rvmPoly'`)

For regression using package **kernlab** with tuning parameters:

- Scale (`scale`, numeric)
- Polynomial Degree (`degree`, numeric)

Relevance Vector Machines with Radial Basis Function Kernel (`method = 'rvmRadial'`)

For regression using package **kernlab** with tuning parameters:

- Sigma (`sigma`, numeric)

Ridge Regression (`method = 'ridge'`)

For regression using package **elasticnet** with tuning parameters:

- Weight Decay (`lambda`, numeric)

Ridge Regression with Variable Selection (`method = 'foba'`)

For regression using package **foba** with tuning parameters:

- Number of Variables Retained (`k`, numeric)
- L2 Penalty (`lambda`, numeric)

Robust Linear Discriminant Analysis (`method = 'Linda'`)

For classification using package **rrcov** with no tuning parameters

Robust Linear Model (`method = 'rlm'`)

For regression using package **MASS** with no tuning parameters

Robust Mixture Discriminant Analysis (`method = 'rmda'`)

For classification using package **robustDA** with tuning parameters:

- Number of Subclasses Per Class (`K`, numeric)
- Model (`model`, character)

Robust Quadratic Discriminant Analysis (`method = 'QdaCov'`)

For classification using package **rrcov** with no tuning parameters

Robust Regularized Linear Discriminant Analysis (`method = 'rrlda'`)

For classification using package **rrlda** with tuning parameters:

- Penalty Parameter (`lambda`, numeric)
- Robustness Parameter (`hp`, numeric)
- Penalty Type (`penalty`, character)

Robust SIMCA (`method = 'RSimca'`)

For classification using package **rrcovHD** with no tuning parameters

ROC-Based Classifier (`method = 'rocc'`)

For classification using package **rocc** with tuning parameters:

- Number of Variables Retained (`xgenes`, numeric)

Rule-Based Classifier (`method = 'JRip'`)

For classification using package **RWeka** with tuning parameters:

- Number of Optimizations (`NumOpt`, numeric)

Rule-Based Classifier (`method = 'PART'`)

For classification using package **RWeka** with tuning parameters:

- Confidence Threshold (`threshold`, numeric)
- Confidence Threshold (`pruned`, character)

Self-Organizing Map (`method = 'bdk'`)

For classification and regression using package **kohonen** with tuning parameters:

- Row (`xdim`, numeric)
- Columns (`ydim`, numeric)
- X Weight (`xweight`, numeric)
- Topology (`topo`, character)

Self-Organizing Maps (`method = 'xyf'`)

For classification and regression using package **kohonen** with tuning parameters:

- Row (`xdim`, numeric)
- Columns (`ydim`, numeric)
- X Weight (`xweight`, numeric)
- Topology (`topo`, character)

Shrinkage Discriminant Analysis (`method = 'sda'`)

For classification using package **sda** with tuning parameters:

- Diagonalize (`diagonal`, logical)
- shrinkage (`lambda`, numeric)

SIMCA (`method = 'CSimca'`)

For classification using package **rrcovHD** with no tuning parameters

Simplified TSK Fuzzy Rules (`method = 'FS.HGD'`)

For regression using package **frbs** with tuning parameters:

- Number of Fuzzy Terms (`num.labels`, numeric)
- Max. Iterations (`max.iter`, numeric)

Single C5.0 Ruleset (`method = 'C5.0Rules'`)

For classification using package **C50** with no tuning parameters

Single C5.0 Tree (`method = 'C5.0Tree'`)

For classification using package **C50** with no tuning parameters

Single Rule Classification (`method = 'OneR'`)

For classification using package **RWeka** with no tuning parameters

Sparse Linear Discriminant Analysis (`method = 'sparseLDA'`)

For classification using package **sparseLDA** with tuning parameters:

- Number of Predictors (NumVars, numeric)
- Lambda (lambda, numeric)

Sparse Mixture Discriminant Analysis (method = 'smda')

For classification using package **sparseLDA** with tuning parameters:

- Number of Predictors (NumVars, numeric)
- Lambda (lambda, numeric)
- Number of Subclasses (R, numeric)

Sparse Partial Least Squares (method = 'spls')

For classification and regression using package **spls** with tuning parameters:

- Number of Components (K, numeric)
- Threshold (eta, numeric)
- Kappa (kappa, numeric)

Stabilized Linear Discriminant Analysis (method = 'slda')

