Package 'MachineShop'

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Type Package

Title Machine Learning Models and Tools

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Description Meta-package for statistical and machine learning with a unified interface for model fitting, prediction, performance assessment, and presentation of results. Approaches for model fitting and prediction of numerical, categorical, or censored time-to-event outcomes include traditional regression models, regularization methods, tree-based methods, support vector machines, neural networks, ensembles, data preprocessing, filtering, and model tuning and selection. Performance metrics are provided for model assessment and can be estimated with independent test sets, split sampling, cross-validation, or bootstrap resampling. Resample estimation can be executed in parallel for faster processing and nested in cases of model tuning and selection. Modeling results can be summarized with descriptive statistics; calibration curves; variable importance; partial dependence plots; confusion matrices; and ROC, lift, and other performance curves.

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MachineShop-package

MachineShop: Machine Learning Models and Tools

Description

Meta-package for statistical and machine learning with a unified interface for model fitting, prediction, performance assessment, and presentation of results. Approaches for model fitting and prediction of numerical, categorical, or censored time-to-event outcomes include traditional regression models, regularization methods, tree-based methods, support vector machines, neural networks, ensembles, data preprocessing, filtering, and model tuning and selection. Performance metrics are provided for model assessment and can be estimated with independent test sets, split sampling, cross-validation, or bootstrap resampling. Resample estimation can be executed in parallel for faster processing and nested in cases of model tuning and selection. Modeling results can be summarized with descriptive statistics; calibration curves; variable importance; partial dependence plots; confusion matrices; and ROC, lift, and other performance curves.

Details

The following set of model fitting, prediction, and performance assessment functions are available for **MachineShop** models.

Training:

fit Model fitting
resample Resample estimation of model performance

Tuning Grids:

expand_modelModel expansion over tuning parametersexpand_modelgridModel tuning grid expansionexpand_paramsModel parameters expansionexpand_stepsRecipe step parameters expansion

Response Values:

response Observed predict Predicted

Performance Assessment:

calibration Model calibration
confusion Confusion matrix
dependence Parital dependence

diff Model performance differences
lift Lift curves
performance metrics Model performance metrics
performance_curve
rfe Model performance curves
Recursive feature elimination

varimp Variable importance

Methods for resample estimation include

BootControlSimple bootstrapBootOptimismControlOptimism-corrected bootstrapCVControlRepeated K-fold cross-validationCVOptimismControlOptimism-corrected cross-validationOOBControlOut-of-bootstrapSplitControlSplit training-testingTrainControlTraining resubstitution

Graphical and tabular summaries of modeling results can be obtained with

plot
print
summary

Further information on package features is available with

metricinfo Performance metric information
modelinfo Model information
settings Global settings

Custom metrics and models can be created with the MLMetric and MLModel constructors.

Author(s)

Maintainer: Brian J Smith <bri> smith@uiowa.edu>

See Also

Useful links:

- https://brian-j-smith.github.io/MachineShop/
- Report bugs at https://github.com/brian-j-smith/MachineShop/issues

AdaBagModel 7

AdaBagModel	Bagging with Classification Trees	
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Description

Fits the Bagging algorithm proposed by Breiman in 1996 using classification trees as single classifiers.

Usage

```
AdaBagModel(
    mfinal = 100,
    minsplit = 20,
    minbucket = round(minsplit/3),
    cp = 0.01,
    maxcompete = 4,
    maxsurrogate = 5,
    usesurrogate = 2,
    xval = 10,
    surrogatestyle = 0,
    maxdepth = 30
)
```

Arguments

mfinal number of trees to use.

minisplit minimum number of observations that must exist in a node in order for a split to

be attempted.

minbucket minimum number of observations in any terminal node.

cp complexity parameter.

maxcompete number of competitor splits retained in the output.

maxsurrogate number of surrogate splits retained in the output.

usesurrogate how to use surrogates in the splitting process.

xval number of cross-validations.

surrogatestyle controls the selection of a best surrogate.

maximum depth of any node of the final tree, with the root node counted as

depth 0.

Details

Response types: factor

Automatic tuning of grid parameters: mfinal, maxdepth

Further model details can be found in the source link below.

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Value

MLModel class object.

See Also

```
bagging, fit, resample
```

Examples

```
## Requires prior installation of suggested package adabag to run
fit(Species ~ ., data = iris, model = AdaBagModel(mfinal = 5))
```

AdaBoostModel

Boosting with Classification Trees

Description

Fits the AdaBoost.M1 (Freund and Schapire, 1996) and SAMME (Zhu et al., 2009) algorithms using classification trees as single classifiers.

Usage

```
AdaBoostModel(
  boos = TRUE,
  mfinal = 100,
  coeflearn = c("Breiman", "Freund", "Zhu"),
  minsplit = 20,
  minbucket = round(minsplit/3),
  cp = 0.01,
  maxcompete = 4,
  maxsurrogate = 5,
  usesurrogate = 2,
  xval = 10,
  surrogatestyle = 0,
  maxdepth = 30
)
```

Arguments

boos if TRUE, then bootstrap samples are drawn from the training set using the obser-

vation weights at each iteration. If FALSE, then all observations are used with

their weights.

mfinal number of iterations for which boosting is run.

coeflearn learning algorithm.

as.data.frame

minsplit minimum number of observations that must exist in a node in order for a split to

be attempted.

minbucket minimum number of observations in any terminal node.

cp complexity parameter.

maxcompete number of competitor splits retained in the output.

maxsurrogate number of surrogate splits retained in the output.

usesurrogate how to use surrogates in the splitting process.

xval number of cross-validations.

surrogatestyle controls the selection of a best surrogate.

maximum depth of any node of the final tree, with the root node counted as

depth 0.

Details

Response types: factor

Automatic tuning of grid parameters: mfinal, maxdepth, coeflearn*

* excluded from grids by default

Further model details can be found in the source link below.

Value

MLModel class object.

See Also

```
boosting, fit, resample
```

Examples

```
## Requires prior installation of suggested package adabag to run
fit(Species ~ ., data = iris, model = AdaBoostModel(mfinal = 5))
```

as.data.frame

Coerce to a Data Frame

Description

Functions to coerce objects to data frames.

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Usage

```
## S3 method for class 'ModelFrame'
as.data.frame(x, ...)

## S3 method for class 'Resample'
as.data.frame(x, ...)

## S3 method for class 'TabularArray'
as.data.frame(x, ...)
```

Arguments

x ModelFrame, resample results, resampled performance estimates, model performance differences, or t-test comparisons of the differences.

... arguments passed to other methods.

Value

data.frame class object.

as.MLInput

Coerce to an MLInput

Description

Function to coerce an object to MLInput.

Usage

```
as.MLInput(x, ...)
## S3 method for class 'MLModelFit'
as.MLInput(x, ...)
## S3 method for class 'ModelSpecification'
as.MLInput(x, ...)
```

Arguments

x model fit result or **MachineShop** model specification.

... arguments passed to other methods.

Value

MLInput class object.

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as.MLModel

Coerce to an MLModel

Description

Function to coerce an object to MLModel.

Usage

```
as.MLModel(x, ...)
## S3 method for class 'MLModelFit'
as.MLModel(x, ...)
## S3 method for class 'ModelSpecification'
as.MLModel(x, ...)
## S3 method for class 'model_spec'
as.MLModel(x, ...)
```

Arguments

x model fit result, **MachineShop** model specification, or **parsnip** model specification.

... arguments passed to other methods.

Value

MLModel class object.

See Also

ParsnipModel

 ${\tt BARTMachine Model}$

Bayesian Additive Regression Trees Model

Description

Builds a BART model for regression or classification.

12 BARTMachineModel

Usage

```
BARTMachineModel(
  num_trees = 50,
  num_burn = 250,
  num_iter = 1000,
  alpha = 0.95,
  beta = 2,
  k = 2,
  q = 0.9,
  nu = 3,
  mh_prob_steps = c(2.5, 2.5, 4)/9,
  verbose = FALSE,
  ...
)
```

Arguments

num_trees	number of trees to be grown in the sum-of-trees model.
num_burn	number of MCMC samples to be discarded as "burn-in".
num_iter	number of MCMC samples to draw from the posterior distribution.
alpha, beta	base and power hyperparameters in tree prior for whether a node is nonterminal or not.
k	regression prior probability that $E(Y X)$ is contained in the interval (y_{min},y_{max}) , based on a normal distribution.
q	quantile of the prior on the error variance at which the data-based estimate is placed.
nu	regression degrees of freedom for the inverse $sigma^2$ prior.
mh_prob_steps	vector of prior probabilities for proposing changes to the tree structures: (GROW, PRUNE, CHANGE).
verbose	logical indicating whether to print progress information about the algorithm.
	additional arguments to bartMachine.

Details

Response types: binary factor, numeric

Automatic tuning of grid parameters: alpha, beta, k, nu

Further model details can be found in the source link below.

In calls to varimp for BARTMachineModel, argument type may be specified as "splits" (default) for the proportion of time each predictor is chosen for a splitting rule or as "trees" for the proportion of times each predictor appears in a tree. Argument num_replicates is also available to control the number of BART replicates used in estimating the inclusion proportions [default: 5]. Variable importance is automatically scaled to range from 0 to 100. To obtain unscaled importance values, set scale = FALSE. See example below.

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Value

MLModel class object.

See Also

```
bartMachine, fit, resample
```

Examples

BARTModel

Bayesian Additive Regression Trees Model

Description

Flexible nonparametric modeling of covariates for continuous, binary, categorical and time-to-event outcomes.

Usage

```
BARTModel(
 K = integer(),
  sparse = FALSE,
  theta = 0,
  omega = 1,
  a = 0.5,
  b = 1,
  rho = numeric(),
  augment = FALSE,
  xinfo = matrix(NA, 0, 0),
  usequants = FALSE,
  sigest = NA,
  sigdf = 3,
  sigquant = 0.9,
  lambda = NA,
  k = 2,
  power = 2,
  base = 0.95,
  tau.num = numeric(),
  offset = numeric(),
```

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```
ntree = integer(),
numcut = 100,
ndpost = 1000,
nskip = integer(),
keepevery = integer(),
printevery = 1000
```

Arguments

K if provided, then coarsen the times of survival responses per the quantiles 1/K, 2/K, ..., K/K

to reduce computational burdern.

sparse logical indicating whether to perform variable selection based on a sparse Dirich-

let prior rather than simply uniform; see Linero 2016.

theta, omega theta and omega parameters; zero means random.

a, b sparse parameters for Beta(a, b) prior: $0.5 \le a \le 1$ where lower values

induce more sparsity and typically b = 1.

rho sparse parameter: typically rho = p where p is the number of covariates under

consideration.

augment whether data augmentation is to be performed in sparse variable selection. xinfo optional matrix whose rows are the covariates and columns their cutpoints.

usequants whether covariate cutpoints are defined by uniform quantiles or generated uni-

formly.

sigest normal error variance prior for numeric response variables.

sigdf degrees of freedom for error variance prior.

sigquant quantile at which a rough estimate of the error standard deviation is placed.

lambda scale of the prior error variance.

number of standard deviations f(x) is away from +/-3 for categorical response

variables.

power, base power and base parameters for tree prior.

tau.num numerator in the tau definition, i.e., tau = tau.num/(k*sqrt(ntree)).

offset override for the default offset of $F^{-1}(mean(y))$ in the multivariate response

probability P(y[j] = 1|x) = F(f(x)[j] + offset[j]).

ntree number of trees in the sum.

numcut number of possible covariate cutoff values.

ndpost number of posterior draws returned.

nskip number of MCMC iterations to be treated as burn in.

keepevery interval at which to keep posterior draws.

printevery interval at which to print MCMC progress.

Details

Response types: factor, numeric, Surv

Default argument values and further model details can be found in the source See Also links below.

BlackBoostModel 15

Value

MLModel class object.

See Also

```
gbart, mbart, surv.bart, fit, resample
```

Examples

```
## Requires prior installation of suggested package BART to run
fit(sale_amount ~ ., data = ICHomes, model = BARTModel)
```

BlackBoostModel

Gradient Boosting with Regression Trees

Description

Gradient boosting for optimizing arbitrary loss functions where regression trees are utilized as base-learners.

Usage

```
BlackBoostModel(
  family = NULL,
  mstop = 100,
  nu = 0.1,
  risk = c("inbag", "oobag", "none"),
  stopintern = FALSE,
  trace = FALSE,
  teststat = c("quadratic", "maximum"),
  testtype = c("Teststatistic", "Univariate", "Bonferroni", "MonteCarlo"),
  mincriterion = 0,
  minsplit = 10,
  minbucket = 4,
  maxdepth = 2,
  saveinfo = FALSE,
  ...
)
```

Arguments

```
family optional Family object. Set automatically according to the class type of the response variable.

mstop number of initial boosting iterations.
```

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step size or shrinkage parameter between 0 and 1. nu method to use in computing the empirical risk for each boosting iteration. risk stopintern logical inidicating whether the boosting algorithm stops internally when the outof-bag risk increases at a subsequent iteration. trace logical indicating whether status information is printed during the fitting process. teststat type of the test statistic to be applied for variable selection. how to compute the distribution of the test statistic. testtype mincriterion value of the test statistic or 1 - p-value that must be exceeded in order to implement a split. minsplit minimum sum of weights in a node in order to be considered for splitting. minimum sum of weights in a terminal node. minbucket maxdepth maximum depth of the tree. logical indicating whether to store information about variable selection in info saveinfo slot of each partynode.

Details

. . .

Response types: binary factor, BinomialVariate, NegBinomialVariate, numeric, PoissonVariate, Surv

Automatic tuning of grid parameters: mstop, maxdepth

Default argument values and further model details can be found in the source See Also links below.

additional arguments to ctree_control.

Value

MLModel class object.

See Also

```
blackboost, Family, ctree_control, fit, resample
```

```
## Requires prior installation of suggested packages mboost and partykit to run
data(Pima.tr, package = "MASS")
fit(type ~ ., data = Pima.tr, model = BlackBoostModel)
```

C50Model 17

C50Model

C5.0 Decision Trees and Rule-Based Model

Description

Fit classification tree models or rule-based models using Quinlan's C5.0 algorithm.

Usage

```
C50Model(
  trials = 1,
  rules = FALSE,
  subset = TRUE,
  bands = 0,
  winnow = FALSE,
  noGlobalPruning = FALSE,
  CF = 0.25,
  minCases = 2,
  fuzzyThreshold = FALSE,
  sample = 0,
  earlyStopping = TRUE
)
```

Arguments

trials	integer	number	οf	hoosting	iterations.
ti iais	mucgu	Humber	O1	ooosung	ncianons.

rules logical indicating whether to decompose the tree into a rule-based model.

subset logical indicating whether the model should evaluate groups of discrete predic-

tors for splits.

bands integer between 2 and 1000 specifying a number of bands into which to group

rules ordered by their affect on the error rate.

winnow logical indicating use of predictor winnowing (i.e. feature selection).

noGlobalPruning

logical indicating a final, global pruning step to simplify the tree.

CF number in (0, 1) for the confidence factor.

minCases integer for the smallest number of samples that must be put in at least two of the

splits.

fuzzyThreshold logical indicating whether to evaluate possible advanced splits of the data.

sample value between (0, 0.999) that specifies the random proportion of data to use in

training the model.

earlyStopping logical indicating whether the internal method for stopping boosting should be

used.

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Details

Response types: factor

Automatic tuning of grid parameters: trials, rules, winnow

Latter arguments are passed to C5.0Control. Further model details can be found in the source link below

In calls to varimp for C50Model, argument type may be specified as "usage" (default) for the percentage of training set samples that fall into all terminal nodes after the split of each predictor or as "splits" for the percentage of splits associated with each predictor. Variable importance is automatically scaled to range from 0 to 100. To obtain unscaled importance values, set scale = FALSE. See example below.

Value

MLModel class object.

See Also

```
C5.0, fit, resample
```

Examples

```
## Requires prior installation of suggested package C50 to run

model_fit <- fit(Species ~ ., data = iris, model = C50Model)
varimp(model_fit, method = "model", type = "splits", scale = FALSE)</pre>
```

calibration

Model Calibration

Description

Calculate calibration estimates from observed and predicted responses.

Usage

```
calibration(
    x,
    y = NULL,
    weights = NULL,
    breaks = 10,
    span = 0.75,
    distr = character(),
    pool = FALSE,
    na.rm = TRUE,
    ...
)
```

calibration 19

Arguments

x	observed responses or resample result containing observed and predicted responses.
У	predicted responses if not contained in x.
weights	numeric vector of non-negative case weights for the observed x responses [default: equal weights].
breaks	value defining the response variable bins within which to calculate observed mean values. May be specified as a number of bins, a vector of breakpoints, or NULL to fit smooth curves with splines for predicted survival probabilities and with loess for others.
span	numeric parameter controlling the degree of loess smoothing.
distr	character string specifying a distribution with which to estimate the observed survival mean. Possible values are "empirical" for the Kaplan-Meier estimator, "exponential", "extreme", "gaussian", "loggaussian", "logistic", "loglogistic", "lognormal", "rayleigh", "t", or "weibull". Defaults to the distribution that was used in predicting mean survival times.
pool	logical indicating whether to compute a single calibration curve on predictions pooled over all resampling iterations or to compute them for each iteration individually and return the mean calibration curve. Pooling can result in large memory allocation errors when fitting smooth curves with breaks = NULL. The current default is changed from versions <= 3.8.0 of the package which only implemented pool = TRUE.
na.rm	logical indicating whether to remove observed or predicted responses that are NA when calculating metrics.

Value

Calibration class object that inherits from data.frame.

arguments passed to other methods.

See Also

```
c, plot
```

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case_weights

Extract Case Weights

Description

Extract the case weights from an object.

Usage

```
case_weights(object, newdata = NULL)
```

Arguments

object model fit result, ModelFrame, or recipe.

newdata dataset from which to extract the weights if given; otherwise, object is used.

The dataset should be given as a ModelFrame or as a data frame if object con-

tains a ModelFrame or a recipe, respectively.