For classification using package **ipred** with no tuning parameters

Stacked AutoEncoder Deep Neural Network (method = 'dnn')

For classification and regression using package **deepnet** with tuning parameters:

- Hidden Layer 1 (layer1, numeric)
- Hidden Layer 2 (layer2, numeric)
- Hidden Layer 3 (layer3, numeric)
- Hidden Dropouts (hidden_dropout, numeric)
- Visible Dropout (visible_dropout, numeric)

Stepwise Diagonal Linear Discriminant Analysis (method = 'sddaLDA')

For classification using package **SDDA** with no tuning parameters

Stepwise Diagonal Quadratic Discriminant Analysis (method = 'sddaQDA')

For classification using package **SDDA** with no tuning parameters

Stochastic Gradient Boosting (method = 'gbm')

For classification and regression using packages **gbm** and **plyr** with tuning parameters:

- Number of Boosting Iterations (n.trees, numeric)
- Max Tree Depth (interaction.depth, numeric)
- Shrinkage (shrinkage, numeric)

Subtractive Clustering and Fuzzy c-Means Rules (method = 'SBC')

For regression using package **frbs** with tuning parameters:

- Radius (r.a, numeric)
- Upper Threshold (eps.high, numeric)

- Lower Threshold (`eps.low`, numeric)

Supervised Principal Component Analysis (`method = 'superpc'`)

For regression using package **superpc** with tuning parameters:

- Threshold (`threshold`, numeric)
- Number of Components (`n.components`, numeric)

Support Vector Machines with Boundrange String Kernel (`method = 'svmBoundrangeString'`)

For classification and regression using package **kernlab** with tuning parameters:

- length (`length`, numeric)
- Cost (`C`, numeric)

Support Vector Machines with Class Weights (`method = 'svmRadialWeights'`)

For classification using package **kernlab** with tuning parameters:

- Sigma (`sigma`, numeric)
- Cost (`C`, numeric)
- Weight (`Weight`, numeric)

Support Vector Machines with Exponential String Kernel (`method = 'svmExpoString'`)

For classification and regression using package **kernlab** with tuning parameters:

- lambda (`lambda`, numeric)
- Cost (`C`, numeric)

Support Vector Machines with Linear Kernel (`method = 'svmLinear'`)

For classification and regression using package **kernlab** with tuning parameters:

- Cost (`C`, numeric)

Support Vector Machines with Polynomial Kernel (`method = 'svmPoly'`)

For classification and regression using package **kernlab** with tuning parameters:

- Polynomial Degree (`degree`, numeric)
- Scale (`scale`, numeric)
- Cost (`C`, numeric)

Support Vector Machines with Radial Basis Function Kernel (`method = 'svmRadial'`)

For classification and regression using package **kernlab** with tuning parameters:

- Sigma (`sigma`, numeric)
- Cost (`C`, numeric)

Support Vector Machines with Radial Basis Function Kernel (`method = 'svmRadialCost'`)

For classification and regression using package **kernlab** with tuning parameters:

- Cost (`C`, numeric)

Support Vector Machines with Spectrum String Kernel (`method = 'svmSpectrumString'`)

For classification and regression using package **kernlab** with tuning parameters:

- length (`length`, numeric)
- Cost (`C`, numeric)

The lasso (`method = 'lasso'`)

For regression using package **elasticnet** with tuning parameters:

- Fraction of Full Solution (`fraction`, numeric)

Tree Models from Genetic Algorithms (`method = 'evtree'`)

For classification and regression using package **evtree** with tuning parameters:

- Complexity Parameter (`alpha`, numeric)

Tree-Based Ensembles (`method = 'nodeHarvest'`)

For classification and regression using package **nodeHarvest** with tuning parameters:

- Maximum Interaction Depth (`maxinter`, numeric)
- Prediction Mode (`mode`, character)

Variational Bayesian Multinomial Probit Regression (`method = 'vbmpRadial'`)

For classification using package **vbmp** with tuning parameters:

- Theta Estimated (`estimateTheta`, character)

Wang and Mendel Fuzzy Rules (`method = 'WM'`)

For regression using package **frbs** with tuning parameters:

- Number of Fuzzy Terms (`num.labels`, numeric)
- Membership Function (`type.mf`, character)

Weighted Subspace Random Forest (`method = 'wsrf'`)

For classification using package **wsrf** with tuning parameters:

- Number of Randomly Selected Predictors (`mtry`, numeric)

References

"Using your own model in `train`" (`http://caret.r-forge.r-project.org/custom_models.html`)

twoClassSim *Simulation Functions*

Description

This function simulates regression and classification data with truly important predictors and irrelevant predictions.

Usage

```
twoClassSim(n = 100, intercept = -5, linearVars = 10,
        noiseVars = 0, corrVars = 0,
            corrType = "AR1", corrValue = 0, mislabel = 0)

SLC14_1(n = 100, noiseVars = 0, corrVars = 0,
    corrType = "AR1", corrValue = 0)

SLC14_2(n = 100, noiseVars = 0, corrVars = 0,
    corrType = "AR1", corrValue = 0)

LPH07_1(n = 100, noiseVars = 0, corrVars = 0,
    corrType = "AR1", corrValue = 0)

LPH07_2(n = 100, noiseVars = 0, corrVars = 0,
    corrType = "AR1", corrValue = 0)
```

Arguments

n	The number of simulated data points
intercept	The intercept, which controls the class balance. The default value produces a roughly balanced data set when the other defaults are used.
linearVars	The number of linearly important effects. See Details below.
noiseVars	The number of uncorrelated irrelevant predictors to be included.
corrVars	The number of correlated irrelevant predictors to be included.
corrType	The correlation structure of the correlated irrelevant predictors. Values of "AR1" and "exch" are available (see Details below)
corrValue	The correlation value.
mislabel	The proportion of data that is possibly mislabeled. See Details below.

Details

The first function (twoClassSim) generates two class data. The data are simulated in different sets. First, two multivariate normal predictors (denoted here as A and B) are created with a correlation our about 0.65. They change the log-odds using main effects and an interaction:

```
intercept - 4A + 4B + 2AB
```

The intercept is a parameter for the simulation and can be used to control the amount of class imbalance.

The second set of effects are linear with coefficients that alternate signs and have values between 2.5 and 0.025. For example, if there were six predictors in this set, their contribution to the log-odds would be

```
-2.50C + 2.05D -1.60E + 1.15F -0.70G + 0.25H
```

The third set is a nonlinear function of a single predictor ranging between [0, 1] called J here:

```
(J^3) + 2exp(-6(J-0.3)^2)
```

The fourth set of informative predictors are copied from one of Friedman's systems and use two more predictors (K and L):

```
2sin(KL)
```

All of these effects are added up to model the log-odds. This is used to calculate the probability of a sample being in the first class and a random uniform number is used to actually make the assignment of the actual class. To mislabel the data, the probability is reversed (i.e. p = 1 - p) before the random number generation.

The remaining functions simulate regression data sets. LPH07_1 and LPH07_2 are from van der Laan et al. (2007). The first function uses random Bernoulli variables that have a 40% probability of being a value of 1. The true regression equation is:

```
2*w_1*w_10 + 4*w_2*w_7 + 3*w_4*w_5
- 5*w_6*w_10 + 3*w_8*w_9 + w_1*w_2*w_4
- 2*w_7*(1-w_6)*w_2*w_9
- 4*(1 - w_10)*w_1*(1-w_4)
```

The simulated error term is a standard normal (i.e. Gaussian). The noise variables are simulated in the same manner as described above but are made binary based on whether the normal random variable is above or below 0. The second function (LPH07_2) uses 20 independent Gaussians with mean zero and variance 16. The functional form here is:

```
x_1*x_2 + x_10^2 - x_3*x_17
- x_15*x_4 + x_9*x_5 + x_19
- x_20^2 + x_9*x_8
```

The error term is also Gaussian with mean zero and variance 16.

The function SLC14_1 simulates a system from Sapp et al. (2014). All informative predictors are independent Gaussian random variables with mean zero and a variance of 9. The prediction equation is:

```
x_1 + sin(x_2) + log(abs(x_3)) + x_4^2 + x_5*x_6 +
I(x_7*x_8*x_9 < 0) + I(x_10 > 0) + x_11*I(x_11 > 0) +
sqrt(abs(x_12)) + cos(x_13) + 2*x_14 + abs(x_15) +
I(x_16 < -1) + x_17*I(x_17 < -1) - 2 * x_18 - x_19*x_20
```

The random error here is also Gaussian with mean zero and a variance of 9.