```
## Training and test sets
inds <- sample(nrow(ICHomes), nrow(ICHomes) * 2 / 3)</pre>
trainset <- ICHomes[inds, ]</pre>
testset <- ICHomes[-inds, ]</pre>
## ModelFrame case weights
trainmf <- ModelFrame(sale_amount ~ . - built, data = trainset, weights = built)</pre>
testmf <- ModelFrame(formula(trainmf), data = testset, weights = built)</pre>
mf_fit <- fit(trainmf, model = GLMModel)</pre>
rmse(response(mf_fit, testmf), predict(mf_fit, testmf),
     case_weights(mf_fit, testmf))
## Recipe case weights
library(recipes)
rec <- recipe(sale_amount ~ ., data = trainset) %>%
  role_case(weight = built, replace = TRUE)
rec_fit <- fit(rec, model = GLMModel)</pre>
rmse(response(rec_fit, testset), predict(rec_fit, testset),
     case_weights(rec_fit, testset))
```

CForestModel 21

CForestModel Conditional Random Forest Model	orestModel
--	------------

Description

An implementation of the random forest and bagging ensemble algorithms utilizing conditional inference trees as base learners.

Usage

```
CForestModel(
  teststat = c("quad", "max"),
  testtype = c("Univariate", "Teststatistic", "Bonferroni", "MonteCarlo"),
  mincriterion = 0,
  ntree = 500,
  mtry = 5,
  replace = TRUE,
  fraction = 0.632
)
```

Arguments

character specifying the type of the test statistic to be applied. teststat testtype character specifying how to compute the distribution of the test statistic. mincriterion value of the test statistic that must be exceeded in order to implement a split. number of trees to grow in a forest. ntree number of input variables randomly sampled as candidates at each node for mtry random forest like algorithms. replace logical indicating whether sampling of observations is done with or without replacement. fraction fraction of number of observations to draw without replacement (only relevant if replace = FALSE).

Details

Response types: factor, numeric, Surv **Automatic tuning of grid parameter:** mtry

Supplied arguments are passed to cforest_control. Further model details can be found in the source link below.

Value

MLModel class object.

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See Also

```
cforest, fit, resample
```

Examples

```
fit(sale_amount ~ ., data = ICHomes, model = CForestModel)
```

combine

Combine MachineShop Objects

Description

Combine one or more **MachineShop** objects of the same class.

Usage

```
## S3 method for class 'Calibration'
c(...)

## S3 method for class 'ConfusionList'
c(...)

## S3 method for class 'ConfusionMatrix'
c(...)

## S3 method for class 'LiftCurve'
c(...)

## S3 method for class 'ListOf'
c(...)

## S3 method for class 'PerformanceCurve'
c(...)

## S3 method for class 'Resample'
c(...)

## S4 method for signature 'SurvMatrix,SurvMatrix'
e1 + e2
```

Arguments

named or unnamed calibration, confusion, lift, performance curve, summary, or resample results. Curves must have been generated with the same performance metrics and resamples with the same resampling control.

e1, e2 objects.

confusion 23

Value

Object of the same class as the arguments.

confusion

Confusion Matrix

Description

Calculate confusion matrices of predicted and observed responses.

Usage

```
confusion(
    x,
    y = NULL,
    weights = NULL,
    cutoff = MachineShop::settings("cutoff"),
    na.rm = TRUE,
    ...
)
ConfusionMatrix(data = NA, ordered = FALSE)
```

Arguments

X	factor of observed responses or resample result containing observed and predicted responses.
У	predicted responses if not contained in x.
weights	numeric vector of non-negative case weights for the observed x responses [default: equal weights].
cutoff	numeric (0, 1) threshold above which binary factor probabilities are classified as events and below which survival probabilities are classified. If NULL, then factor responses are summed directly over predicted class probabilities, whereas a default cutoff of 0.5 is used for survival probabilities. Class probability summations and survival will appear as decimal numbers that can be interpreted as expected counts.
na.rm	logical indicating whether to remove observed or predicted responses that are NA when calculating metrics.
	arguments passed to other methods.
data	square matrix, or object that can be converted to one, of cross-classified predicted and observed values in the rows and columns, respectively.
ordered	logical indicating whether the confusion matrix row and columns should be regarded as ordered.

24 CoxModel

Value

The return value is a ConfusionMatrix class object that inherits from table if x and y responses are specified or a ConfusionList object that inherits from list if x is a Resample object.

See Also

```
c, plot, summary
```

Examples

```
## Requires prior installation of suggested package gbm to run
res <- resample(Species ~ ., data = iris, model = GBMModel)
(conf <- confusion(res))
plot(conf)</pre>
```

CoxModel

Proportional Hazards Regression Model

Description

Fits a Cox proportional hazards regression model. Time dependent variables, time dependent strata, multiple events per subject, and other extensions are incorporated using the counting process formulation of Andersen and Gill.

Usage

```
CoxModel(ties = c("efron", "breslow", "exact"), ...)
CoxStepAICModel(
  ties = c("efron", "breslow", "exact"),
  ...,
  direction = c("both", "backward", "forward"),
  scope = list(),
  k = 2,
  trace = FALSE,
  steps = 1000
)
```

Arguments

```
ties character string specifying the method for tie handling.... arguments passed to coxph.control.direction mode of stepwise search, can be one of "both" (default), "backward", or "forward".
```

dependence	25
------------	----

scope	defines the range of models examined in the stepwise search. This should be a list containing components upper and lower, both formulae.
k	multiple of the number of degrees of freedom used for the penalty. Only $k=2$ gives the genuine AIC; $k=.(\log(nobs))$ is sometimes referred to as BIC or SBC.
trace	if positive, information is printed during the running of stepAIC. Larger values may give more information on the fitting process.
steps	maximum number of steps to be considered.

Details

Response types: Surv

Default argument values and further model details can be found in the source See Also links below.

In calls to varimp for CoxModel and CoxStepAICModel, numeric argument base may be specified for the (negative) logarithmic transformation of p-values [defaul: exp(1)]. Transformed p-values are automatically scaled in the calculation of variable importance to range from 0 to 100. To obtain unscaled importance values, set scale = FALSE.

Value

MLModel class object.

See Also

```
coxph, coxph.control, stepAIC, fit, resample
```

Examples

```
library(survival)
fit(Surv(time, status) ~ ., data = veteran, model = CoxModel)
```

dependence	Partial Dependence

Description

Calculate partial dependence of a response on select predictor variables.

26 dependence

Usage

```
dependence(
  object,
  data = NULL,
  select = NULL,
  interaction = FALSE,
  n = 10,
  intervals = c("uniform", "quantile"),
  distr = character(),
  method = character(),
  stats = MachineShop::settings("stats.PartialDependence"),
  na.rm = TRUE
)
```

Arguments

object	model fit result.
data	data frame containing all predictor variables. If not specified, the training data will be used by default.
select	expression indicating predictor variables for which to compute partial dependence (see subset for syntax) [default: all].
interaction	logical indicating whether to calculate dependence on the interacted predictors.
n	number of predictor values at which to perform calculations.
intervals	character string specifying whether the n values are spaced uniformly ("uniform") or according to variable quantiles ("quantile").
distr, method	arguments passed to predict.
stats	function, function name, or vector of these with which to compute response variable summary statistics over non-selected predictor variables.
na.rm	logical indicating whether to exclude missing predicted response values from

Value

PartialDependence class object that inherits from data.frame.

the calculation of summary statistics.

See Also

plot

```
## Requires prior installation of suggested package gbm to run
gbm_fit <- fit(Species ~ ., data = iris, model = GBMModel)
(pd <- dependence(gbm_fit, select = c(Petal.Length, Petal.Width)))
plot(pd)</pre>
```

diff 27

diff

Model Performance Differences

Description

Pairwise model differences in resampled performance metrics.

Usage

```
## S3 method for class 'MLModel'
diff(x, ...)
## S3 method for class 'Performance'
diff(x, ...)
## S3 method for class 'Resample'
diff(x, ...)
```

Arguments

x model performance or resample result.... arguments passed to other methods.

Value

PerformanceDiff class object that inherits from Performance.

See Also

```
t.test, plot, summary
```

```
## Requires prior installation of suggested package gbm to run

## Survival response example
library(survival)

fo <- Surv(time, status) ~ .
    control <- CVControl()

gbm_res1 <- resample(fo, data = veteran, GBMModel(n.trees = 25), control)
gbm_res2 <- resample(fo, data = veteran, GBMModel(n.trees = 50), control)
gbm_res3 <- resample(fo, data = veteran, GBMModel(n.trees = 100), control)

res <- c(GBM1 = gbm_res1, GBM2 = gbm_res2, GBM3 = gbm_res3)
res_diff <- diff(res)
summary(res_diff)</pre>
```

28 Discrete Variate

```
plot(res_diff)
```

DiscreteVariate

Discrete Variate Constructors

Description

Create a variate of binomial counts, discrete numbers, negative binomial counts, or Poisson counts.

Usage

```
BinomialVariate(x = integer(), size = integer())
DiscreteVariate(x = integer(), min = -Inf, max = Inf)
NegBinomialVariate(x = integer())
PoissonVariate(x = integer())
```

Arguments

x numeric vector.

size number or numeric vector of binomial trials.

min, max minimum and maximum bounds for discrete numbers.

Value

BinomialVariate object class, DiscreteVariate that inherits from numeric, or NegBinomialVariate or PoissonVariate that inherit from DiscreteVariate.

See Also

```
role_binom
```

```
BinomialVariate(rbinom(25, 10, 0.5), size = 10)
PoissonVariate(rpois(25, 10))
```

EarthModel 29

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Multivariate Adaptive Regression Splines Model

Description

Build a regression model using the techniques in Friedman's papers "Multivariate Adaptive Regression Splines" and "Fast MARS".

Usage

```
EarthModel(
  pmethod = c("backward", "none", "exhaustive", "forward", "seqrep", "cv"),
  trace = 0,
  degree = 1,
  nprune = integer(),
  nfold = 0,
  ncross = 1,
  stratify = TRUE
)
```

Arguments

pmethod	pruning method.
trace	level of execution information to display.
degree	maximum degree of interaction.
nprune	maximum number of terms (including intercept) in the pruned model.
nfold	number of cross-validation folds.
ncross	number of cross-validations if nfold > 1.
stratify	logical indicating whether to stratify cross-validation samples by the response levels.

Details

Response types: factor, numeric

Automatic tuning of grid parameters: nprune, degree*

Default argument values and further model details can be found in the source See Also link below.

In calls to varimp for EarthModel, argument type may be specified as "nsubsets" (default) for the number of model subsets that include each predictor, as "gcv" for the generalized cross-validation decrease over all subsets that include each predictor, or as "rss" for the residual sums of squares decrease. Variable importance is automatically scaled to range from 0 to 100. To obtain unscaled importance values, set scale = FALSE. See example below.

^{*} excluded from grids by default

30 expand_model

Value

MLModel class object.

See Also

```
earth, fit, resample
```

Examples

```
## Requires prior installation of suggested package earth to run
model_fit <- fit(Species ~ ., data = iris, model = EarthModel)
varimp(model_fit, method = "model", type = "gcv", scale = FALSE)</pre>
```

expand_model

Model Expansion Over Tuning Parameters

Description

Expand a model over all combinations of a grid of tuning parameters.

Usage

```
expand_model(object, ..., random = FALSE)
```

Arguments

object model function, function name, or object; or another object that can be coerced

to a model.

... named vectors or factors or a list of these containing the parameter values over

which to expand object.

random number of points to be randomly sampled from the parameter grid or FALSE if

all points are to be returned.

Value

list of expanded models.

See Also

SelectedModel

expand_modelgrid 31

Examples

expand_modelgrid

Model Tuning Grid Expansion

Description

Expand a model grid of tuning parameter values.

Usage

```
expand_modelgrid(...)
## S3 method for class 'formula'
expand_modelgrid(formula, data, model, info = FALSE, ...)
## S3 method for class 'matrix'
expand_modelgrid(x, y, model, info = FALSE, ...)
## S3 method for class 'ModelFrame'
expand_modelgrid(input, model, info = FALSE, ...)
## S3 method for class 'recipe'
expand_modelgrid(input, model, info = FALSE, ...)
## S3 method for class 'ModelSpecification'
expand_modelgrid(object, ...)
## S3 method for class 'MLModel'
expand_modelgrid(model, ...)
## S3 method for class 'MLModelFunction'
expand_modelgrid(model, ...)
```

32 expand_modelgrid

Arguments

	arguments passed from the generic function to its methods and from the MLModel and MLModelFunction methods to others. The first argument of each expand_modelgrid method is positional and, as such, must be given first in calls to them.
formula, data	formula defining the model predictor and response variables and a data frame containing them.
model	model function, function name, or object; or another object that can be coerced to a model. A model can be given first followed by any of the variable specifications.
info	logical indicating whether to return model-defined grid construction information rather than the grid values.
x, y	matrix and object containing predictor and response variables.
input	input object defining and containing the model predictor and response variables.
object	model specification.

Details

The expand_modelgrid function enables manual extraction and viewing of grids created automatically when a TunedModel is fit.

Value

A data frame of parameter values or NULL if data are required for construction of the grid but not supplied.

See Also

TunedModel

expand_params 33

expand_params

Model Parameters Expansion

Description

Create a grid of parameter values from all combinations of supplied inputs.

Usage

```
expand_params(..., random = FALSE)
```

Arguments

... named data frames or vectors or a list of these containing the parameter values

over which to create the grid.

random number of points to be randomly sampled from the parameter grid or FALSE if

all points are to be returned.

Value

A data frame containing one row for each combination of the supplied inputs.

See Also

TunedModel

```
## Requires prior installation of suggested package gbm to run

data(Boston, package = "MASS")

grid <- expand_params(
   n.trees = c(50, 100),
   interaction.depth = 1:2
)

fit(medv ~ ., data = Boston, model = TunedModel(GBMModel, grid = grid))</pre>
```

34 expand_steps

expand_steps

Recipe Step Parameters Expansion

Description

Create a grid of parameter values from all combinations of lists supplied for steps of a preprocessing recipe.

Usage

```
expand_steps(..., random = FALSE)
```

Arguments

... one or more lists containing parameter values over which to create the grid. For

each list an argument name should be given as the id of the recipe step to which

it corresponds.

random number of points to be randomly sampled from the parameter grid or FALSE if

all points are to be returned.

Value

RecipeGrid class object that inherits from data. frame.

See Also

TunedInput

extract 35

extract

Extract Elements of an Object

Description

Operators acting on data structures to extract elements.

Usage

```
## S3 method for class 'BinomialVariate'
x[i, j, ..., drop = FALSE]
## S4 method for signature 'DiscreteVariate, ANY, missing, missing'
x[i]
## S4 method for signature 'ListOf, ANY, missing, missing'
x[i]
## S4 method for signature 'ModelFrame, ANY, ANY, ANY'
x[i, j, ..., drop = FALSE]
## S4 method for signature 'ModelFrame, ANY, missing, ANY'
x[i, j, ..., drop = FALSE]
## S4 method for signature 'ModelFrame, missing, ANY, ANY'
x[i, j, ..., drop = FALSE]
## S4 method for signature 'ModelFrame, missing, missing, ANY'
x[i, j, ..., drop = FALSE]
## S4 method for signature 'RecipeGrid, ANY, ANY, ANY'
x[i, j, ..., drop = FALSE]
## S4 method for signature 'Resample, ANY, ANY, ANY'
x[i, j, ..., drop = FALSE]
## S4 method for signature 'Resample, ANY, missing, ANY'
x[i, j, ..., drop = FALSE]
## S4 method for signature 'Resample, missing, missing, ANY'
x[i, j, ..., drop = FALSE]
## S4 method for signature 'SurvMatrix,ANY,ANY,ANY'
x[i, j, ..., drop = FALSE]
## S4 method for signature 'SurvTimes, ANY, missing, missing'
x[i]
```

FDAModel FDAModel

Arguments

X	object from which to extract elements.
i, j,	indices specifying elements to extract.
drop	logical indicating that the result be returned as an object coerced to the lowest dimension possible if TRUE or with the original dimensions and class otherwise.

FDAModel

Flexible and Penalized Discriminant Analysis Models

Description

Performs flexible discriminant analysis.

Usage

```
FDAModel(
   theta = matrix(NA, 0, 0),
   dimension = integer(),
   eps = .Machine$double.eps,
   method = .(mda::polyreg),
   ...
)

PDAModel(lambda = 1, df = numeric(), ...)
```

Arguments

theta	optional matrix of class scores, typically with number of columns less than one minus the number of classes.
dimension	dimension of the discriminant subspace, less than the number of classes, to use for prediction.
eps	numeric threshold for small singular values for excluding discriminant variables.
method	regression function used in optimal scaling. The default of linear regression is provided by polyreg from the mda package. For penalized discriminant analysis, gen.ridge is appropriate. Other possibilities are mars for multivariate adaptive regression splines and bruto for adaptive backfitting of additive splines. Use the . operator to quote specified functions.
	$additional \ arguments \ to \ {\tt method} \ for \ {\tt FDAModel} \ and \ to \ {\tt FDAModel} \ for \ {\tt PDAModel}.$
lambda	shrinkage penalty coefficient.
df	alternative specification of lambda in terms of equivalent degrees of freedom.

fit 37

Details

```
Response types: factor

Automatic tuning of grid parameters:
• PDAModel: lambda

* excluded from grids by default
```

The predict function for this model additionally accepts the following argument.

prior prior class membership probabilities for prediction data if different from the training set.

Default argument values and further model details can be found in the source See Also links below.

Value

MLModel class object.

See Also

```
fda, predict.fda, fit, resample
```

Examples

```
## Requires prior installation of suggested package mda to run
fit(Species ~ ., data = iris, model = FDAModel)

## Requires prior installation of suggested package mda to run
fit(Species ~ ., data = iris, model = PDAModel)
```

fit

Model Fitting

Description

Fit a model to estimate its parameters from a data set.

Usage

```
fit(...)
## S3 method for class 'formula'
fit(formula, data, model, ...)
## S3 method for class 'matrix'
```

38 fit

```
fit(x, y, model, ...)
## S3 method for class 'ModelFrame'
fit(input, model, ...)
## S3 method for class 'recipe'
fit(input, model, ...)
## S3 method for class 'ModelSpecification'
fit(object, verbose = FALSE, ...)
## S3 method for class 'MLModel'
fit(model, ...)
## S3 method for class 'MLModelFunction'
fit(model, ...)
```

Arguments

arguments passed from the generic function to its methods, from the MLModel and MLModelFunction methods to first arguments of others, and from others to the ModelSpecification method. The first argument of each fit method is positional and, as such, must be given first in calls to them. formula defining the model predictor and response variables and a data frame formula, data containing them. model model function, function name, or object; or another object that can be coerced to a model. A model can be given first followed by any of the variable specifimatrix and object containing predictor and response variables. x, y input object defining and containing the model predictor and response variables. input object model specification. verbose logical indicating whether to display printed output generated by some model-

Details

User-specified case weights may be specified for ModelFrames upon creation with the weights argument in its constructor.

specific fit functions to aid in monitoring progress and diagnosing errors.

Variables in recipe specifications may be designated as case weights with the role_case function.

Value

MLModelFit class object.

See Also

```
as.MLModel, response, predict, varimp
```

GAMBoostModel 39

Examples

```
## Requires prior installation of suggested package gbm to run
## Survival response example
library(survival)
gbm_fit <- fit(Surv(time, status) ~ ., data = veteran, model = GBMModel)
varimp(gbm_fit)</pre>
```

GAMBoostModel

Gradient Boosting with Additive Models

Description

Gradient boosting for optimizing arbitrary loss functions, where component-wise arbitrary base-learners, e.g., smoothing procedures, are utilized as additive base-learners.

Usage