`SLC14_2` is also from Sapp et al. (2014). Two hundred independent Gaussian variables are generated, each having mean zero and variance 16. The functional form is

```
-1 + log(abs(x_1)) + ... + log(abs(x_200))
```

and the error term is Gaussian with mean zero and a variance of 25.

For each simulation, the user can also add non-informative predictors to the data. These are random standard normal predictors and can be optionally added to the data in two ways: a specified number of independent predictors or a set number of predictors that follow a particular correlation structure. The only two correlation structure that have been implemented are

- compound-symmetry (aka exchangeable) where there is a constant correlation between all the predictors
- auto-regressive 1 [AR(1)]. While there is no time component to these data, this structure can be used to add predictors of varying levels of correlation. For example, if there were 4 predictors and `r` was the correlation parameter, the between predictor correlation matrix would be

```
| 1             sym   |
| r    1              |
| r^2  r    1         |
| r^3  r^2  r    1    |
| r^4  r^3  r^2  r  1 |
```

Value

a data frame with columns:

`Class` A factor with levels "Class1" and "Class2"

`TwoFactor1, TwoFactor2`
Correlated multivariate normal predictors (denoted as `A` and `B` above)

`Nonlinear1, Nonlinear2, Nonlinear3`
Uncorrelated random uniform predictors (`J`, `K` and `L` above).

`Linear1, ...` Optional uncorrelated standard normal predictors (`C` through `H` above)

`Noise1, ...` Optional uncorrelated standard normal predictions

`Corr1, ...` Optional correlated multivariate normal predictors (each with unit variances)

.

Author(s)

Max Kuhn

References

van der Laan, M. J., & Polley Eric, C. (2007). Super learner. Statistical Applications in Genetics and Molecular Biology, 6(1), 1-23.

Sapp, S., van der Laan, M. J., & Canny, J. (2014). Subsemble: an ensemble method for combining subset-specific algorithm fits. Journal of Applied Statistics, 41(6), 1247-1259.

Examples

```
example <- twoClassSim(100, linearVars = 1)
splom(~example[, 1:6], groups = example$Class)
```

`update.safs` *Update or Re-fit a SA or GA Model*

Description

`update` allows a user to over-ride the search iteration selection process.

Usage

```
## S3 method for class 'gafs'
update(object, iter, x, y, ...)

## S3 method for class 'safs'
update(object, iter, x, y, ...)
```

Arguments

`object`	An object produced by `gafs` or `safs`
`iter`	a single numeric integer
`x, y`	the original training data used in the call to `gafs` or `safs`
`...`	not currently used

Details

Based on the results of plotting a `gafs` or `safs` object, these functions can be used to supersede the number of iterations determined analytically from the resamples.

Any values of `...` originally passed to `gafs` or `safs` are automatically passed on to the updated model (i.e. they do not need to be supplied again to `update`.

Value

an object of class `gafs` or `safs`

Author(s)

Max Kuhn

See Also

gafs, safs

Examples

```
## Not run:
set.seed(1)
train_data <- twoClassSim(100, noiseVars = 10)
test_data  <- twoClassSim(10,  noiseVars = 10)

## A short example
ctrl <- safsControl(functions = rfSA,
                    method = "cv",
                    number = 3)

rf_search <- safs(x = train_data[, -ncol(train_data)],
                  y = train_data$Class,
                  iters = 3,
                  safsControl = ctrl)

rf_search2 <- update(rf_search,
                 iter = 1,
                 x = train_data[, -ncol(train_data)],
                     y = train_data$Class)
rf_search2

## End(Not run)
```

---

update.train *Update or Re-fit a Model*

Description

update allows a user to over-ride the tuning parameter selection process by specifying a set of tuning parameters or to update the model object to the latest version of this package.

Usage

```
## S3 method for class 'train'
update(object, param = NULL, ...)
```

Arguments

object	an object of class train
param	a data frame or named list of all tuning parameters
...	not currently used

Details

If the model object was created with version 5.17-7 or earlier, the underlying package structure was different. To make old `train` objects consistent with the new structure, use `param = NULL` to get the same object back with updates.

To update the model parameters, the training data must be stored in the model object (see the option `returnData` in `trainControl`. Also, all tuning parameters must be specified in the `param` slot. All other options are held constant, including the original pre-processing (if any), options passed in using code... and so on. When printing, the verbiage "The tuning parameter was set manually." is used to describe how the tuning parameters were created.

Value

a new `train` object

Author(s)

Max Kuhn

See Also

`train`, `trainControl`

Examples

```
## Not run:
data(iris)
TrainData <- iris[,1:4]
TrainClasses <- iris[,5]

knnFit1 <- train(TrainData, TrainClasses,
                 method = "knn",
                 preProcess = c("center", "scale"),
                 tuneLength = 10,
                 trControl = trainControl(method = "cv"))

update(knnFit1, list(.k = 3))

## End(Not run)
```

---

varImp *Calculation of variable importance for regression and classification models*

Description

A generic method for calculating variable importance for objects produced by `train` and method specific methods

Usage

```
## S3 method for class 'train'
varImp(object, useModel = TRUE, nonpara = TRUE, scale = TRUE, ...)

## S3 method for class 'earth'
varImp(object, value = "gcv", ...)

## S3 method for class 'fda'
varImp(object, value = "gcv", ...)

## S3 method for class 'rpart'
varImp(object, surrogates = FALSE, competes = TRUE, ...)

## S3 method for class 'randomForest'
varImp(object, ...)

## S3 method for class 'gbm'
varImp(object, numTrees, ...)

## S3 method for class 'classbagg'
varImp(object, ...)

## S3 method for class 'regbagg'
varImp(object, ...)

## S3 method for class 'pamrtrained'
varImp(object, threshold, data, ...)

## S3 method for class 'lm'
varImp(object, ...)

## S3 method for class 'mvr'
varImp(object, estimate = NULL, ...)

## S3 method for class 'bagEarth'
varImp(object, ...)

## S3 method for class 'bagFDA'
varImp(object, ...)

## S3 method for class 'RandomForest'
varImp(object, ...)

## S3 method for class 'rfe'
varImp(object, drop = FALSE, ...)

## S3 method for class 'dsa'
varImp(object, cuts = NULL, ...)
```

```
## S3 method for class 'multinom'
varImp(object, ...)

## S3 method for class 'cubist'
varImp(object, weights = c(0.5, 0.5), ...)

## S3 method for class 'JRip'
varImp(object, ...)

## S3 method for class 'PART'
varImp(object, ...)

## S3 method for class 'C5.0'
varImp(object, ...)

## S3 method for class 'nnet'
varImp(object, ...)

## S3 method for class 'glmnet'
varImp(object, lambda = NULL, ...)

## S3 method for class 'plsda'
varImp(object, ...)
```

Arguments

object	an object corresponding to a fitted model
useModel	use a model based technique for measuring variable importance? This is only used for some models (lm, pls, rf, rpart, gbm, pam and mars)
nonpara	should nonparametric methods be used to assess the relationship between the features and response (only used with useModel = FALSE and only passed to filterVarImp).
scale	should the importance values be scaled to 0 and 100?
...	parameters to pass to the specific varImp methods
numTrees	the number of iterations (trees) to use in a boosted tree model
threshold	the shrinkage threshold (pamr models only)
data	the training set predictors (pamr models only)
value	the statistic that will be used to calculate importance: either gcv, nsubsets, or rss
surrogates	should surrogate splits contribute to the importance calculation?
competes	should competing splits contribute to the importance calculation?
estimate	which estimate of performance should be used? See mvrVal
drop	a logical: should variables not included in the final set be calculated?
cuts	the number of rule sets to use in the model (for partDSA only)

weights	a numeric vector of length two that weighs the usage of variables in the rule conditions and the usage in the linear models (see details below).
lambda	a single value of the penalty parameter

Details

For models that do not have corresponding varImp methods, see filerVarImp.

Otherwise:

Linear Models: the absolute value of the t–statistic for each model parameter is used.

Random Forest: varImp.randomForest and varImp.RandomForest are wrappers around the importance functions from the **randomForest** and **party** packages, respectively.

Partial Least Squares: the variable importance measure here is based on weighted sums of the absolute regression coefficients. The weights are a function of the reduction of the sums of squares across the number of PLS components and are computed separately for each outcome. Therefore, the contribution of the coefficients are weighted proportionally to the reduction in the sums of squares.

Recursive Partitioning: The reduction in the loss function (e.g. mean squared error) attributed to each variable at each split is tabulated and the sum is returned. Also, since there may be candidate variables that are important but are not used in a split, the top competing variables are also tabulated at each split. This can be turned off using the maxcompete argument in rpart.control. This method does not currently provide class–specific measures of importance when the response is a factor.