```
GAMBoostModel(
  family = NULL,
  baselearner = c("bbs", "bols", "btree", "bss", "bns"),
  dfbase = 4,
  mstop = 100,
  nu = 0.1,
  risk = c("inbag", "oobag", "none"),
  stopintern = FALSE,
  trace = FALSE
)
```

Arguments

family optional Family object. Set automatically according to the class type of the

response variable.

baselearner character specifying the component-wise base learner to be used.

dfbase gobal degrees of freedom for P-spline base learners ("bbs").

mstop number of initial boosting iterations.

nu step size or shrinkage parameter between 0 and 1.

risk method to use in computing the empirical risk for each boosting iteration.

stopintern logical inidicating whether the boosting algorithm stops internally when the out-

of-bag risk increases at a subsequent iteration.

trace logical indicating whether status information is printed during the fitting pro-

cess.

40 GBMModel

Details

Response types: binary factor, BinomialVariate, NegBinomialVariate, numeric, PoissonVariate, Surv

Automatic tuning of grid parameter: mstop

Default argument values and further model details can be found in the source See Also links below.

Value

MLModel class object.

See Also

```
gamboost, Family, baselearners, fit, resample
```

Examples

```
## Requires prior installation of suggested package mboost to run
data(Pima.tr, package = "MASS")
fit(type ~ ., data = Pima.tr, model = GAMBoostModel)
```

GBMModel

Generalized Boosted Regression Model

Description

Fits generalized boosted regression models.

Usage

```
GBMModel(
  distribution = character(),
  n.trees = 100,
  interaction.depth = 1,
  n.minobsinnode = 10,
  shrinkage = 0.1,
  bag.fraction = 0.5
)
```

GLMBoostModel 41

Arguments

distribution optional character string specifying the name of the distribution to use or list

with a component name specifying the distribution and any additional parameters needed. Set automatically according to the class type of the response vari-

able.

n. trees total number of trees to fit.

interaction.depth

maximum depth of variable interactions.

n.minobsinnode minimum number of observations in the trees terminal nodes.

shrinkage parameter applied to each tree in the expansion.

bag.fraction fraction of the training set observations randomly selected to propose the next

tree in the expansion.

Details

Response types: factor, numeric, PoissonVariate, Surv

Automatic tuning of grid parameters: n.trees, interaction.depth, shrinkage*, n.minobsinnode*

* excluded from grids by default

Default argument values and further model details can be found in the source See Also link below.

Value

MLModel class object.

See Also

```
gbm, fit, resample
```

Examples

```
## Requires prior installation of suggested package gbm to run
```

```
fit(Species \sim ., data = iris, model = GBMModel)
```

GLMBoostModel

Gradient Boosting with Linear Models

Description

Gradient boosting for optimizing arbitrary loss functions where component-wise linear models are utilized as base-learners.

42 GLMBoostModel

Usage

```
GLMBoostModel(
  family = NULL,
  mstop = 100,
  nu = 0.1,
  risk = c("inbag", "oobag", "none"),
  stopintern = FALSE,
  trace = FALSE
)
```

Arguments

mstop

family optional Family object. Set automatically according to the class type of the response variable.

number of initial boosting iterations.

nu step size or shrinkage parameter between 0 and 1.

risk method to use in computing the empirical risk for each boosting iteration.

stopintern logical inidicating whether the boosting algorithm stops internally when the out-

of-bag risk increases at a subsequent iteration.

trace logical indicating whether status information is printed during the fitting pro-

cess.

Details

Response types: binary factor, BinomialVariate, NegBinomialVariate, numeric, PoissonVariate, Surv

Automatic tuning of grid parameter: mstop

Default argument values and further model details can be found in the source See Also links below.

Value

MLModel class object.

See Also

```
glmboost, Family, fit, resample
```

Examples

```
## Requires prior installation of suggested package mboost to run
data(Pima.tr, package = "MASS")
fit(type ~ ., data = Pima.tr, model = GLMBoostModel)
```

GLMModel 43

GLMModel	Generalized Linear Model
	•

Description

Fits generalized linear models, specified by giving a symbolic description of the linear predictor and a description of the error distribution.

Usage

```
GLMModel(family = NULL, quasi = FALSE, ...)

GLMStepAICModel(
  family = NULL,
  quasi = FALSE,
    ...,
  direction = c("both", "backward", "forward"),
  scope = list(),
  k = 2,
  trace = FALSE,
  steps = 1000
)
```

Arguments

family	optional error distribution and link function to be used in the model. Set automatically according to the class type of the response variable.
quasi	logical indicator for over-dispersion of binomial and Poisson families; i.e., dispersion parameters not fixed at one.
	arguments passed to glm.control.
direction	mode of stepwise search, can be one of "both" (default), "backward", or "forward".
scope	defines the range of models examined in the stepwise search. This should be a list containing components upper and lower, both formulae.
k	multiple of the number of degrees of freedom used for the penalty. Only $k = 2$ gives the genuine AIC; $k = .(log(nobs))$ is sometimes referred to as BIC or SBC.
trace	if positive, information is printed during the running of stepAIC. Larger values may give more information on the fitting process.
steps	maximum number of steps to be considered.

Details

 ${\tt GLMModel} \ \textbf{Response types:} \ {\tt BinomialVariate}, factor, {\tt matrix}, {\tt NegBinomialVariate}, {\tt numeric}, \\ {\tt PoissonVariate}$

44 GLMNetModel

GLMStepAICModel **Response types:** binary factor, BinomialVariate, NegBinomialVariate, numeric, PoissonVariate

Default argument values and further model details can be found in the source See Also links below.

In calls to varimp for GLMModel and GLMStepAICModel, numeric argument base may be specified for the (negative) logarithmic transformation of p-values [defaul: exp(1)]. Transformed p-values are automatically scaled in the calculation of variable importance to range from 0 to 100. To obtain unscaled importance values, set scale = FALSE.

Value

MLModel class object.

See Also

```
glm, glm.control, stepAIC, fit, resample
```

Examples

```
fit(sale_amount ~ ., data = ICHomes, model = GLMModel)
```

GLMNetModel

GLM Lasso or Elasticnet Model

Description

Fit a generalized linear model via penalized maximum likelihood.

Usage

```
GLMNetModel(
  family = NULL,
  alpha = 1,
  lambda = 0,
  standardize = TRUE,
  intercept = logical(),
  penalty.factor = .(rep(1, nvars)),
  standardize.response = FALSE,
  thresh = 1e-07,
  maxit = 1e+05,
  type.gaussian = .(if (nvars < 500) "covariance" else "naive"),
  type.logistic = c("Newton", "modified.Newton"),
  type.multinomial = c("ungrouped", "grouped")
)</pre>
```

GLMNetModel 45

Arguments

family optional response type. Set automatically according to the class type of the

response variable.

alpha elasticnet mixing parameter.

lambda regularization parameter. The default value lambda = 0 performs no regular-

ization and should be increased to avoid model fitting issues if the number of

predictor variables is greater than the number of observations.

standardize logical flag for predictor variable standardization, prior to model fitting.

intercept logical indicating whether to fit intercepts.

penalty.factor vector of penalty factors to be applied to each coefficient.

standardize.response

logical indicating whether to standardize "mgaussian" response variables.

thresh convergence threshold for coordinate descent.

maxit maximum number of passes over the data for all lambda values.

type.gaussian algorithm type for guassian models.
type.logistic algorithm type for logistic models.

type.multinomial

algorithm type for multinomial models.

Details

Response types: Binomial Variate, factor, matrix, numeric, Poisson Variate, Surv

Automatic tuning of grid parameters: lambda, alpha

Default argument values and further model details can be found in the source See Also link below.

Value

MLModel class object.

See Also

```
glmnet, fit, resample
```

Examples

```
## Requires prior installation of suggested package glmnet to run
fit(sale_amount ~ ., data = ICHomes, model = GLMNetModel(lambda = 0.01))
```

46 ICHomes

ICHomes

Iowa City Home Sales Dataset

Description

Characteristics of homes sold in Iowa City, IA from 2005 to 2008 as reported by the county assessor's office.

Usage

ICHomes

Format

A data frame with 753 observations of 17 variables:

sale_amount sale amount in dollars.

sale_year sale year.

sale_month sale month.

built year in which the home was built.

style home stlye (Home/Condo)

construction home construction type.

base_size base foundation size in sq ft.

add_size size of additions made to the base foundation in sq ft.

garage1_size attached garage size in sq ft.

garage2_size detached garage size in sq ft.

lot_size total lot size in sq ft.

bedrooms number of bedrooms.

basement presence of a basement (No/Yes).

ac presence of central air conditioning (No/Yes).

attic presence of a finished attic (No/Yes).

lon,lat home longitude/latitude coordinates.

inputs 47

inputs	Model Inputs	

Description

Model inputs are the predictor and response variables whose relationship is determined by a model fit. Input specifications supported by **MachineShop** are summarized in the table below.

formula Traditional model formula matrix Design matrix of predictors

ModelFrame Model frame ModelSpecification Model specification

recipe Preprocessing recipe roles and steps

Response variable types in the input specifications are defined by the user with the functions and recipe roles:

Response Functions Binomial Variate

DiscreteVariate

factor
matrix

 ${\tt NegBinomialVariate}$

numeric
ordered

PoissonVariate

Surv

Recipe Roles role_binom

role_surv

Inputs may be combined, selected, or tuned with the following meta-input functions.

ModelSpecification Model specification

SelectedInput Input selection from a candidate set TunedInput Input tuning over a parameter grid

See Also

fit, resample

48 KNNModel

KNNModel

Weighted k-Nearest Neighbor Model

Description

Fit a k-nearest neighbor model for which the k nearest training set vectors (according to Minkowski distance) are found for each row of the test set, and prediction is done via the maximum of summed kernel densities.

Usage

```
KNNModel(
   k = 7,
   distance = 2,
   scale = TRUE,
   kernel = c("optimal", "biweight", "cos", "epanechnikov", "gaussian", "inv", "rank",
        "rectangular", "triangular", "triweight")
)
```

Arguments

k numer of neigbors considered. distance Minkowski distance parameter.

scale logical indicating whether to scale predictors to have equal standard deviations.

kernel kernel to use.

Details

```
Response types: factor, numeric, ordinal
Automatic tuning of grid parameters: k, distance*, kernel*
* excluded from grids by default
```

Further model details can be found in the source link below.

Value

MLModel class object.

See Also

```
kknn, fit, resample
```

Examples

```
## Requires prior installation of suggested package kknn to run
fit(Species ~ ., data = iris, model = KNNModel)
```

LARSModel 49

LARSModel	Least Angle Regression, Lasso and Infinitesimal Forward Stagewise Models
-----------	---

Description

Fit variants of Lasso, and provide the entire sequence of coefficients and fits, starting from zero to the least squares fit.

Usage

```
LARSModel(
  type = c("lasso", "lar", "forward.stagewise", "stepwise"),
  trace = FALSE,
  normalize = TRUE,
  intercept = TRUE,
  step = numeric(),
  use.Gram = TRUE
)
```

Arguments

type model type.

trace logical indicating whether status information is printed during the fitting pro-

cess.

normalize whether to standardize each variable to have unit L2 norm.

intercept whether to include an intercept in the model.

step algorithm step number to use for prediction. May be a decimal number indicat-

ing a fractional distance between steps. If specified, the maximum number of algorithm steps will be ceiling(step); otherwise, step will be set equal to the

source package default maximum [default: max.steps].

use. Gram whether to precompute the Gram matrix.

Details

Response types: numeric

Automatic tuning of grid parameter: step

Default argument values and further model details can be found in the source See Also link below.

Value

MLModel class object.

See Also

```
lars, fit, resample
```

50 LDAModel

Examples

```
## Requires prior installation of suggested package lars to run
fit(sale_amount ~ ., data = ICHomes, model = LARSModel)
```

LDAModel

Linear Discriminant Analysis Model

Description

Performs linear discriminant analysis.

Usage

```
LDAModel(
  prior = numeric(),
  tol = 1e-04,
  method = c("moment", "mle", "mve", "t"),
  nu = 5,
  dimen = integer(),
  use = c("plug-in", "debiased", "predictive")
)
```

Arguments

prior	prior probabilities of class membership if specified or the class proportions in the training set otherwise.
tol	tolerance for the determination of singular matrices.
method	type of mean and variance estimator.
nu	degrees of freedom for method = "t".
dimen	dimension of the space to use for prediction.
use	type of parameter estimation to use for prediction.

Details

Response types: factor

Automatic tuning of grid parameter: dimen

The predict function for this model additionally accepts the following argument.

prior prior class membership probabilities for prediction data if different from the training set.

Default argument values and further model details can be found in the source See Also links below.

lift 51

Value

MLModel class object.

See Also

```
lda, predict.lda, fit, resample
```

Examples

```
fit(Species ~ ., data = iris, model = LDAModel)
```

lift

Model Lift Curves

Description

Calculate lift curves from observed and predicted responses.

Usage

```
lift(x, y = NULL, weights = NULL, na.rm = TRUE, ...)
```

Arguments

X	observed responses or resample result containing observed and predicted responses.
у	predicted responses if not contained in x.
weights	numeric vector of non-negative case weights for the observed x responses [default: equal weights].
na.rm	logical indicating whether to remove observed or predicted responses that are NA when calculating metrics.
	arguments passed to other methods.

Value

LiftCurve class object that inherits from PerformanceCurve.

See Also

```
c, plot, summary
```

52 LMModel

Examples

```
## Requires prior installation of suggested package gbm to run
data(Pima.tr, package = "MASS")

res <- resample(type ~ ., data = Pima.tr, model = GBMModel)
lf <- lift(res)
plot(lf)</pre>
```

LMModel

Linear Models

Description

Fits linear models.

Usage

LMModel()

Details

Response types: factor, matrix, numeric

Further model details can be found in the source link below.

In calls to varimp for LModel, numeric argument base may be specified for the (negative) logarithmic transformation of p-values [defaul: exp(1)]. Transformed p-values are automatically scaled in the calculation of variable importance to range from 0 to 100. To obtain unscaled importance values, set scale = FALSE.

Value

MLModel class object.

See Also

```
lm, fit, resample
```

Examples

```
fit(sale_amount ~ ., data = ICHomes, model = LMModel)
```

MDAModel 53

MDAModel

Mixture Discriminant Analysis Model

Description

Performs mixture discriminant analysis.

Usage

```
MDAModel(
   subclasses = 3,
   sub.df = numeric(),
   tot.df = numeric(),
   dimension = sum(subclasses) - 1,
   eps = .Machine$double.eps,
   iter = 5,
   method = .(mda::polyreg),
   trace = FALSE,
   ...
)
```

Arguments

sub.df effective degrees of freedom of the centroids per class if subclass centroid shring age is performed.	nk-
÷ ·	
tot.df specification of the total degrees of freedom as an alternative to sub.df.	
dimension dimension of the discriminant subspace to use for prediction.	
eps numeric threshold for automatically truncating the dimension.	
iter limit on the total number of iterations.	
regression function used in optimal scaling. The default of linear regression provided by polyreg from the mda package. For penalized mixture discrimant models, gen.ridge is appropriate. Other possibilities are mars for multivariate adaptive regression splines and bruto for adaptive backfitting of additises and splines. Use the concentration of the provided functions.	ni- lti-
trace logical indicating whether iteration information is printed.	
additional arguments to mda.start and method.	

Details

Response types: factor

Automatic tuning of grid parameter: subclasses

The predict function for this model additionally accepts the following argument.

prior prior class membership probabilities for prediction data if different from the training set.

Default argument values and further model details can be found in the source See Also links below.

54 metricinfo

Value

MLModel class object.

See Also

```
mda, predict.mda, fit, resample
```

Examples

```
## Requires prior installation of suggested package mda to run
fit(Species ~ ., data = iris, model = MDAModel)
```

metricinfo

Display Performance Metric Information

Description

Display information about metrics provided by the **MachineShop** package.

Usage

```
metricinfo(...)
```

Arguments

metric functions or function names; observed responses; observed and predicted responses; confusion or resample results for which to display information. If none are specified, information is returned on all available metrics by default.

Value

List of named metric elements each containing the following components:

label character descriptor for the metric.

maximize logical indicating whether higher values of the metric correspond to better predictive performance.

arguments closure with the argument names and corresponding default values of the metric func-

response_types data frame of the observed and predicted response variable types supported by the metric.

Examples

```
## All metrics
metricinfo()

## Metrics by observed and predicted response types
names(metricinfo(factor(0)))
names(metricinfo(factor(0), factor(0)))
names(metricinfo(factor(0), matrix(0)))
names(metricinfo(factor(0), numeric(0)))

## Metric-specific information
metricinfo(auc)
```

metrics

Performance Metrics

Description

Compute measures of agreement between observed and predicted responses.

Usage

```
accuracy(
  observed,
  predicted = NULL,
 weights = NULL,
  cutoff = MachineShop::settings("cutoff"),
)
auc(
  observed,
  predicted = NULL,
 weights = NULL,
 multiclass = c("pairs", "all"),
 metrics = c(MachineShop::tpr, MachineShop::fpr),
  stat = MachineShop::settings("stat.Curve"),
)
brier(observed, predicted = NULL, weights = NULL, ...)
cindex(observed, predicted = NULL, weights = NULL, ...)
cross_entropy(observed, predicted = NULL, weights = NULL, ...)
```

```
f_score(
 observed,
 predicted = NULL,
 weights = NULL,
 cutoff = MachineShop::settings("cutoff"),
 beta = 1,
)
fnr(
 observed,
 predicted = NULL,
 weights = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
fpr(
 observed,
 predicted = NULL,
 weights = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
kappa2(
 observed,
 predicted = NULL,
 weights = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
npv(
 observed,
 predicted = NULL,
 weights = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
ppr(
 observed,
 predicted = NULL,
 weights = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
```

```
ppv(
  observed,
  predicted = NULL,
 weights = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
pr_auc(
 observed,
 predicted = NULL,
 weights = NULL,
 multiclass = c("pairs", "all"),
)
precision(
 observed,
  predicted = NULL,
 weights = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
recall(
 observed,
 predicted = NULL,
 weights = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
roc_auc(
  observed,
 predicted = NULL,
 weights = NULL,
 multiclass = c("pairs", "all"),
)
roc_index(
  observed,
 predicted = NULL,
 weights = NULL,
  cutoff = MachineShop::settings("cutoff"),
  fun = function(sensitivity, specificity) (sensitivity + specificity)/2,
```

```
)
sensitivity(
  observed,
  predicted = NULL,
 weights = NULL,
  cutoff = MachineShop::settings("cutoff"),
)
specificity(
  observed,
  predicted = NULL,
 weights = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
tnr(
  observed,
 predicted = NULL,
 weights = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
tpr(
 observed,
 predicted = NULL,
 weights = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
weighted_kappa2(observed, predicted = NULL, weights = NULL, power = 1, ...)
gini(observed, predicted = NULL, weights = NULL, ...)
mae(observed, predicted = NULL, weights = NULL, ...)
mse(observed, predicted = NULL, weights = NULL, ...)
msle(observed, predicted = NULL, weights = NULL, ...)
r2(
  observed,
  predicted = NULL,
  weights = NULL,
```

```
method = c("mse", "pearson", "spearman"),
distr = character(),
...
)

rmse(observed, predicted = NULL, weights = NULL, ...)

rmsle(observed, predicted = NULL, weights = NULL, ...)
```

Arguments

observed observed responses; or confusion, performance curve, or resample result con-

taining observed and predicted responses.

predicted predicted responses if not contained in observed.

weights numeric vector of non-negative case weights for the observed responses [default:

equal weights].

cutoff numeric (0, 1) threshold above which binary factor probabilities are classified

as events and below which survival probabilities are classified. If NULL , then confusion matrix-based metrics are computed on predicted class probabilities if

given.

... arguments passed to or from other methods.

multiclass character string specifying the method for computing generalized area under

the performance curve for multiclass factor responses. Options are to average over areas for each pair of classes ("pairs") or for each class versus all others

("all").

metrics vector of two metric functions or function names that define a curve under which

to calculate area [default: ROC metrics].

stat function or character string naming a function to compute a summary statistic

at each cutoff value of resampled metrics in performance curves, or NULL for

resample-specific metrics.

beta relative importance of recall to precision in the calculation of f_score [default:

F1 score].

fun function to calculate a desired sensitivity-specificity tradeoff.

power power to which positional distances of off-diagonals from the main diagonal in

confusion matrices are raised to calculate weighted_kappa2.

method character string specifying whether to compute r2 as the coefficient of determi-

nation ("mse") or as the square of "pearson" or "spearman" correlation.

distr character string specifying a distribution with which to estimate the observed

survival mean in the total sum of square component of r2. Possible values are "empirical" for the Kaplan-Meier estimator, "exponential", "extreme",

"gaussian", "loggaussian", "logistic", "loglogistic", "lognormal", "rayleigh",

"t", or "weibull". Defaults to the distribution that was used in predicting mean $\,$

survival times.

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References

Hand, D. J., & Till, R. J. (2001). A simple generalisation of the area under the ROC curve for multiple class classification problems. *Machine Learning*, 45, 171-186.

See Also

metricinfo, performance

MLControl

Resampling Controls

Description

Structures to define and control sampling methods for estimation of model predictive performance in the **MachineShop** package.

Usage

```
BootControl(
  samples = 25,
 weights = TRUE,
  seed = sample(.Machine$integer.max, 1)
BootOptimismControl(
  samples = 25,
 weights = TRUE,
  seed = sample(.Machine$integer.max, 1)
CVControl(
  folds = 10,
  repeats = 1,
 weights = TRUE,
  seed = sample(.Machine$integer.max, 1)
CVOptimismControl(
  folds = 10,
  repeats = 1,
 weights = TRUE,
  seed = sample(.Machine$integer.max, 1)
)
00BControl(
  samples = 25,
 weights = TRUE,
```

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```
seed = sample(.Machine$integer.max, 1)
)

SplitControl(
  prop = 2/3,
  weights = TRUE,
  seed = sample(.Machine$integer.max, 1)
)

TrainControl(weights = TRUE, seed = sample(.Machine$integer.max, 1))
```

Arguments

samples	number of bootstrap samples.
weights	logical indicating whether to return case weights in resampled output for the calculation of performance metrics.
seed	integer to set the seed at the start of resampling.
folds	number of cross-validation folds (K).
repeats	number of repeats of the K-fold partitioning.
prop	proportion of cases to include in the training set $(0 < prop < 1)$.

Details

BootControl constructs an MLControl object for simple bootstrap resampling in which models are fit with bootstrap resampled training sets and used to predict the full data set (Efron and Tibshirani 1993).

BootOptimismControl constructs an MLControl object for optimism-corrected bootstrap resampling (Efron and Gong 1983, Harrell et al. 1996).

CVControl constructs an MLControl object for repeated K-fold cross-validation (Kohavi 1995). In this procedure, the full data set is repeatedly partitioned into K-folds. Within a partitioning, prediction is performed on each of the K folds with models fit on all remaining folds.

CVOptimismControl constructs an MLControl object for optimism-corrected cross-validation resampling (Davison and Hinkley 1997, eq. 6.48).

OOBControl constructs an MLControl object for out-of-bootstrap resampling in which models are fit with bootstrap resampled training sets and used to predict the unsampled cases.

SplitControl constructs an MLControl object for splitting data into a separate training and test set (Hastie et al. 2009).

TrainControl constructs an MLControl object for training and performance evaluation to be performed on the same training set (Efron 1986).

Value

Object that inherits from the MLControl class.

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References

Efron, B., & Tibshirani, R. J. (1993). An introduction to the bootstrap. Chapman & Hall/CRC.

Efron, B., & Gong, G. (1983). A leisurely look at the bootstrap, the jackknife, and cross-validation. *The American Statistician*, *37*(1), 36-48.

Harrell, F. E., Lee, K. L., & Mark, D. B. (1996). Multivariable prognostic models: Issues in developing models, evaluating assumptions and adequacy, and measuring and reducing errors. *Statistics in Medicine*, *15*(4), 361-387.

Kohavi, R. (1995). A study of cross-validation and bootstrap for accuracy estimation and model selection. In *IJCAI'95: Proceedings of the 14th International Joint Conference on Artificial Intelligence* (vol. 2, pp. 1137-1143). Morgan Kaufmann Publishers Inc.

Davison, A. C., & Hinkley, D. V. (1997). *Bootstrap methods and their application*. Cambridge University Press.

Hastie, T., Tibshirani, R., & Friedman, J. (2009). *The elements of statistical learning: data mining, inference, and prediction* (2nd ed.). Springer.

Efron, B. (1986). How biased is the apparent error rate of a prediction rule? *Journal of the American Statistical Association*, 81(394), 461-70.

See Also

 $\tt set_monitor, set_predict, set_strata, resample, SelectedInput, SelectedModel, TunedInput, TunedModel$

Examples

```
## Bootstrapping with 100 samples
BootControl(samples = 100)

## Optimism-corrected bootstrapping with 100 samples
BootOptimismControl(samples = 100)

## Cross-validation with 5 repeats of 10 folds
CVControl(folds = 10, repeats = 5)

## Optimism-corrected cross-validation with 5 repeats of 10 folds
CVOptimismControl(folds = 10, repeats = 5)

## Out-of-bootstrap validation with 100 samples
OOBControl(samples = 100)

## Split sample validation with 2/3 training and 1/3 testing
SplitControl(prop = 2/3)

## Training set evaluation
TrainControl()
```

MLMetric 63

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MLMetric Class Constructor

Description

Create a performance metric for use with the MachineShop package.

Usage

```
MLMetric(object, name = "MLMetric", label = name, maximize = TRUE)
MLMetric(object) <- value</pre>
```

Arguments

object	function to compute the metric, defined to accept observed and predicted as the first two arguments and with an ellipsis (\ldots) to accommodate others.
name	character name of the object to which the metric is assigned.
label	optional character descriptor for the model.
maximize	logical indicating whether higher values of the metric correspond to better predictive performance.
value	list of arguments to pass to the MLMetric constructor.

Value

MLMetric class object.

See Also

```
metrics
```

Examples

```
f2_score <- MLMetric(
  function(observed, predicted, ...) {
    f_score(observed, predicted, beta = 2, ...)
},
  name = "f2_score",
  label = "F Score (beta = 2)",
  maximize = TRUE
)</pre>
```

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MLMode1

MLModel and MLModelFunction Class Constructors

Description

Create a model or model function for use with the **MachineShop** package.

Usage

```
MLModel(
  name = "MLModel",
  label = name,
  packages = character(),
  response_types = character(),
  weights = FALSE,
  predictor_encoding = c(NA, "model.frame", "model.matrix"),
  na.rm = FALSE,
  params = list(),
  gridinfo = tibble::tibble(param = character(), get_values = list(), default =
    logical()),
  fit = function(formula, data, weights, ...) stop("No fit function."),
  predict = function(object, newdata, times, ...) stop("No predict function."),
  varimp = function(object, ...) NULL,
)
MLModelFunction(object, ...)
```

Arguments

name character name of the object to which the model is assigned.

label optional character descriptor for the model.

packages character vector of package names upon which the model depends. Each name

may be optionally followed by a comment in parentheses specifying a version requirement. The comment should contain a comparison operator, whitespace

and a valid version number, e.g. "xgboost (>= 1.3.0)".

response_types character vector of response variable types to which the model can be fit. Sup-

ported types are "binary", "BinomialVariate", "DiscreteVariate", "factor", "matrix", "NegBinomialVariate", "numeric", "ordered", "PoissonVariate",

and "Surv".

weights logical value or vector of the same length as response_types indicating whether

case weights are supported for the responses.

predictor_encoding

character string indicating whether the model is fit with predictor variables encoded as a "model.frame", a "model.matrix", or unspecified (default).

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na.rm	character string or logical specifying removal of "all" (TRUE) cases with missing values from model fitting and prediction, "none" (FALSE), or only those whose missing values are in the "response" variable.
params	list of user-specified model parameters to be passed to the fit function.
gridinfo	tibble of information for construction of tuning grids consisting of a character column param with the names of parameters in the grid, a list column get_values with functions to generate grid points for the corresponding parameters, and an optional logical column default indicating which parameters to include by default in regular grids. Values functions may optionally include arguments n and data for the number of grid points to generate and a ModelFrame of the model fit data and formula, respectively; and must include an ellipsis ().
fit	model fitting function whose arguments are a formula, a ModelFrame named data, case weights, and an ellipsis.
predict	model prediction function whose arguments are the object returned by fit, a ModelFrame named newdata of predictor variables, optional vector of times at which to predict survival, and an ellipsis.
varimp	variable importance function whose arguments are the object returned by fit, optional arguments passed from calls to varimp, and an ellipsis.
	arguments passed to other methods.
object	function that returns an MLModel object when called without any supplied argument values.

Details

If supplied, the grid function should return a list whose elements are named after and contain values of parameters to include in a tuning grid to be constructed automatically by the package.

Arguments data and newdata in the fit and predict functions may be converted to data frames with as.data.frame() if needed for their operation. The fit function should return the object resulting from the model fit. Values returned by the predict functions should be formatted according to the response variable types below.

factor matrix whose columns contain the probabilities for multi-level factors or vector of probabilities for the second level of binary factors.

matrix matrix of predicted responses.

numeric vector or column matrix of predicted responses.

Surv matrix whose columns contain survival probabilities at times if supplied or a vector of predicted survival means otherwise.

The varimp function should return a vector of importance values named after the predictor variables or a matrix or data frame whose rows are named after the predictors.

The predict and varimp functions are additionally passed a list named .MachineShop containing the input and model from fit. This argument may be included in the function definitions as needed for their implementations. Otherwise, it will be captured by the ellipsis.

Value

An MLModel or MLModelFunction class object.

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See Also

```
models, fit, resample
```

Examples

```
## Logistic regression model
LogisticModel <- MLModel(</pre>
  name = "LogisticModel",
  response_types = "binary",
  weights = TRUE,
  fit = function(formula, data, weights, ...) {
   glm(formula, data = as.data.frame(data), weights = weights,
        family = binomial, ...)
  predict = function(object, newdata, ...) {
   predict(object, newdata = as.data.frame(newdata), type = "response")
  varimp = function(object, ...) {
    pchisq(coef(object)^2 / diag(vcov(object)), 1)
)
data(Pima.tr, package = "MASS")
res <- resample(type ~ ., data = Pima.tr, model = LogisticModel)</pre>
summary(res)
```

ModelFrame

ModelFrame Class

Description

Class for storing data, formulas, and other attributes for MachineShop model fitting.

Usage

```
ModelFrame(...)
## S3 method for class 'formula'
ModelFrame(
  formula,
  data,
  groups = NULL,
  strata = NULL,
  weights = NULL,
  na.rm = TRUE,
  ...
)
```

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```
## S3 method for class 'matrix'
ModelFrame(
    x,
    y = NULL,
    offsets = NULL,
    groups = NULL,
    strata = NULL,
    weights = NULL,
    na.rm = TRUE,
    ...
)
```

Arguments

	arguments passed from the generic function to its methods. The first argument of each ModelFrame method is positional and, as such, must be given first in calls to them.
formula, data	formula defining the model predictor and response variables and a data frame containing them. In the associated method, arguments groups, strata, and weights will be evaluated as expressions, whose objects are searched for first in the accompanying data environment and, if not found there, next in the calling environment.
groups	vector of values defining groupings of case observations, such as repeated measurements, to keep together during resampling [default: none].
strata	vector of values to use in conducting stratified resample estimation of model performance [default: none].
weights	numeric vector of non-negative case weights for the y response variable [default: equal weights].
na.rm	character string or logical specifying removal of "all" (TRUE) cases with missing values, "none" (FALSE), or only those whose missing values are in the "response" variable.
x, y	matrix and object containing predictor and response variables.
offsets	numeric vector, matrix, or data frame of values to be added with a fixed coefficient of 1 to linear predictors in compatible regression models.

Value

ModelFrame class object that inherits from data.frame.

See Also

```
fit, resample, response, SelectedInput
```

Examples

```
## Requires prior installation of suggested package gbm to run
```

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modelinfo

Display Model Information

Description

Display information about models supplied by the **MachineShop** package.

Usage

```
modelinfo(...)
```

Arguments

. . .

model functions, function names, or objects; observed responses for which to display information. If none are specified, information is returned on all available models by default.

Value

List of named model elements each containing the following components:

label character descriptor for the model.

packages character vector of source packages required to use the model. These need only be installed with the install.packages function or by equivalent means; but need not be loaded with, for example, the library function.

response_types character vector of response variable types supported by the model.

weights logical value or vector of the same length as response_types indicating whether case weights are supported for the responses.

arguments closure with the argument names and corresponding default values of the model function.

grid logical indicating whether automatic generation of tuning parameter grids is implemented for the model.

varimp logical indicating whether model-specific variable importance is defined.

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Examples

```
## All models
modelinfo()

## Models by response types
names(modelinfo(factor(0)))
names(modelinfo(factor(0), numeric(0)))

## Model-specific information
modelinfo(GBMModel)
```

models *Models*

Description

Model constructor functions supplied by **MachineShop** are summarized in the table below according to the types of response variables with which each can be used.

Function	Categorical	Continuous	Survival
AdaBagModel	f		
AdaBoostModel	f		
BARTModel	f	n	S
BARTMachineModel	b	n	
BlackBoostModel	b	n	S
C50Model	f		
CForestModel	f	n	S
CoxModel			S
CoxStepAICModel			S
EarthModel	f	n	
FDAModel	f		
GAMBoostModel	b	n	S
GBMModel	f	n	S
GLMBoostModel	b	n	S
GLMModel	f	m,n	
GLMStepAICModel	b	n	
GLMNetModel	f	m,n	S
KNNModel	f,o	n	
LARSModel		n	
LDAModel	f		
LMModel	f	m,n	
MDAModel	f		
NaiveBayesModel	f		
NNetModel	f	n	
ParsnipModel	f	m,n	S
PDAModel	f		

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DI CM- d-1	f		
PLSMode1	_	n	
POLRModel	0		
QDAMode1	f		
RandomForestModel	f	n	
RangerModel	f	n	S
RFSRCModel	f	m,n	S
RFSRCFastModel	f	m,n	S
RPartModel	f	n	S
SurvRegModel			S
SurvRegStepAICModel			S
SVMModel	f	n	
SVMANOVAModel	f	n	
SVMBesselModel	f	n	
SVMLaplaceModel	f	n	
SVMLinearModel	f	n	
SVMPolyModel	f	n	
SVMRadialModel	f	n	
SVMSplineModel	f	n	
SVMTanhModel	f	n	
TreeModel	f	n	
XGBModel	f	n	S
XGBDARTModel	f	n	S
XGBLinearModel	f	n	S
XGBTreeModel	f	n	S

Categorical: b = binary, f = factor, o = ordered

Continuous: m = matrix, n = numeric

Survival: S = Surv

Models may be combined, tuned, or selected with the following meta-model functions.

ModelSpecificationModel specificationStackedModelStacked regressionSuperModelSuper learner

SelectedModel Model selection from a candidate set
TunedModel Model tuning over a parameter grid

See Also

modelinfo, fit, resample

 ${\tt Model Specification} \qquad {\tt Model Specification}$

ModelSpecification 71

Description

Specification of a relationship between response and predictor variables and a model to define a relationship between them.

Usage

```
ModelSpecification(...)
## Default S3 method:
ModelSpecification(
  input,
  model,
  control = MachineShop::settings("control"),
 metrics = NULL,
  cutoff = MachineShop::settings("cutoff"),
  stat = MachineShop::settings("stat.TrainingParams"),
)
## S3 method for class 'formula'
ModelSpecification(formula, data, model, ...)
## S3 method for class 'matrix'
ModelSpecification(x, y, model, ...)
## S3 method for class 'ModelFrame'
ModelSpecification(input, model, ...)
## S3 method for class 'recipe'
ModelSpecification(input, model, ...)
```

Arguments

control

arguments passed from the generic function to its methods. The first argument of each ModelSpecification method is positional and, as such, must be given first in calls to them.

input input object defining and containing the model predictor and response variables.

model model function, function name, or object; or another object that can be coerced to a model.

to a model.

control function, function name, or object defining the resampling method to be employed. If NULL or if the model specification contains any SelectedInput or SelectedModel objects, then object-specific control structures and training parameters are used for selection and tuning, as usual, and objects are trained sequentially with nested resampling. Otherwise,

• tuning of input and model objects is performed simultaneously over a global grid of their parameter values, and

72 NaiveBayesModel

	• the specified control method and training parameters below override those of any included TunedInput or TunedModel.
metrics	metric function, function name, or vector of these with which to calculate performance. If not specified, default metrics defined in the performance functions are used. Model selection is based on the first calculated metric.
cutoff	argument passed to the metrics functions.
stat	function or character string naming a function to compute a summary statistic on resampled metric values for model tuning.
formula, data	formula defining the model predictor and response variables and a data frame containing them.
x, y	matrix and object containing predictor and response variables.

Value

ModelSpecification class object.

See Also

```
fit, resample, set_monitor, set_optim
```

Examples

```
## Requires prior installation of suggested package gbm to run
modelspec <- ModelSpecification(
   sale_amount ~ ., data = ICHomes, model = GBMModel
)
fit(modelspec)</pre>
```

NaiveBayesModel

Naive Bayes Classifier Model

Description

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

Usage

```
NaiveBayesModel(laplace = 0)
```

Arguments

laplace

positive numeric controlling Laplace smoothing.

NNetModel 73

Details

```
Response types: factor
```

Further model details can be found in the source link below.

Value

MLModel class object.

See Also

```
naiveBayes, fit, resample
```

Examples

```
## Requires prior installation of suggested package e1071 to run
fit(Species ~ ., data = iris, model = NaiveBayesModel)
```

NNetModel

Neural Network Model

Description

Fit single-hidden-layer neural network, possibly with skip-layer connections.