Bagged Trees: The same methodology as a single tree is applied to all bootstrapped trees and the total importance is returned

Boosted Trees: varImp.gbm is a wrapper around the function from that package (see the **gbm** package vignette)

Multivariate Adaptive Regression Splines: MARS models include a backwards elimination feature selection routine that looks at reductions in the generalized cross-validation (GCV) estimate of error. The varImp function tracks the changes in model statistics, such as the GCV, for each predictor and accumulates the reduction in the statistic when each predictor's feature is added to the model. This total reduction is used as the variable importance measure. If a predictor was never used in any of the MARS basis functions in the final model (after pruning), it has an importance value of zero. Prior to June 2008, the package used an internal function for these calculations. Currently, the varImp is a wrapper to the evimp function in the earth package. There are three statistics that can be used to estimate variable importance in MARS models. Using varImp(object, value = "gcv") tracks the reduction in the generalized cross-validation statistic as terms are added. However, there are some cases when terms are retained in the model that result in an increase in GCV. Negative variable importance values for MARS are set to zero. Alternatively, using varImp(object, value = "rss") monitors the change in the residual sums of squares (RSS) as terms are added, which will never be negative. Also, the option varImp(object, value =" nsubsets"), which counts the number of subsets where the variable is used (in the final, pruned model).

Nearest shrunken centroids: The difference between the class centroids and the overall centroid is used to measure the variable influence (see pamr.predict). The larger the difference between the class centroid and the overall center of the data, the larger the separation between the classes. The training set predictions must be supplied when an object of class pamrtrained is given to varImp.

Cubist: The Cubist output contains variable usage statistics. It gives the percentage of times where each variable was used in a condition and/or a linear model. Note that this output will probably be inconsistent with the rules shown in the output from `summary.cubist`. At each split of the tree, Cubist saves a linear model (after feature selection) that is allowed to have terms for each variable used in the current split or any split above it. Quinlan (1992) discusses a smoothing algorithm where each model prediction is a linear combination of the parent and child model along the tree. As such, the final prediction is a function of all the linear models from the initial node to the terminal node. The percentages shown in the Cubist output reflects all the models involved in prediction (as opposed to the terminal models shown in the output). The variable importance used here is a linear combination of the usage in the rule conditions and the model.

PART and **JRip**: For these rule-based models, the importance for a predictor is simply the number of rules that involve the predictor.

C5.0: C5.0 measures predictor importance by determining the percentage of training set samples that fall into all the terminal nodes after the split. For example, the predictor in the first split automatically has an importance measurement of 100 percent since all samples are affected by this split. Other predictors may be used frequently in splits, but if the terminal nodes cover only a handful of training set samples, the importance scores may be close to zero. The same strategy is applied to rule-based models and boosted versions of the model. The underlying function can also return the number of times each predictor was involved in a split by using the option `metric = "usage"`.

Neural Networks: The method used here is based on Gevrey et al (2003), which uses combinations of the absolute values of the weights. For classification models, the class-specific importances will be the same.

Recursive Feature Elimination: Variable importance is computed using the ranking method used for feature selection. For the final subset size, the importances for the models across all resamples are averaged to compute an overall value.

Feature Selection via Univariate Filters, the percentage of resamples that a predictor was selected is determined. In other words, an importance of 0.50 means that the predictor survived the filter in half of the resamples.

Value

A data frame with class `c("varImp.train", "data.frame")` for `varImp.train` or a matrix for other models.

Author(s)

Max Kuhn

References

Gevrey, M., Dimopoulos, I., & Lek, S. (2003). Review and comparison of methods to study the contribution of variables in artificial neural network models. Ecological Modelling, 160(3), 249-264.

Quinlan, J. (1992). Learning with continuous classes. Proceedings of the 5th Australian Joint Conference On Artificial Intelligence, 343-348.

varImp.gafs *Variable importances for GAs and SAs*

Description

Variable importance scores for safs and gafs objects.

Usage

```
## S3 method for class 'gafs'
varImp(object,
       metric = object$control$metric["external"],
       maximize = object$control$maximize["external"], ...)

## S3 method for class 'safs'
varImp(object,
       metric = object$control$metric["external"],
       maximize = object$control$maximize["external"], ...)
```

Arguments

object	an safs or gafs object
metric	a metric to compute importance (see Details below)
maximize	are larger values of the metric better?
...	not currently uses

Details

A crude measure of importance is computed for thee two search procedures. At the end of a search process, the difference in the fitness values is computed for models with and without each feature (based on the search history). If a predictor has at least two subsets that include and did not include the predictor, a t-statistic is computed (otherwise a value of NA is assigned to the predictor).