```
NNetModel(
    size = 1,
    linout = logical(),
    entropy = logical(),
    softmax = logical(),
    censored = FALSE,
    skip = FALSE,
    rang = 0.7,
    decay = 0,
    maxit = 100,
    trace = FALSE,
    MaxNWts = 1000,
    abstol = 1e-04,
    reltol = 1e-08
)
```

74 NNetModel

Arguments

size	number of units in the hidden layer.
linout	switch for linear output units. Set automatically according to the class type of the response variable [numeric: TRUE, other: FALSE].
entropy	switch for entropy (= maximum conditional likelihood) fitting.
softmax	switch for softmax (log-linear model) and maximum conditional likelihood fitting.
censored	a variant on softmax, in which non-zero targets mean possible classes.
skip	switch to add skip-layer connections from input to output.
rang	Initial random weights on [-rang, rang].
decay	parameter for weight decay.
maxit	maximum number of iterations.
trace	switch for tracing optimization.
MaxNWts	maximum allowable number of weights.
abstol	stop if the fit criterion falls below abstol, indicating an essentially perfect fit.
reltol	stop if the optimizer is unable to reduce the fit criterion by a factor of at least 1 - reltol.

Details

Response types: factor, numeric

Automatic tuning of grid parameters: size, decay

Default argument values and further model details can be found in the source See Also link below.

Value

MLModel class object.

See Also

```
nnet, fit, resample
```

```
fit(sale_amount ~ ., data = ICHomes, model = NNetModel)
```

ParameterGrid 75

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Tuning Parameters Grid

Description

Defines a tuning grid from a set of parameters.

Usage

```
ParameterGrid(...)
## S3 method for class 'param'
ParameterGrid(..., size = 3, random = FALSE)
## S3 method for class 'list'
ParameterGrid(object, size = 3, random = FALSE, ...)
## S3 method for class 'parameters'
ParameterGrid(object, size = 3, random = FALSE, ...)
```

Arguments

	named param objects as defined in the dials package.
size	single integer or vector of integers whose positions or names match the given parameters and which specify the number of values used to construct the grid.
random	number of unique points to sample at random from the grid defined by size, or FALSE for all points.
object	list of named param objects or a parameters object. This is a positional argument that must be given first in calls to its methods.

Value

ParameterGrid class object that inherits from parameters and TuningGrid.

See Also

TunedModel

```
## GBMModel tuning parameters
grid <- ParameterGrid(
   n.trees = dials::trees(),
   interaction.depth = dials::tree_depth(),
   random = 5
)
TunedModel(GBMModel, grid = grid)</pre>
```

76 ParsnipModel

ParsnipModel

Parsnip Model

Description

Convert a model specification from the **parsnip** package to one that can be used with the **MachineShop** package.

Usage

```
ParsnipModel(object, ...)
```

Arguments

object model specification from the **parsnip** package.
... tuning parameters with which to update object.

Value

ParsnipModel class object that inherits from MLModel.

See Also

```
as.MLModel, fit, resample
```

```
## Requires prior installation of suggested package parsnip to run
prsp_model <- parsnip::linear_reg(engine = "glmnet")
model <- ParsnipModel(prsp_model, penalty = 1, mixture = 1)
model

model_fit <- fit(sale_amount ~ ., data = ICHomes, model = model)
predict(model_fit)</pre>
```

performance 77

performance

Model Performance Metrics

Description

Compute measures of model performance.

```
performance(x, ...)
## S3 method for class 'BinomialVariate'
performance(
 х,
 у,
 weights = NULL,
 metrics = MachineShop::settings("metrics.numeric"),
 na.rm = TRUE,
)
## S3 method for class 'factor'
performance(
 х,
 у,
 weights = NULL,
 metrics = MachineShop::settings("metrics.factor"),
 cutoff = MachineShop::settings("cutoff"),
 na.rm = TRUE,
)
## S3 method for class 'matrix'
performance(
 Х,
 у,
 weights = NULL,
 metrics = MachineShop::settings("metrics.matrix"),
 na.rm = TRUE,
)
## S3 method for class 'numeric'
performance(
 х,
 у,
 weights = NULL,
```

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```
metrics = MachineShop::settings("metrics.numeric"),
 na.rm = TRUE,
)
## S3 method for class 'Surv'
performance(
 Х,
 у,
 weights = NULL,
 metrics = MachineShop::settings("metrics.Surv"),
 cutoff = MachineShop::settings("cutoff"),
 na.rm = TRUE,
)
## S3 method for class 'ConfusionList'
performance(x, ...)
## S3 method for class 'ConfusionMatrix'
performance(x, metrics = MachineShop::settings("metrics.ConfusionMatrix"), ...)
## S3 method for class 'MLModel'
performance(x, ...)
## S3 method for class 'Resample'
performance(x, ...)
## S3 method for class 'TrainingStep'
performance(x, ...)
```

Arguments

X	observed responses; or confusion, trained model fit, resample, or rfe result.
	arguments passed from the Resample method to the response type-specific methods or from the method for ConfusionList to ConfusionMatrix. Elliptical arguments in the response type-specific methods are passed to metrics supplied as a single MLMetric function and are ignored otherwise.
У	predicted responses if not contained in x.
weights	numeric vector of non-negative case weights for the observed x responses [default: equal weights].
metrics	metric function, function name, or vector of these with which to calculate performance.
na.rm	logical indicating whether to remove observed or predicted responses that are NA when calculating metrics.
cutoff	numeric (0, 1) threshold above which binary factor probabilities are classified as events and below which survival probabilities are classified.

performance_curve 79

See Also

```
plot, summary
```

Examples

```
## Requires prior installation of suggested package gbm to run

res <- resample(Species ~ ., data = iris, model = GBMModel)
(perf <- performance(res))
summary(perf)
plot(perf)

## Survival response example
library(survival)

gbm_fit <- fit(Surv(time, status) ~ ., data = veteran, model = GBMModel)

obs <- response(gbm_fit, newdata = veteran)
pred <- predict(gbm_fit, newdata = veteran)
performance(obs, pred)</pre>
```

performance_curve

Model Performance Curves

Description

Calculate curves for the analysis of tradeoffs between metrics for assessing performance in classifying binary outcomes over the range of possible cutoff probabilities. Available curves include receiver operating characteristic (ROC) and precision recall.

```
performance_curve(x, ...)

## Default S3 method:
performance_curve(
    x,
    y,
    weights = NULL,
    metrics = c(MachineShop::tpr, MachineShop::fpr),
    na.rm = TRUE,
    ...
)

## S3 method for class 'Resample'
performance_curve(
```

80 performance_curve

```
x,
metrics = c(MachineShop::tpr, MachineShop::fpr),
na.rm = TRUE,
...
)
```

Arguments

x	observed responses or resample result containing observed and predicted responses.
	arguments passed to other methods.
У	predicted responses if not contained in x.
weights	numeric vector of non-negative case weights for the observed x responses [default: equal weights].
metrics	list of two performance metrics for the analysis [default: ROC metrics]. Precision recall curves can be obtained with c(precision, recall).
na.rm	logical indicating whether to remove observed or predicted responses that are NA when calculating metrics.

Value

PerformanceCurve class object that inherits from data.frame.

See Also

```
auc, c, plot, summary
```

```
## Requires prior installation of suggested package gbm to run
data(Pima.tr, package = "MASS")
res <- resample(type ~ ., data = Pima.tr, model = GBMModel)
## ROC curve
roc <- performance_curve(res)
plot(roc)
auc(roc)</pre>
```

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plot

Model Performance Plots

Description

Plot measures of model performance and predictor variable importance.

```
## S3 method for class 'Calibration'
plot(x, type = c("line", "point"), se = FALSE, ...)
## S3 method for class 'ConfusionList'
plot(x, ...)
## S3 method for class 'ConfusionMatrix'
plot(x, ...)
## S3 method for class 'LiftCurve'
plot(
 Χ,
 find = numeric(),
 diagonal = TRUE,
  stat = MachineShop::settings("stat.Curve"),
)
## S3 method for class 'MLModel'
plot(
 х,
 metrics = NULL,
 stat = MachineShop::settings("stat.TrainingParams"),
  type = c("boxplot", "density", "errorbar", "line", "violin"),
)
## S3 method for class 'PartialDependence'
plot(x, stats = NULL, ...)
## S3 method for class 'Performance'
plot(
 х,
 metrics = NULL,
 stat = MachineShop::settings("stat.Resample"),
  type = c("boxplot", "density", "errorbar", "violin"),
)
```

82 plot

```
## S3 method for class 'PerformanceCurve'
plot(
  type = c("tradeoffs", "cutoffs"),
  diagonal = FALSE,
  stat = MachineShop::settings("stat.Curve"),
)
## S3 method for class 'Resample'
plot(
  х,
 metrics = NULL,
  stat = MachineShop::settings("stat.Resample"),
  type = c("boxplot", "density", "errorbar", "violin"),
)
## S3 method for class 'TrainingStep'
plot(
  х,
 metrics = NULL,
  stat = MachineShop::settings("stat.TrainingParams"),
  type = c("boxplot", "density", "errorbar", "line", "violin"),
)
## S3 method for class 'VariableImportance'
plot(x, n = Inf, ...)
```

Arguments

X	calibration, confusion, lift, trained model fit, partial dependence, performance,
	performance curve, recample, rfe, or variable importance result

performance curve, resample, rfe, or variable importance result.

type type of plot to construct.

se logical indicating whether to include standard error bars.

... arguments passed to other methods.

find numeric true positive rate at which to display reference lines identifying the

corresponding rates of positive predictions.

diagonal logical indicating whether to include a diagonal reference line.

stat function or character string naming a function to compute a summary statistic on

resampled metrics for trained MLModel line plots and Resample model ordering. The original ordering is preserved if a value of NULL is given. For LiftCurve and PerformanceCurve classes, plots are of resampled metrics aggregated by

the statistic if given or of resample-specific metrics if NULL.

metrics vector of numeric indexes or character names of performance metrics to plot.

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stats vector of numeric indexes or character names of partial dependence summary

statistics to plot.

n number of most important variables to include in the plot.

Examples

```
## Requires prior installation of suggested package gbm to run
## Factor response example

fo <- Species ~ .
    control <- CVControl()

gbm_fit <- fit(fo, data = iris, model = GBMModel, control = control)
plot(varimp(gbm_fit))

gbm_res1 <- resample(fo, iris, GBMModel(n.trees = 25), control)
gbm_res2 <- resample(fo, iris, GBMModel(n.trees = 50), control)
gbm_res3 <- resample(fo, iris, GBMModel(n.trees = 100), control)
plot(gbm_res3)

res <- c(GBM1 = gbm_res1, GBM2 = gbm_res2, GBM3 = gbm_res3)
plot(res)</pre>
```

PLSModel

Partial Least Squares Model

Description

Function to perform partial least squares regression.

Usage

```
PLSModel(ncomp = 1, scale = FALSE)
```

Arguments

ncomp number of components to include in the model.

scale logical indicating whether to scale the predictors by the sample standard devia-

tion.

Details

Response types: factor, numeric

Automatic tuning of grid parameters: ncomp

Further model details can be found in the source link below.

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Value

MLModel class object.

See Also

```
mvr, fit, resample
```

Examples

```
## Requires prior installation of suggested package pls to run
fit(sale_amount ~ ., data = ICHomes, model = PLSModel)
```

POLRModel

Ordered Logistic or Probit Regression Model

Description

Fit a logistic or probit regression model to an ordered factor response.

Usage

```
POLRModel(method = c("logistic", "probit", "loglog", "cloglog", "cauchit"))
```

Arguments

method

logistic or probit or (complementary) log-log or cauchit (corresponding to a Cauchy latent variable).

Details

Response types: ordered

Further model details can be found in the source link below.

In calls to varimp for POLRModel, numeric argument base may be specified for the (negative) logarithmic transformation of p-values [defaul: exp(1)]. Transformed p-values are automatically scaled in the calculation of variable importance to range from 0 to 100. To obtain unscaled importance values, set scale = FALSE.

Value

MLModel class object.

See Also

```
polr, fit, resample
```

predict 85

Examples

predict

Model Prediction

Description

Predict outcomes with a fitted model.

Usage

```
## S3 method for class 'MLModelFit'
predict(
  object,
  newdata = NULL,
  times = numeric(),
  type = c("response", "raw", "numeric", "prob", "default"),
  cutoff = MachineShop::settings("cutoff"),
  distr = character(),
  method = character(),
  verbose = FALSE,
  ...
)

## S4 method for signature 'MLModelFit'
predict(object, ...)
```

Arguments

object model fit result.

newdata optional data frame with which to obtain predictions. If not specified, the train-

ing data will be used by default.

times numeric vector of follow-up times at which to predict survival events/probabilities

or NULL for predicted survival means.

type specifies prediction on the original outcome ("response"), numeric ("numeric"),

or probability ("prob") scale; or the "raw" predictions returned by the model. Option "default" is deprecated and will be removed in the future; use "raw"

instead.

86 print

cutoff	numeric (0, 1) threshold above which binary factor probabilities are classified as events and below which survival probabilities are classified.
distr	character string specifying distributional approximations to estimated survival curves. Possible values are "empirical", "exponential", "rayleigh", or "weibull"; with defaults of "empirical" for predicted survival events/probabilities and "weibull" for predicted survival means.
method	character string specifying the empirical method of estimating baseline survival curves for Cox proportional hazards-based models. Choices are "breslow" or "efron" (default).
verbose	logical indicating whether to display printed output generated by some model- specific predict functions to aid in monitoring progress and diagnosing errors.
	arguments passed from the S4 to the S3 method.

See Also

```
confusion, performance, metrics
```

Examples

```
## Requires prior installation of suggested package gbm to run
## Survival response example
library(survival)

gbm_fit <- fit(Surv(time, status) ~ ., data = veteran, model = GBMModel)
predict(gbm_fit, newdata = veteran, times = c(90, 180, 360), type = "prob")</pre>
```

print

Print MachineShop Objects

Description

Print methods for objects defined in the MachineShop package.

```
## S3 method for class 'BinomialVariate'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'Calibration'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'DiscreteVariate'
print(x, n = MachineShop::settings("print_max"), ...)
```

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```
## S3 method for class 'ListOf'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'MLControl'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'MLMetric'
print(x, ...)
## S3 method for class 'MLModel'
print(x, n = MachineShop::settings("print_max"), id = FALSE, ...)
## S3 method for class 'MLModelFunction'
print(x, ...)
## S3 method for class 'ModelFrame'
print(x, n = MachineShop::settings("print_max"), id = FALSE, data = TRUE, ...)
## S3 method for class 'ModelRecipe'
print(x, n = MachineShop::settings("print_max"), id = FALSE, data = TRUE, ...)
## S3 method for class 'ModelSpecification'
print(x, n = MachineShop::settings("print_max"), id = FALSE, ...)
## S3 method for class 'Performance'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'PerformanceCurve'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'RecipeGrid'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'Resample'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'SurvMatrix'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'SurvTimes'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'TrainingStep'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'VariableImportance'
print(x, n = MachineShop::settings("print_max"), ...)
```

88 QDAModel

Arguments

X	object to print.
n	integer number of models or data frame rows to show.
	arguments passed to other methods, including the one described below.
	<pre>level = 0 current nesting level of the corresponding object in recursive calls to print. The amount of information displayed decreases and increases with positive and negative levels, respectively.</pre>
id	logical indicating whether to show object identifiers.
data	logical indicating whether to show model data.

QDAModel

Quadratic Discriminant Analysis Model

Description

Performs quadratic discriminant analysis.

Usage

```
QDAModel(
  prior = numeric(),
  method = c("moment", "mle", "mve", "t"),
  nu = 5,
  use = c("plug-in", "predictive", "debiased", "looCV")
)
```

Arguments

prior prior probabilities of class membership if specified or the class proportions in

the training set otherwise.

method type of mean and variance estimator. nu degrees of freedom for method = "t".

use type of parameter estimation to use for prediction.

Details

Response types: factor

The predict function for this model additionally accepts the following argument.

prior prior class membership probabilities for prediction data if different from the training set.

Default argument values and further model details can be found in the source See Also links below.

Value

MLModel class object.

quote 89

See Also

```
qda, predict.qda, fit, resample
```

Examples

```
fit(Species ~ ., data = iris, model = QDAModel)
```

quote

Quote Operator

Description

Shorthand notation for the quote function. The quote operator simply returns its argument unevaluated and can be applied to any R expression.

Usage

```
.(expr)
```

Arguments

expr

any syntactically valid R expression.

Details

Useful for calling model functions with quoted parameter values defined in terms of one or more of the following variables.

```
nobs number of observations in data to be fit.
```

nvars number of predictor variables.

y the response variable.

Value

The quoted (unevaluated) expression.

See Also

quote

```
## Stepwise variable selection with BIC glm_fit \leftarrow fit(sale_amount \sim ., ICHomes, GLMStepAICModel(k = .(log(nobs)))) varimp(glm_fit)
```

90 RandomForestModel

RandomForestModel

Random Forest Model

Description

Implementation of Breiman's random forest algorithm (based on Breiman and Cutler's original Fortran code) for classification and regression.

Usage

```
RandomForestModel(
  ntree = 500,
  mtry = .(if (is.factor(y)) floor(sqrt(nvars)) else max(floor(nvars/3), 1)),
  replace = TRUE,
  nodesize = .(if (is.factor(y)) 1 else 5),
  maxnodes = integer()
)
```

Arguments

ntree number of trees to grow.

number of variables randomly sampled as candidates at each split. replace should sampling of cases be done with or without replacement?

nodesize minimum size of terminal nodes.

maximum number of terminal nodes trees in the forest can have.

Details

```
Response types: factor, numeric
```

Automatic tuning of grid parameters: mtry, nodesize*

* excluded from grids by default

Default argument values and further model details can be found in the source See Also link below.

Value

MLModel class object.

See Also

```
randomForest, fit, resample
```

```
## Requires prior installation of suggested package randomForest to run
fit(sale_amount ~ ., data = ICHomes, model = RandomForestModel)
```

RangerModel 91

RangerModel Fast Random Forest Mode

Description

Fast implementation of random forests or recursive partitioning.

Usage

```
RangerModel(
  num.trees = 500,
 mtry = integer(),
  importance = c("impurity", "impurity_corrected", "permutation"),
 min.node.size = integer(),
  replace = TRUE,
  sample.fraction = if (replace) 1 else 0.632,
  splitrule = character(),
  num.random.splits = 1,
  alpha = 0.5,
  minprop = 0.1,
  split.select.weights = numeric(),
  always.split.variables = character(),
  respect.unordered.factors = character(),
  scale.permutation.importance = FALSE,
  verbose = FALSE
)
```

Arguments

```
number of trees.
num.trees
                  number of variables to possibly split at in each node.
mtry
                  variable importance mode.
importance
min.node.size
                  minimum node size.
replace
                  logical indicating whether to sample with replacement.
sample.fraction
                  fraction of observations to sample.
splitrule
                  splitting rule.
num.random.splits
                  number of random splits to consider for each candidate splitting variable in the
                  "extratrees" rule.
alpha
                  significance threshold to allow splitting in the "maxstat" rule.
                  lower quantile of covariate distribution to be considered for splitting in the
minprop
                  "maxstat" rule.
```

92 recipe_roles

```
split.select.weights
```

numeric vector with weights between 0 and 1, representing the probability to select variables for splitting.

always.split.variables

character vector with variable names to be always selected in addition to the mtry variables tried for splitting.

 ${\tt respect.unordered.factors}$

handling of unordered factor covariates.

scale.permutation.importance

scale permutation importance by standard error.

verbose show computation status and estimated runtime.

Details

Response types: factor, numeric, Surv

Automatic tuning of grid parameters: mtry, min.node.size*, splitrule*

* excluded from grids by default

Default argument values and further model details can be found in the source See Also link below.

Value

MLModel class object.

See Also

```
ranger, fit, resample
```

Examples

```
## Requires prior installation of suggested package ranger to run
fit(Species ~ ., data = iris, model = RangerModel)
```

recipe_roles

Set Recipe Roles

Description

Add to or replace the roles of variables in a preprocessing recipe.

recipe_roles 93

Usage

```
role_binom(recipe, x, size)
role_case(recipe, group, stratum, weight, replace = FALSE)
role_pred(recipe, offset, replace = FALSE)
role_surv(recipe, time, event)
```

Arguments

recipe	existing recipe object.
x, size	number of counts and trials for the specification of a BinomialVariate out-
	come.
group	variable defining groupings of case observations, such as repeated measurements, to keep together during resampling [default: none].
stratum	variable to use in conducting stratified resample estimation of model performance.
weight	numeric variable of case weights for model fitting.
replace	logical indicating whether to replace existing roles.
offset	numeric variable to be added to a linear predictor, such as in a generalized linear model, with known coefficient 1 rather than an estimated coefficient.
time, event	numeric follow up time and 0-1 numeric or logical event indicator for specification of a Surv outcome. If the event indicator is omitted, all cases are assumed to have events.

Value

An updated recipe object.

See Also

recipe

```
library(survival)
library(recipes)

df <- within(veteran, {
   y <- Surv(time, status)
   remove(time, status)
})

rec <- recipe(y ~ ., data = df) %>%
   role_case(stratum = y)

(res <- resample(rec, model = CoxModel))
summary(res)</pre>
```

94 resample

resample

Resample Estimation of Model Performance

Description

Estimation of the predictive performance of a model estimated and evaluated on training and test samples generated from an observed data set.

Usage

```
resample(...)
## S3 method for class 'formula'
resample(formula, data, model, ...)
## S3 method for class 'matrix'
resample(x, y, model, ...)
## S3 method for class 'ModelFrame'
resample(input, model, ...)
## S3 method for class 'recipe'
resample(input, model, ...)
## S3 method for class 'ModelSpecification'
resample(object, control = MachineShop::settings("control"), ...)
## S3 method for class 'MLModel'
resample(model, ...)
## S3 method for class 'MLModelFunction'
resample(model, ...)
```

Arguments

	arguments passed from the generic function to its methods, from the MLModel and MLModelFunction methods to first arguments of others, and from others to the ModelSpecification method. The first argument of each fit method is positional and, as such, must be given first in calls to them.
formula, data	formula defining the model predictor and response variables and a data frame containing them.
model	model function, function name, or object; or another object that can be coerced to a model. A model can be given first followed by any of the variable specifications.
x, y	matrix and object containing predictor and response variables.
input	input object defining and containing the model predictor and response variables.

resample 95

object model input or specification.

control control function, function name, or object defining the resampling method to be

employed.

Details

Stratified resampling is performed automatically for the formula and matrix methods according to the type of response variable. In general, strata are constructed from numeric proportions for BinomialVariate; original values for character, factor, logical, and ordered; first columns of values for matrix; original values for numeric; and numeric times within event statuses for Surv. Numeric values are stratified into quantile bins and categorical values into factor levels defined by MLControl.

Resampling stratification variables may be specified manually for ModelFrames upon creation with the strata argument in their constructor. Resampling of this class is unstratified by default.

Stratification variables may be designated in recipe specifications with the role_case function. Resampling will be unstratified otherwise.

Value

Resample class object.

See Also

```
c, metrics, performance, plot, summary
```

```
## Requires prior installation of suggested package gbm to run
## Factor response example

fo <- Species ~ .
    control <- CVControl()

gbm_res1 <- resample(fo, iris, GBMModel(n.trees = 25), control)
    gbm_res2 <- resample(fo, iris, GBMModel(n.trees = 50), control)
    gbm_res3 <- resample(fo, iris, GBMModel(n.trees = 100), control)

summary(gbm_res1)

plot(gbm_res1)

res <- c(GBM1 = gbm_res1, GBM2 = gbm_res2, GBM3 = gbm_res3)
    summary(res)
    plot(res)</pre>
```

96 response

response

Extract Response Variable

Description

Extract the response variable from an object.

Usage

```
response(object, ...)
## S3 method for class 'MLModelFit'
response(object, newdata = NULL, ...)
## S3 method for class 'ModelFrame'
response(object, newdata = NULL, ...)
## S3 method for class 'ModelSpecification'
response(object, newdata = NULL, ...)
## S3 method for class 'recipe'
response(object, newdata = NULL, ...)
```

Arguments

object model fit, input, or specification containing predictor and response variables.

... arguments passed to other methods.

newdata data frame from which to extract the response variable values if given; other-

wise, object is used.

```
## Survival response example
library(survival)

mf <- ModelFrame(Surv(time, status) ~ ., data = veteran)
response(mf)</pre>
```

rfe 97

rfe

Recursive Feature Elimination

Description

A wrapper method of backward feature selection in which a given model is fit to nested subsets of most important predictor variables in order to select the subset whose resampled predictive performance is optimal.

```
rfe(...)
## S3 method for class 'formula'
rfe(formula, data, model, ...)
## S3 method for class 'matrix'
rfe(x, y, model, ...)
## S3 method for class 'ModelFrame'
rfe(input, model, ...)
## S3 method for class 'recipe'
rfe(input, model, ...)
## S3 method for class 'ModelSpecification'
rfe(
  object,
  select = NULL,
  control = MachineShop::settings("control"),
  props = 4,
  sizes = integer(),
  random = FALSE,
  recompute = TRUE,
  optimize = c("global", "local"),
  samples = c(rfe = 1, varimp = 1),
 metrics = NULL,
  stat = c(resample = MachineShop::settings("stat.Resample"), permute =
    MachineShop::settings("stat.TrainingParams")),
  progress = FALSE,
)
## S3 method for class 'MLModel'
rfe(model, ...)
## S3 method for class 'MLModelFunction'
```

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```
rfe(model, ...)
```

Arguments

arguments passed from the generic function to its methods, from the MLModel and MLModelFunction methods to first arguments of others, and from others to the ModelSpecification method. The first argument of each fit method is positional and, as such, must be given first in calls to them.

formula, data formula defining the model predictor and response variables and a data frame

containing them.

model model function, function name, or object; or another object that can be coerced to a model. A model can be given first followed by any of the variable specifi-

cations.

x, y matrix and object containing predictor and response variables.

input object defining and containing the model predictor and response variables.

object model input or specification.

select expression indicating predictor variables that can be eliminated (see subset for

syntax) [default: all].

control control function, function name, or object defining the resampling method to be

mployed.

props numeric vector of the proportions of most important predictor variables to retain

in fitted models or an integer number of equal spaced proportions to generate

automatically; ignored if sizes are given.

sizes integer vector of the set sizes of most important predictor variables to retain.

random logical indicating whether to eliminate variables at random with probabilities

proportional to their importance.

recompute logical indicating whether to recompute variable importance after eliminating

each set of variables.

optimize character string specifying a search through all props to identify the globally

optimal model ("global") or a search that stops after identifying the first locally

optimal model ("local").

samples numeric vector or list giving the number of permutation samples for each of

the rfe and varimp algorithms. One or both of the values may be specified as named arguments or in the order in which their defaults appear. Larger numbers of samples decrease variability in estimated model performances and variable importances at the expense of increased computation time. Samples are more

expensive computationally for rfe than for varimp.

metrics metric function, function name, or vector of these with which to calculate per-

formance. If not specified, default metrics defined in the performance functions

are used.

stat functions or character strings naming functions to compute summary statistics

on resampled metric values and permuted samples. One or both of the values may be specified as named arguments or in the order in which their defaults

appear.

progress logical indicating whether to display iterative progress during elimination.

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Value

TrainingStep class object containing a summary of the numbers of predictor variables retained (size), their names (terms), logical indicators for the optimal model selected (selected), and associated performance metrics (metrics).

See Also

```
performance, plot, summary, varimp
```

Examples

```
## Requires prior installation of suggested package gbm to run
(res <- rfe(sale_amount ~ ., data = ICHomes, model = GBMModel))
summary(res)
summary(performance(res))
plot(res, type = "line")</pre>
```

RFSRCModel

Fast Random Forest (SRC) Model

Description

Fast OpenMP computing of Breiman's random forest for a variety of data settings including right-censored survival, regression, and classification.

```
RFSRCModel(
  ntree = 1000,
 mtry = integer(),
  nodesize = integer(),
  nodedepth = integer(),
  splitrule = character(),
  nsplit = 10,
  block.size = integer(),
  samptype = c("swor", "swr"),
  membership = FALSE,
  sampsize = if (samptype == "swor") function(x) 0.632 \times x else function(x) x,
  nimpute = 1,
  ntime = integer(),
  proximity = c(FALSE, TRUE, "inbag", "oob", "all"),
  distance = c(FALSE, TRUE, "inbag", "oob", "all"),
  forest.wt = c(FALSE, TRUE, "inbag", "oob", "all"),
  xvar.wt = numeric(),
```

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```
split.wt = numeric(),
  var.used = c(FALSE, "all.trees", "by.tree"),
  split.depth = c(FALSE, "all.trees", "by.tree"),
  do.trace = FALSE,
  statistics = FALSE
)

RFSRCFastModel(
  ntree = 500,
  sampsize = function(x) min(0.632 * x, max(x^0.75, 150)),
  ntime = 50,
  terminal.qualts = FALSE,
  ...
)
```

Arguments

ntree number of trees.

mtry number of variables randomly selected as candidates for splitting a node.

nodesize minumum size of terminal nodes.

nodedepth maximum depth to which a tree should be grown.

splitrule splitting rule (see rfsrc).

nsplit non-negative integer value for number of random splits to consider for each

candidate splitting variable.

block.size interval number of trees at which to compute the cumulative error rate.

samptype whether bootstrap sampling is with or without replacement.

membership logical indicating whether to return terminal node membership.

sampsize function specifying the bootstrap size.

nimpute number of iterations of the missing data imputation algorithm.

ntime integer number of time points to constrain ensemble calculations for survival

outcomes.

proximity whether and how to return proximity of cases as measured by the frequency of

sharing the same terminal nodes.

distance whether and how to return distance between cases as measured by the ratio of

the sum of edges from each case to the root node.

forest.wt whether and how to return the forest weight matrix.

xvar.wt vector of non-negative weights representing the probability of selecting a vari-

able for splitting.

split.wt vector of non-negative weights used for multiplying the split statistic for a vari-

able.

var.used whether and how to return variables used for splitting.

split.depth whether and how to return minimal depth for each variable.

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do.trace number of seconds between updates to the user on approximate time to comple-

tion.

statistics logical indicating whether to return split statistics.

terminal.qualts

logical indicating whether to return terminal node membership information.

... arguments passed to RFSRCModel.

Details

Response types: factor, matrix, numeric, Surv

Automatic tuning of grid parameters: mtry, nodesize

Default argument values and further model details can be found in the source See Also links below.

In calls to varimp for RFSRCModel, argument type may be specified as "anti" (default) for cases assigned to the split opposite of the random assignments, as "permute" for permutation of OOB cases, or as "random" for permutation replaced with random assignment. Variable importance is automatically scaled to range from 0 to 100. To obtain unscaled importance values, set scale = FALSE. See example below.

Value

MLModel class object.

See Also

```
rfsrc, rfsrc.fast, fit, resample
```

Examples

```
## Requires prior installation of suggested package randomForestSRC to run
model_fit <- fit(sale_amount ~ ., data = ICHomes, model = RFSRCModel)
varimp(model_fit, method = "model", type = "random", scale = TRUE)</pre>
```

RPartModel

Recursive Partitioning and Regression Tree Models

Description

Fit an rpart model.

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Usage

```
RPartModel(
  minsplit = 20,
  minbucket = round(minsplit/3),
  cp = 0.01,
  maxcompete = 4,
  maxsurrogate = 5,
  usesurrogate = 2,
  xval = 10,
  surrogatestyle = 0,
  maxdepth = 30
)
```

Arguments

minsplit minimum number of observations that must exist in a node in order for a split to

be attempted.

minbucket minimum number of observations in any terminal node.

cp complexity parameter.

maxcompete number of competitor splits retained in the output.

maxsurrogate number of surrogate splits retained in the output.

usesurrogate how to use surrogates in the splitting process.

xval number of cross-validations.

surrogatestyle controls the selection of a best surrogate.

maximum depth of any node of the final tree, with the root node counted as

depth 0.

Details

Response types: factor, numeric, Surv **Automatic tuning of grid parameter:** cp

Further model details can be found in the source link below.

Value

MLModel class object.

See Also

```
rpart, fit, resample
```

```
## Requires prior installation of suggested packages rpart and partykit to run fit(Species \sim ., data = iris, model = RPartModel)
```

SelectedInput 103

SelectedInput

Selected Model Inputs

Description

Formula, design matrix, model frame, or recipe selection from a candidate set.

```
SelectedInput(...)
## S3 method for class 'formula'
SelectedInput(
  ...,
  data,
  control = MachineShop::settings("control"),
 metrics = NULL,
 cutoff = MachineShop::settings("cutoff"),
  stat = MachineShop::settings("stat.TrainingParams")
)
## S3 method for class 'matrix'
SelectedInput(
  . . . ,
 у,
  control = MachineShop::settings("control"),
 metrics = NULL,
  cutoff = MachineShop::settings("cutoff"),
  stat = MachineShop::settings("stat.TrainingParams")
)
## S3 method for class 'ModelFrame'
SelectedInput(
 control = MachineShop::settings("control"),
 metrics = NULL,
  cutoff = MachineShop::settings("cutoff"),
  stat = MachineShop::settings("stat.TrainingParams")
)
## S3 method for class 'recipe'
SelectedInput(
  control = MachineShop::settings("control"),
 metrics = NULL,
  cutoff = MachineShop::settings("cutoff"),
  stat = MachineShop::settings("stat.TrainingParams")
```

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```
## S3 method for class 'ModelSpecification'
SelectedInput(
    ...,
    control = MachineShop::settings("control"),
    metrics = NULL,
    cutoff = MachineShop::settings("cutoff"),
    stat = MachineShop::settings("stat.TrainingParams")
)
## S3 method for class 'list'
SelectedInput(x, ...)
```

Arguments

	inputs defining relationships between model predictor and response variables. Supplied inputs must all be of the same type and may be named or unnamed.
data	data frame containing predictor and response variables.
control	control function, function name, or object defining the resampling method to be employed.
metrics	metric function, function name, or vector of these with which to calculate performance. If not specified, default metrics defined in the performance functions are used. Recipe selection is based on the first calculated metric.
cutoff	argument passed to the metrics functions.
stat	function or character string naming a function to compute a summary statistic on resampled metric values for recipe selection.
у	response variable.
x	list of inputs followed by arguments passed to their method function.

Value

SelectedModelFrame, SelectedModelRecipe, or SelectedModelSpecification class object that inherits from SelectedInput and ModelFrame, recipe, or ModelSpecification, respectively.

See Also

```
fit, resample
```

```
## Selected model frame
sel_mf <- SelectedInput(
   sale_amount ~ sale_year + built + style + construction,
   sale_amount ~ sale_year + base_size + bedrooms + basement,
   data = ICHomes
)</pre>
```

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```
fit(sel_mf, model = GLMModel)

## Selected recipe
library(recipes)
data(Boston, package = "MASS")

rec1 <- recipe(medv ~ crim + zn + indus + chas + nox + rm, data = Boston)
rec2 <- recipe(medv ~ chas + nox + rm + age + dis + rad + tax, data = Boston)
sel_rec <- SelectedInput(rec1, rec2)

fit(sel_rec, model = GLMModel)</pre>
```

SelectedModel

Selected Model

Description

Model selection from a candidate set.

```
SelectedModel(...)
## Default S3 method:
SelectedModel(
  control = MachineShop::settings("control"),
 metrics = NULL,
 cutoff = MachineShop::settings("cutoff"),
  stat = MachineShop::settings("stat.TrainingParams")
)
## S3 method for class 'ModelSpecification'
SelectedModel(
  control = MachineShop::settings("control"),
 metrics = NULL,
  cutoff = MachineShop::settings("cutoff"),
  stat = MachineShop::settings("stat.TrainingParams")
)
## S3 method for class 'list'
SelectedModel(x, ...)
```

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Arguments

	model functions, function names, objects; other objects that can be coerced to models; vectors of these to serve as the candidate set from which to select, such as that returned by expand_model; or model specifications.
control	control function, function name, or object defining the resampling method to be employed.
metrics	metric function, function name, or vector of these with which to calculate performance. If not specified, default metrics defined in the performance functions are used. Model selection is based on the first calculated metric.
cutoff	argument passed to the metrics functions.
stat	function or character string naming a function to compute a summary statistic on resampled metric values for model selection.
x	list of models followed by arguments passed to their method function.

Details

Response types: factor, numeric, ordered, Surv

Value

 $Selected \texttt{Model or Selected Model Specification class object that inherits from \texttt{MLModel or Model Specification}, respectively.$

See Also

```
fit, resample
```

```
## Requires prior installation of suggested package gbm and glmnet to run
model_fit <- fit(
    sale_amount ~ ., data = ICHomes,
    model = SelectedModel(GBMModel, GLMNetModel, SVMRadialModel)
)
(selected_model <- as.MLModel(model_fit))
summary(selected_model)</pre>
```

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settings

MachineShop Settings

Description

Allow the user to view or change global settings which affect default behaviors of functions in the **MachineShop** package.

Usage

```
settings(...)
```

Arguments

character names of settings to view, name = value pairs giving the values of settings to change, a vector of these, "reset" to restore all package defaults, or no arguments to view all settings. Partial matching of setting names is supported.

Value

The setting value if only one is specified to view. Otherwise, a list of the values of specified settings as they existed prior to any requested changes. Such a list can be passed as an argument to settings to restore their values.

Settings

control function, function name, or object defining a default resampling method [default: "CVControl"].

- cutoff numeric (0, 1) threshold above which binary factor probabilities are classified as events and below which survival probabilities are classified [default: 0.5].
- distr.SurvMeans character string specifying distributional approximations to estimated survival curves for predicting survival means. Choices are "empirical" for the Kaplan-Meier estimator, "exponential", "rayleigh", or "weibull" (default).
- distr.SurvProbs character string specifying distributional approximations to estimated survival curves for predicting survival events/probabilities. Choices are "empirical" (default) for the Kaplan-Meier estimator, "exponential", "rayleigh", or "weibull".
- grid size argument to TuningGrid indicating the number of parameter-specific values to generate automatically for tuning of models that have pre-defined grids or a TuningGrid function, function name, or object [default: 3].
- method. Empirical Surv character string specifying the empirical method of estimating baseline survival curves for Cox proportional hazards-based models. Choices are "breslow" or "efron" (default).
- metrics.ConfusionMatrix function, function name, or vector of these with which to calculate
 performance metrics for confusion matrices [default: c(Accuracy = "accuracy", Kappa =
 "kappa2", `Weighted Kappa` = "weighted_kappa2", Sensitivity = "sensitivity", Specificity
 = "specificity")].

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- metrics.matrix function, function name, or vector of these with which to calculate performance metrics for matrix responses [default: c(RMSE = "rmse", R2 = "r2", MAE = "mae")].
- metrics.numeric function, function name, or vector of these with which to calculate performance metrics for numeric responses [default: c(RMSE = "rmse", R2 = "r2", MAE = "mae")].
- metrics.Surv function, function name, or vector of these with which to calculate performance metrics for survival responses [default: c(`C-Index` = "cindex", Brier = "brier", `ROC AUC` = "roc_auc", Accuracy = "accuracy")].
- print_max number of models or data rows to show with print methods or Inf to show all [default: 10].
- require names of installed packages to load during parallel execution of resampling algorithms [default: "MachineShop"].
- reset character names of settings to reset to their default values.
- RHS.formula non-modifiable character vector of operators and functions allowed in traditional formula specifications.
- stat. Curve function or character string naming a function to compute one summary statistic at each cutoff value of resampled metrics in performance curves, or NULL for resample-specific metrics [default: "base::mean"].
- stat.Resample function or character string naming a function to compute one summary statistic to control the ordering of models in plots [default: "base::mean"].
- stat. TrainingParams function or character string naming a function to compute one summary statistic on resampled performance metrics for input selection or tuning or for model selection or tuning [default: "base::mean"].
- stats.PartialDependence function, function name, or vector of these with which to compute partial dependence summary statistics [default: c(Mean = "base::mean")].
- stats.Resample function, function name, or vector of these with which to compute summary
 statistics on resampled performance metrics [default: c(Mean = "base::mean", Median = "stats::median",
 SD = "stats::sd", Min = "base::min", Max = "base::max")].