This computation is done separately for each resample and the t-statistics are averaged (NA values are ignored) and this average is reported as the importance. If the fitness value should be minimized, the negative value of the t-statistic is used in the average.

As such, the importance score reflects the standardized increase in fitness that occurs when the predict is included in the subset. Values near zero (or negative) indicate that the predictor may not be important to the model.

Value

a data frame where the rownames are the predictor names and the column is the average t-statistic

Author(s)

Max Kuhn

See Also

safs, gafs

---

xyplot.resamples *Lattice Functions for Visualizing Resampling Results*

Description

Lattice functions for visualizing resampling results across models

Usage

```
## S3 method for class 'resamples'
xyplot(x, data = NULL, what = "scatter", models = NULL,
       metric = x$metric[1], units = "min", ...)

## S3 method for class 'resamples'
dotplot(x, data = NULL, models = x$models,
        metric = x$metric, conf.level = 0.95, ...)

## S3 method for class 'resamples'
densityplot(x, data = NULL, models = x$models, metric = x$metric, ...)

## S3 method for class 'resamples'
bwplot(x, data = NULL, models = x$models, metric = x$metric, ...)

## S3 method for class 'resamples'
splom(x, data = NULL, variables = "models",
      models = x$models, metric = NULL, panelRange = NULL, ...)

## S3 method for class 'resamples'
parallelplot(x, data = NULL, models = x$models, metric = x$metric[1], ...)
```

Arguments

x	an object generated by resamples
data	Not used
models	a character string for which models to plot. Note: xyplot requires one or two models whereas the other methods can plot more than two.
metric	a character string for which metrics to use as conditioning variables in the plot. splom requires exactly one metric when variables = "models" and at least two when variables = "metrics".
variables	either "models" or "metrics"; which variable should be treated as the scatter plot variables?

panelRange	a common range for the panels. If NULL, the panel ranges are derived from the values across all the models
what	for xyplot, the type of plot. Valid options are: "scatter" (for a plot of the resampled results between two models), "BlandAltman" (a Bland-Altman, aka MA plot between two models), "tTime" (for the total time to run train versus the metric), "mTime" (for the time to build the final model) or "pTime" (the time to predict samples - see the timingSamps options in trainControl, rfeControl, or sbfControl)
units	either "sec", "min" or "hour"; which what is either "tTime", "mTime" or "pTime", how should the timings be scaled?
conf.level	the confidence level for intervals about the mean (obtained using t.test)
...	further arguments to pass to either histogram, densityplot, xyplot, dotplot or splom

Details

The ideas and methods here are based on Hothorn et al. (2005) and Eugster et al. (2008).

dotplot plots the average performance value (with two-sided confidence limits) for each model and metric.

densityplot and bwplot display univariate visualizations of the resampling distributions while splom shows the pair-wise relationships.

Value

a lattice object

Author(s)

Max Kuhn

References

Hothorn et al. The design and analysis of benchmark experiments. Journal of Computational and Graphical Statistics (2005) vol. 14 (3) pp. 675-699

Eugster et al. Exploratory and inferential analysis of benchmark experiments. Ludwigs-Maximilians-Universitat Munchen, Department of Statistics, Tech. Rep (2008) vol. 30

See Also

resamples, dotplot, bwplot, densityplot, xyplot, splom

Examples

```
## Not run:
#load(url("http://topepo.github.io/caret/exampleModels.RData"))

resamps <- resamples(list(CART = rpartFit,
                          CondInfTree = ctreeFit,
```

```
                          MARS = earthFit))

dotplot(resamps,
        scales =list(x = list(relation = "free")),
        between = list(x = 2))

bwplot(resamps,
       metric = "RMSE")

densityplot(resamps,
            auto.key = list(columns = 3),
            pch = "|")

xyplot(resamps,
       models = c("CART", "MARS"),
       metric = "RMSE")

splom(resamps, metric = "RMSE")
splom(resamps, variables = "metrics")

parallelplot(resamps, metric = "RMSE")



## End(Not run)
```

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