```
## View all current settings
settings()

## Change settings
presets <- settings(control = "BootControl", grid = 10)

## View one setting
settings("control")

## View multiple settings
settings("control", "grid")</pre>
```

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```
## Restore the previous settings
settings(presets)
```

set_monitor

Training Parameters Monitoring Control

Description

Set parameters that control the monitoring of resample estimation of model performance and of tuning parameter optimization.

Usage

```
set_monitor(object, ...)
## S3 method for class 'MLControl'
set_monitor(object, progress = TRUE, verbose = FALSE, ...)
## S3 method for class 'MLOptimization'
set_monitor(object, progress = FALSE, verbose = FALSE, ...)
## S3 method for class 'ModelSpecification'
set_monitor(object, which = c("all", "control", "optim"), ...)
```

Arguments

object	resampling control, tuning parameter optimization, or model specification object.
	arguments passed from the ModelSpecification method to the others.
progress	logical indicating whether to display iterative progress during resampling or optimization. In the case of resampling, a progress bar will be displayed if a computing cluster is not registered or is registered with the doSNOW package.
verbose	numeric or logical value specifying the level of progress detail to print, with 0 (FALSE) indicating none and 1 (TRUE) or higher indicating increasing amounts of detail.
which	character string specifying the monitoring parameters to set as "all", "control", or optimization ("optim").

Value

Argument object updated with the supplied parameters.

See Also

```
resample, set_optim, set_predict, set_strata
```

Examples

```
CVControl() %>% set_monitor(verbose = TRUE)
```

set_optim

Tuning Parameter Optimization

Description

Set the optimization method and control parameters for tuning of model parameters.

Usage

```
set_optim_bayes(object, ...)
## S3 method for class 'ModelSpecification'
set_optim_bayes(
 object,
 num_init = 5,
  times = 10,
  each = 1,
  acquisition = c("ucb", "ei", "eips", "poi"),
  kappa = stats::qnorm(conf),
  conf = 0.995,
  epsilon = 0,
  control = list(),
  packages = c("ParBayesianOptimization", "rBayesianOptimization"),
  random = FALSE,
 progress = verbose,
 verbose = 0,
)
set_optim_bfgs(object, ...)
## S3 method for class 'ModelSpecification'
set_optim_bfgs(
 object,
  times = 10,
 control = list(),
  random = FALSE,
 progress = FALSE,
 verbose = 0,
)
set_optim_grid(object, ...)
```

```
## S3 method for class 'TrainingParams'
set_optim_grid(object, random = FALSE, progress = FALSE, ...)
## S3 method for class 'ModelSpecification'
set_optim_grid(object, ...)
## S3 method for class 'TunedInput'
set_optim_grid(object, ...)
## S3 method for class 'TunedModel'
set_optim_grid(object, ...)
set_optim_pso(object, ...)
## S3 method for class 'ModelSpecification'
set_optim_pso(
 object,
 times = 10,
 each = NULL,
 control = list(),
 random = FALSE,
 progress = FALSE,
 verbose = 0,
)
set_optim_sann(object, ...)
## S3 method for class 'ModelSpecification'
set_optim_sann(
 object,
  times = 10,
  control = list(),
  random = FALSE,
 progress = FALSE,
 verbose = 0,
)
set_optim_method(object, ...)
## S3 method for class 'ModelSpecification'
set_optim_method(
 object,
  fun,
  label = "Optimization Function",
  packages = character(),
```

```
params = list(),
random = FALSE,
progress = FALSE,
verbose = FALSE,
...
)
```

Arguments

object input or model object.

 $\dots \qquad \text{arguments passed to the TrainingParams method of } \mathsf{set_optim_grid} \ from \ its$

other methods.

num_init number of grid points to sample for the initialization of Bayesian optimization.

times maximum number of times to repeat the optimization step. Multiple sets of

model parameters are evaluated automatically at each step of the BFGS algo-

rithm to compute a finite-difference approximation to the gradient.

each number of times to sample and evaluate model parameters at each optimization

step. This is the swarm size in particle swarm optimization, which defaults to

floor(10 + 2 * sqrt(length(bounds))).

acquisition character string specifying the acquisition function as "ucb" (upper confidence

bound), "ei" (expected improvement), "eips" (expected improvement per sec-

ond), or "poi" (probability of improvement).

kappa, conf upper confidence bound ("ucb") quantile or its probability to balance exploita-

tion against exploration. Argument kappa takes precedence if both are given and multiplies the predictive standard deviation added to the predictive mean in the acquisition function. Larger values encourage exploration of the model

parameter space.

epsilon improvement methods ("ei", "eips", and "poi") parameter to balance ex-

ploitation against exploration. Values should be between -0.1 and 0.1 with larger

ones encouraging exploration.

control list of control parameters passed to bayesOpt by set_optim_bayes with pack-

age "ParBayesianOptimization", to BayesianOptimization by set_optim_bayes with package "rBayesianOptimization", to optim by set_optim_bfgs and

set_optim_sann, and to psoptim by set_optim_pso.

packages R package or packages to use for the optimization method, or an empty vec-

tor if none are needed. The first package in set_optim_bayes is used unless

otherwise specified by the user.

random number of points to sample for a random grid search, or FALSE for an exhaustive

grid search. Used when a grid search is specified or as the fallback method for non-numeric model parameters present during other optimization methods.

progress logical indicating whether to display iterative progress during optimization.

verbose numeric or logical value specifying the level of progress detail to print, with 0

(FALSE) indicating none and 1 (TRUE) or higher indicating increasing amounts

of detail.

fun

user-defined optimization function to which the arguments below are passed in order. An ellipsis can be included in the function definition when using only a subset of the arguments and ignoring others. A tibble returned by the function with the same number of rows as model evaluations will be included in a TrainingStep summary of optimization results; other types of return values will be ignored.

optim function that takes a numeric vector or list of named model parameters as the first argument, optionally accepts the maximum number of iterations as argument max_iter, and returns a scalar measure of performance to be maximized. Parameter names are available from the grid and bounds arguments described below. If the function cannot be evaluated at a given set of parameter values, then -Inf is returned.

grid data frame containing a tuning grid of all model parameters.

bounds named list of lower and upper bounds for each finite numeric model parameter in grid. The types (integer or double) of the original parameter values are preserved in the bounds.

params list of optimization parameters as supplied to set_optim_method.

monitor list of the progress and verbose values.

label character descriptor for the optimization method.

params list of user-specified model parameters to be passed to fun.

Details

The optimization functions implement the following methods.

set_optim_bayes Bayesian optimization with a Gaussian process model (Snoek et al. 2012).

set_optim_bfgs limited-memory modification of quasi-Newton BFGS optimization (Byrd et al. 1995).

set_optim_grid exhaustive or random grid search.

set_optim_pso particle swarm optimization (Bratton and Kennedy 2007, Zambrano-Bigiarini et al. 2013).

set_optim_sann simulated annealing (Belisle 1992). This method depends critically on the control parameter settings. It is not a general-purpose method but can be very useful in getting to good parameter values on a very rough optimization surface.

set_optim_method user-defined optimization function.

The package-defined optimization functions evaluate and return values of the tuning parameters that are of same type (e.g. integer, double, character) as given in the object grid. Sequential optimization of numeric tuning parameters is performed over a hypercube defined by their minimum and maximum grid values. Non-numeric parameters are optimized with grid searches.

Value

Argument object updated with the specified optimization method and control parameters.

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References

Belisle, C. J. P. (1992). Convergence theorems for a class of simulated annealing algorithms on Rd. *Journal of Applied Probability*, 29, 885–895.

Bratton, D. & Kennedy, J. (2007), Defining a standard for particle swarm optimization. In *IEEE Swarm Intelligence Symposium*, 2007 (pp. 120-127).

Byrd, R. H., Lu, P., Nocedal, J., & Zhu, C. (1995). A limited memory algorithm for bound constrained optimization. *SIAM Journal on Scientific Computing*, *16*, 1190–1208.

Snoek, J., Larochelle, H., & Adams, R.P. (2012). Practical Bayesian Optimization of Machine Learning Algorithms. arXiv:1206.2944 [stat.ML].

Zambrano-Bigiarini, M., Clerc, M., & Rojas, R. (2013). Standard particle swarm optimisation 2011 at CEC-2013: A baseline for future PSO improvements. In *IEEE Congress on Evolutionary Computation*, 2013 (pp. 2337-2344).

See Also

BayesianOptimization, bayesOpt, optim, psoptim, set_monitor, set_predict, set_strata

Examples

```
ModelSpecification(
  sale_amount ~ ., data = ICHomes,
  model = TunedModel(GBMModel)
) %>% set_optim_bayes
```

set_predict

Resampling Prediction Control

Description

Set parameters that control prediction during resample estimation of model performance.

Usage

```
set_predict(
  object,
  times = numeric(),
  distr = character(),
  method = character(),
  ...
)
```

Arguments

```
object control object.

times, distr, method
arguments passed to predict.
... arguments passed to other methods.
```

set_strata 115

Value

Argument object updated with the supplied parameters.

See Also

```
resample, set_monitor, set_optim, set_strata
```

Examples

```
CVControl() %>% set_predict(times = 1:3)
```

set_strata

Resampling Stratification Control

Description

Set parameters that control the construction of strata during resample estimation of model performance.

Usage

```
set_strata(object, breaks = 4, nunique = 5, prop = 0.1, size = 20, ...)
```

Arguments

object control object.

breaks number of quantile bins desired for stratification of numeric data during resampling.

nunique number of unique values at or below which numeric data are stratified as categorical.

prop minimum proportion of data in each strata.

size minimum number of values in each strata.

... arguments passed to other methods.

Details

The arguments control resampling strata which are constructed from numeric proportions for BinomialVariate; original values for character, factor, logical, numeric, and ordered; first columns of values for matrix; and numeric times within event statuses for Surv. Stratification of survival data by event status only can be achieved by setting breaks = 1. Numeric values are stratified into quantile bins and categorical values into factor levels. The number of bins will be the largest integer less than or equal to breaks satisfying the prop and size control argument thresholds. Categorical levels below the thresholds will be pooled iteratively by reassigning values in the smallest nominal level to the remaining ones at random and by combining the smallest adjacent ordinal levels. Missing values are replaced with non-missing values sampled at random with replacement.

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Value

Argument object updated with the supplied parameters.

See Also

```
resample, set_monitor, set_optim, set_predict
```

Examples

```
CVControl() %>% set_strata(breaks = 3)
```

StackedModel

Stacked Regression Model

Description

Fit a stacked regression model from multiple base learners.

Usage

```
StackedModel(
    ...,
    control = MachineShop::settings("control"),
    weights = numeric()
)
```

Arguments

... model functions, function names, objects; other objects that can be coerced to

models; or vector of these to serve as base learners.

control control function, function name, or object defining the resampling method to be

employed for the estimation of base learner weights.

weights optional fixed base learner weights.

Details

```
Response types: factor, numeric, ordered, Surv
```

Value

StackedModel class object that inherits from MLModel.

References

Breiman, L. (1996). Stacked regression. Machine Learning, 24, 49-64.

step_kmeans 117

See Also

```
fit, resample
```

Examples

```
## Requires prior installation of suggested packages gbm and glmnet to run
model <- StackedModel(GBMModel, SVMRadialModel, GLMNetModel(lambda = 0.01))
model_fit <- fit(sale_amount ~ ., data = ICHomes, model = model)
predict(model_fit, newdata = ICHomes)</pre>
```

step_kmeans

K-Means Clustering Variable Reduction

Description

Creates a *specification* of a recipe step that will convert numeric variables into one or more by averaging within k-means clusters.

Usage

```
step_kmeans(
  recipe,
  ...,
  k = 5,
  center = TRUE,
  scale = TRUE,
  algorithm = c("Hartigan-Wong", "Lloyd", "Forgy", "MacQueen"),
 max_iter = 10,
  num_start = 1,
  replace = TRUE,
  prefix = "KMeans",
  role = "predictor",
  skip = FALSE,
  id = recipes::rand_id("kmeans")
## S3 method for class 'step_kmeans'
tidy(x, ...)
## S3 method for class 'step_kmeans'
tunable(x, ...)
```

step_kmeans

Arguments

recipe	recipe object to which the step will be added.
	one or more selector functions to choose which variables will be used to compute the components. See selections for more details. These are not currently used by the tidy method.
k	number of k-means clusterings of the variables. The value of k is constrained to be between 1 and one less than the number of original variables.
center, scale	logicals indicating whether to mean center and standard deviation scale the original variables prior to deriving components, or functions or names of functions for the centering and scaling.
algorithm	character string specifying the clustering algorithm to use.
max_iter	maximum number of algorithm iterations allowed.
num_start	number of random cluster centers generated for starting the Hartigan-Wong algorithm.
replace	logical indicating whether to replace the original variables.
prefix	character string prefix added to a sequence of zero-padded integers to generate names for the resulting new variables.
role	analysis role that added step variables should be assigned. By default, they are designated as model predictors.
skip	logical indicating whether to skip the step when the recipe is baked. While all operations are baked when prep is run, some operations may not be applicable to new data (e.g. processing outcome variables). Care should be taken when using skip = TRUE as it may affect the computations for subsequent operations.
id	unique character string to identify the step.
x	step_kmeans object.

Details

K-means clustering partitions variables into k groups such that the sum of squares between the variables and their assigned cluster means is minimized. Variables within each cluster are then averaged to derive a new set of k variables.

Value

Function step_kmeans creates a new step whose class is of the same name and inherits from step_lincomp, adds it to the sequence of existing steps (if any) in the recipe, and returns the updated recipe. For the tidy method, a tibble with columns terms (selectors or variables selected), cluster assignments, sqdist (squared distance from cluster centers), and name of the new variable names.

References

Forgy, E. W. (1965). Cluster analysis of multivariate data: efficiency versus interpretability of classifications. *Biometrics*, 21, 768-769.

step_kmedoids 119

Hartigan, J. A., & Wong, M. A. (1979). A K-means clustering algorithm. *Applied Statistics*, 28, 100-108.

Lloyd, S. P. (1982). Least squares quantization in PCM. *IEEE Transactions on Information Theory*, 28(2), 129-137.

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

See Also

kmeans, recipe, prep, bake

Examples

```
library(recipes)

rec <- recipe(rating ~ ., data = attitude)
kmeans_rec <- rec %>%
    step_kmeans(all_predictors(), k = 3)
kmeans_prep <- prep(kmeans_rec, training = attitude)
kmeans_data <- bake(kmeans_prep, attitude)

pairs(kmeans_data, lower.panel = NULL)

tidy(kmeans_rec, number = 1)
tidy(kmeans_prep, number = 1)</pre>
```

step_kmedoids

K-Medoids Clustering Variable Selection

Description

Creates a *specification* of a recipe step that will partition numeric variables according to k-medoids clustering and select the cluster medoids.

Usage

```
step_kmedoids(
  recipe,
    ...,
  k = 5,
  center = TRUE,
  scale = TRUE,
  method = c("pam", "clara"),
  metric = "euclidean",
  optimize = FALSE,
  num_samp = 50,
```

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```
samp_size = 40 + 2 * k,
replace = TRUE,
prefix = "KMedoids",
role = "predictor",
skip = FALSE,
id = recipes::rand_id("kmedoids")
)

## S3 method for class 'step_kmedoids'
tunable(x, ...)
```

Arguments

recipe object to which the step will be added.

... one or more selector functions to choose which variables will be used to compute the components. See selections for more details. These are not currently used

by the tidy method.

k number of k-medoids clusterings of the variables. The value of k is constrained

to be between 1 and one less than the number of original variables.

center, scale logicals indicating whether to mean center and median absolute deviation scale

the original variables prior to cluster partitioning, or functions or names of func-

tions for the centering and scaling; not applied to selected variables.

method character string specifying one of the clustering methods provided by the **cluster**

package. The clara (clustering large applications) method is an extension of

pam (partitioning around medoids) designed to handle large datasets.

metric character string specifying the distance metric for calculating dissimilarities

between observations as "euclidean", "manhattan", or "jaccard" (clara

only).

optimize logical indicator or 0:5 integer level specifying optimization for the pam cluster-

ing method.

num_samp number of sub-datasets to sample for the clara clustering method.

samp_size number of cases to include in each sub-dataset.

replace logical indicating whether to replace the original variables.

prefix if the original variables are not replaced, the selected variables are added to

the dataset with the character string prefix added to their names; otherwise, the

original variable names are retained.

role analysis role that added step variables should be assigned. By default, they are

designated as model predictors.

skip logical indicating whether to skip the step when the recipe is baked. While all

operations are baked when prep is run, some operations may not be applicable to new data (e.g. processing outcome variables). Care should be taken when using skip = TRUE as it may affect the computations for subsequent operations.

id unique character string to identify the step.

x step_kmedoids object.

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Details

K-medoids clustering partitions variables into k groups such that the dissimilarity between the variables and their assigned cluster medoids is minimized. Cluster medoids are then returned as a set of k variables.

Value

Function step_kmedoids creates a new step whose class is of the same name and inherits from step_sbf, adds it to the sequence of existing steps (if any) in the recipe, and returns the updated recipe. For the tidy method, a tibble with columns terms (selectors or variables selected), cluster assignments, selected (logical indicator of selected cluster medoids), silhouette (silhouette values), and name of the selected variable names.

References

Kaufman, L., & Rousseeuw, P. J. (1990). Finding groups in data: An introduction to cluster analysis. Wiley.

Reynolds, A., Richards, G., de la Iglesia, B., & Rayward-Smith, V. (1992). Clustering rules: A comparison of partitioning and hierarchical clustering algorithms. *Journal of Mathematical Modelling and Algorithms*, 5, 475-504.

See Also

```
pam, clara, recipe, prep, bake
```

Examples

```
## Requires prior installation of suggested package cluster to run
library(recipes)

rec <- recipe(rating ~ ., data = attitude)
kmedoids_rec <- rec %>%
    step_kmedoids(all_predictors(), k = 3)
kmedoids_prep <- prep(kmedoids_rec, training = attitude)
kmedoids_data <- bake(kmedoids_prep, attitude)

pairs(kmedoids_data, lower.panel = NULL)

tidy(kmedoids_rec, number = 1)
tidy(kmedoids_prep, number = 1)</pre>
```

step_lincomp

step_lincomp

Linear Components Variable Reduction

Description

Creates a *specification* of a recipe step that will compute one or more linear combinations of a set of numeric variables according to a user-specified transformation matrix.

Usage

```
step_lincomp(
  recipe,
  . . . ,
  transform,
  num\_comp = 5,
  options = list(),
  center = TRUE,
  scale = TRUE,
  replace = TRUE,
  prefix = "LinComp",
  role = "predictor",
  skip = FALSE,
  id = recipes::rand_id("lincomp")
)
## S3 method for class 'step_lincomp'
tidy(x, ...)
## S3 method for class 'step_lincomp'
tunable(x, ...)
```

Arguments

recipe recipe object to which the step will be added.

one or more selector functions to choose which variables will be used to compute the components. See selections for more details. These are not currently used

by the tidy method.

transform function whose first argument x is a matrix of variables with which to compute

linear combinations and second argument step is the current step. The function should return a transformation matrix or Matrix of variable weights in its columns, or return a list with element `weights` containing the transformation matrix and possibly with other elements to be included as attributes in output

from the tidy method.

num_comp number of components to derive. The value of num_comp will be constrained to

a minimum of 1 and maximum of the number of original variables when prep

is run.

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options	list of elements to be added to the step object for use in the transform function.
center, scale	logicals indicating whether to mean center and standard deviation scale the original variables prior to deriving components, or functions or names of functions for the centering and scaling.
replace	logical indicating whether to replace the original variables.
prefix	character string prefix added to a sequence of zero-padded integers to generate names for the resulting new variables.
role	analysis role that added step variables should be assigned. By default, they are designated as model predictors.
skip	logical indicating whether to skip the step when the recipe is baked. While all operations are baked when prep is run, some operations may not be applicable to new data (e.g. processing outcome variables). Care should be taken when using skip = TRUE as it may affect the computations for subsequent operations.
id	unique character string to identify the step.
x	step_lincomp object.

Value

An updated version of recipe with the new step added to the sequence of existing steps (if any). For the tidy method, a tibble with columns terms (selectors or variables selected), weight of each variable in the linear transformations, and name of the new variable names.

See Also

```
recipe, prep, bake
```

Examples

step_sbf

step_sbf

Variable Selection by Filtering

Description

Creates a *specification* of a recipe step that will select variables from a candidate set according to a user-specified filtering function.

Usage

```
step_sbf(
  recipe,
    ...,
  filter,
  multivariate = FALSE,
  options = list(),
  replace = TRUE,
  prefix = "SBF",
  role = "predictor",
  skip = FALSE,
  id = recipes::rand_id("sbf")
)

## S3 method for class 'step_sbf'
tidy(x, ...)
```

Arguments

rocino	racina oh	iact to	which the	cton will	be added.
recipe	recipe ob	וככנ נט	willen the	Step will	be added.

... one or more selector functions to choose which variables will be used to compute the components. See selections for more details. These are not currently used

by the tidy method.

filter function whose first argument x is a univariate vector or a multivariate data

frame of candidate variables from which to select, second argument y is the response variable as defined in preceding recipe steps, and third argument step is the current step. The function should return a logical value or vector of length equal the number of variables in x indicating whether to select the corresponding variable, or return a list or data frame with element `selected` containing the logical(s) and possibly with other elements of the same length to be included in

output from the tidy method.

multivariate logical indicating that candidate variables be passed to the x argument of the

filter function separately as univariate vectors if FALSE, or altogether in one

multivariate data frame if TRUE.

options list of elements to be added to the step object for use in the filter function.

replace logical indicating whether to replace the original variables.

step_sbf

prefix	if the original variables are not replaced, the selected variables are added to the dataset with the character string prefix added to their names; otherwise, the original variable names are retained.
role	analysis role that added step variables should be assigned. By default, they are designated as model predictors.
skip	logical indicating whether to skip the step when the recipe is baked. While all operations are baked when prep is run, some operations may not be applicable to new data (e.g. processing outcome variables). Care should be taken when using skip = TRUE as it may affect the computations for subsequent operations.
id	unique character string to identify the step.
X	step_sbf object.

Value

An updated version of recipe with the new step added to the sequence of existing steps (if any). For the tidy method, a tibble with columns terms (selectors or variables selected), selected (logical indicator of selected variables), and name of the selected variable names.

See Also

```
recipe, prep, bake
```

Examples

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step_spca

Sparse Principal Components Analysis Variable Reduction

Description

Creates a *specification* of a recipe step that will derive sparse principal components from one or more numeric variables.

Usage

```
step_spca(
  recipe,
  . . . ,
  num\_comp = 5,
  sparsity = 0,
  num_var = integer(),
  shrinkage = 1e-06,
  center = TRUE,
  scale = TRUE,
 max_iter = 200,
  tol = 0.001,
  replace = TRUE,
  prefix = "SPCA",
  role = "predictor",
  skip = FALSE,
  id = recipes::rand_id("spca")
)
## S3 method for class 'step_spca'
tunable(x, ...)
```

Arguments

recipe recipe object to which the step will be added.

one or more selector functions to choose which variables will be used to compute the components. See selections for more details. These are not currently used

by the tidy method.

num_comp number of components to derive. The value of num_comp will be constrained to

a minimum of 1 and maximum of the number of original variables when prep

sparsity, num_var

sparsity (L1 norm) penalty for each component or number of variables with non-zero component loadings. Larger sparsity values produce more zero loadings. Argument sparsity is ignored if num_var is given. The argument value may be a single number applied to all components or a vector of component-specific numbers.

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shrinkage	numeric shrinkage (quadratic) penalty for the components to improve conditioning; larger values produce more shrinkage of component loadings toward zero.
center, scale	logicals indicating whether to mean center and standard deviation scale the original variables prior to deriving components, or functions or names of functions for the centering and scaling.
max_iter	maximum number of algorithm iterations allowed.
tol	numeric tolerance for the convergence criterion.
replace	logical indicating whether to replace the original variables.
prefix	character string prefix added to a sequence of zero-padded integers to generate names for the resulting new variables.
role	analysis role that added step variables should be assigned. By default, they are designated as model predictors.
skip	logical indicating whether to skip the step when the recipe is baked. While all operations are baked when prep is run, some operations may not be applicable to new data (e.g. processing outcome variables). Care should be taken when using skip = TRUE as it may affect the computations for subsequent operations.
id	unique character string to identify the step.
x	step_spca object.

Details

Sparse principal components analysis (SPCA) is a variant of PCA in which the original variables may have zero loadings in the linear combinations that form the components.

Value

Function step_spca creates a new step whose class is of the same name and inherits from step_lincomp, adds it to the sequence of existing steps (if any) in the recipe, and returns the updated recipe. For the tidy method, a tibble with columns terms (selectors or variables selected), weight of each variable loading in the components, and name of the new variable names; and with attribute pev containing the proportions of explained variation.

References

Zou, H., Hastie, T., & Tibshirani, R. (2006). Sparse principal component analysis. *Journal of Computational and Graphical Statistics*, 15(2), 265-286.

See Also

```
spca, recipe, prep, bake
```

Examples

```
## Requires prior installation of suggested package elasticnet to run
library(recipes)
```

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```
rec <- recipe(rating ~ ., data = attitude)
spca_rec <- rec %>%
    step_spca(all_predictors(), num_comp = 5, sparsity = 1)
spca_prep <- prep(spca_rec, training = attitude)
spca_data <- bake(spca_prep, attitude)

pairs(spca_data, lower.panel = NULL)

tidy(spca_rec, number = 1)
tidy(spca_prep, number = 1)</pre>
```

summary

Model Performance Summaries

Description

Summary statistics for resampled model performance metrics.

Usage

```
## S3 method for class 'ConfusionList'
summary(object, ...)
## S3 method for class 'ConfusionMatrix'
summary(object, ...)
## S3 method for class 'MLModel'
summary(
 object,
  stats = MachineShop::settings("stats.Resample"),
 na.rm = TRUE,
)
## S3 method for class 'MLModelFit'
summary(object, .type = c("default", "glance", "tidy"), ...)
## S3 method for class 'Performance'
summary(
 object,
  stats = MachineShop::settings("stats.Resample"),
 na.rm = TRUE,
)
## S3 method for class 'PerformanceCurve'
```

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```
summary(object, stat = MachineShop::settings("stat.Curve"), ...)
## S3 method for class 'Resample'
summary(
  object,
  stats = MachineShop::settings("stats.Resample"),
  na.rm = TRUE,
  ...
)

## S3 method for class 'TrainingStep'
summary(object, ...)
```

Arguments

object	confusion, lift, trained model fit, performance, performance curve, resample, or rfe result.
	arguments passed to other methods.
stats	function, function name, or vector of these with which to compute summary statistics.
na.rm	logical indicating whether to exclude missing values.
.type	character string specifying that unMLModelFit(object) be passed to summary ("default"), glance, or tidy.
stat	function or character string naming a function to compute a summary statistic at each cutoff value of resampled metrics in PerformanceCurve, or NULL for resample-specific metrics.

Value

An object of summary statistics.

Examples

```
## Requires prior installation of suggested package gbm to run
## Factor response example
fo <- Species ~ .
control <- CVControl()

gbm_res1 <- resample(fo, iris, GBMModel(n.trees = 25), control)
gbm_res2 <- resample(fo, iris, GBMModel(n.trees = 50), control)
gbm_res3 <- resample(fo, iris, GBMModel(n.trees = 100), control)
summary(gbm_res3)

res <- c(GBM1 = gbm_res1, GBM2 = gbm_res2, GBM3 = gbm_res3)
summary(res)</pre>
```

SuperModel SuperModel

SuperModel	Su	per	^Mo	del
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Super Learner Model

Description

Fit a super learner model to predictions from multiple base learners.

Usage

```
SuperModel(
    ...,
    model = GBMModel,
    control = MachineShop::settings("control"),
    all_vars = FALSE
)
```

Arguments

	model functions, function names, objects; other objects that can be coerced to models; or vector of these to serve as base learners.
mode1	model function, function name, or object defining the super model; or another object that can be coerced to the model.
control	control function, function name, or object defining the resampling method to be employed for the estimation of base learner weights.
all_vars	logical indicating whether to include the original predictor variables in the super model.

Details

```
Response types: factor, numeric, ordered, Surv
```

Value

SuperModel class object that inherits from MLModel.

References

van der Laan, M. J., Polley, E. C., & Hubbard, A. E. (2007). Super learner. *Statistical Applications in Genetics and Molecular Biology*, 6(1).

See Also

```
fit, resample
```

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Examples

```
## Requires prior installation of suggested packages gbm and glmnet to run
model <- SuperModel(GBMModel, SVMRadialModel, GLMNetModel(lambda = 0.01))
model_fit <- fit(sale_amount ~ ., data = ICHomes, model = model)
predict(model_fit, newdata = ICHomes)</pre>
```

SurvMatrix

SurvMatrix Class Constructors

Description

Create a matrix of survival events or probabilites.

Usage

```
SurvEvents(data = NA, times = numeric(), distr = character())
SurvProbs(data = NA, times = numeric(), distr = character())
```

Arguments

data	matrix, or object that can be coerced to one, with survival events or probabilities at points in time in the columns and cases in the rows.
times	numeric vector of survival times for the columns.
distr	character string specifying the survival distribution from which the matrix values were derived.

Value

Object that is of the same class as the constructor name and inherits from SurvMatrix. Examples of these are predicted survival events and probabilities returned by the predict function.

See Also

```
performance, metrics
```

SurvRegModel SurvRegModel

SurvRegModel

Parametric Survival Model

Description

Fits the accelerated failure time family of parametric survival models.

Usage

```
SurvRegModel(
 dist = c("weibull", "exponential", "gaussian", "logistic", "lognormal",
    "logloglogistic"),
  scale = 0,
 parms = list(),
)
SurvRegStepAICModel(
 dist = c("weibull", "exponential", "gaussian", "logistic", "lognormal",
    "logloglogistic"),
  scale = 0,
 parms = list(),
 direction = c("both", "backward", "forward"),
  scope = list(),
 k = 2,
  trace = FALSE,
  steps = 1000
)
```

Arguments

dist	assumed distribution for y variable.
scale	optional fixed value for the scale.
parms	list of fixed parameters.
	arguments passed to survreg.control.
direction	mode of stepwise search, can be one of "both" (default), "backward", or "forward".
scope	defines the range of models examined in the stepwise search. This should be a list containing components upper and lower, both formulae.
k	multiple of the number of degrees of freedom used for the penalty. Only $k = 2$ gives the genuine AIC; $k = .(log(nobs))$ is sometimes referred to as BIC or SBC.
trace	if positive, information is printed during the running of stepAIC. Larger values may give more information on the fitting process.
steps	maximum number of steps to be considered.

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Details

Response types: Surv

Default argument values and further model details can be found in the source See Also links below.

Value

MLModel class object.

See Also

```
psm, survreg.control, stepAIC, fit, resample
stepAIC, fit, resample
```

Examples

```
## Requires prior installation of suggested packages rms and Hmisc to run
library(survival)
fit(Surv(time, status) ~ ., data = veteran, model = SurvRegModel)
```

SVMModel

Support Vector Machine Models

Description

Fits the well known C-svc, nu-svc, (classification) one-class-svc (novelty) eps-svr, nu-svr (regression) formulations along with native multi-class classification formulations and the bound-constraint SVM formulations.

Usage

```
SVMModel(
    scaled = TRUE,
    type = character(),
    kernel = c("rbfdot", "polydot", "vanilladot", "tanhdot", "laplacedot", "besseldot",
        "anovadot", "splinedot"),
    kpar = "automatic",
    C = 1,
    nu = 0.2,
    epsilon = 0.1,
    prob.model = FALSE,
    cache = 40,
    tol = 0.001,
    shrinking = TRUE
```

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```
SVMANOVAModel(sigma = 1, degree = 1, ...)

SVMBesselModel(sigma = 1, order = 1, degree = 1, ...)

SVMLaplaceModel(sigma = numeric(), ...)

SVMLinearModel(...)

SVMPolyModel(degree = 1, scale = 1, offset = 1, ...)

SVMRadialModel(sigma = numeric(), ...)

SVMSplineModel(...)

SVMTanhModel(scale = 1, offset = 1, ...)
```

Arguments

scaled logical vector indicating the variables to be scaled.

type type of support vector machine.

kernel kernel function used in training and predicting.

kpar list of hyper-parameters (kernel parameters).

C cost of constraints violation defined as the regularization term in the Lagrange

formulation.

nu parameter needed for nu-svc, one-svc, and nu-svr.

epsilon parameter in the insensitive-loss function used for eps-svr, nu-svr and eps-bsvm.

prob.model logical indicating whether to calculate the scaling parameter of the Laplacian

distribution fitted on the residuals of numeric response variables. Ignored in the

case of a factor response variable.

cache cache memory in MB.

tol tolerance of termination criterion.

shrinking whether to use the shrinking-heuristics.

sigma inverse kernel width used by the ANOVA, Bessel, and Laplacian kernels.

degree degree of the ANOVA, Bessel, and polynomial kernel functions.

... arguments passed to SVMModel from the other constructors.

order order of the Bessel function to be used as a kernel.

scale scaling parameter of the polynomial and hyperbolic tangent kernels as a conve-

nient way of normalizing patterns without the need to modify the data itself.

offset used in polynomial and hyperbolic tangent kernels.

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Details

Response types: factor, numeric

Automatic tuning of grid parameters: • SVMModel: NULL

• SVMANOVAModel: C, degree • SVMBesselModel: C, order, degree

 $\bullet \ SVMLaplace Model: \ C, \ sigma$

• SVMLinearModel: C

• SVMPolyModel: C, degree, scale

• SVMRadialModel: C, sigma

The kernel-specific constructor functions SVMANOVAModel, SVMBesselModel, SVMLaplaceModel, SVMLinearModel, SVMPolyModel, SVMRadialModel, SVMSplineModel, and SVMTanhModel are special cases of SVMModel which automatically set its kernel and kpar arguments. These are called directly in typical usage unless SVMModel is needed to specify a more general model.

Default argument values and further model details can be found in the source See Also link below.

Value

MLModel class object.

See Also

```
ksvm, fit, resample
```

Examples

```
fit(sale_amount ~ ., data = ICHomes, model = SVMRadialModel)
```

t.test

Paired t-Tests for Model Comparisons

Description

Paired t-test comparisons of resampled performance metrics from different models.

Usage

```
## S3 method for class 'PerformanceDiff'
t.test(x, adjust = "holm", ...)
```

Arguments

x performance difference result.

adjust method of p-value adjustment for multiple statistical comparisons as imple-

mented by p.adjust.

... arguments passed to other methods.

136 t.test

Details

The t-test statistic for pairwise model differences of R resampled performance metric values is calculated as

$$t = \frac{\bar{x}_R}{\sqrt{Fs_R^2/R}},$$

where \bar{x}_R and s_R^2 are the sample mean and variance. Statistical testing for a mean difference is then performed by comparing t to a t_{R-1} null distribution. The sample variance in the t statistic is known to underestimate the true variances of cross-validation mean estimators. Underestimation of these variances will lead to increased probabilities of false-positive statistical conclusions. Thus, an additional factor F is included in the t statistic to allow for variance corrections. A correction of F=1+K/(K-1) was found by Nadeau and Bengio (2003) to be a good choice for cross-validation with K folds and is thus used for that resampling method. The extension of this correction by Bouchaert and Frank (2004) to F=1+TK/(K-1) is used for cross-validation with K folds repeated T times. For other resampling methods F=1.

Value

PerformanceDiffTest class object that inherits from array. p-values and mean differences are contained in the lower and upper triangular portions, respectively, of the first two dimensions. Model pairs are contained in the third dimension.

References

Nadeau, C., & Bengio, Y. (2003). Inference for the generalization error. *Machine Learning*, 52, 239–81.

Bouckaert, R. R., & Frank, E. (2004). Evaluating the replicability of significance tests for comparing learning algorithms. In H. Dai, R. Srikant, & C. Zhang (Eds.), *Advances in knowledge discovery and data mining* (pp. 3–12). Springer.

Examples

```
## Numeric response example
fo <- sale_amount ~ .
control <- CVControl()

gbm_res1 <- resample(fo, ICHomes, GBMModel(n.trees = 25), control)
gbm_res2 <- resample(fo, ICHomes, GBMModel(n.trees = 50), control)
gbm_res3 <- resample(fo, ICHomes, GBMModel(n.trees = 100), control)

res <- c(GBM1 = gbm_res1, GBM2 = gbm_res2, GBM3 = gbm_res3)
res_diff <- diff(res)
t.test(res_diff)</pre>
```

Requires prior installation of suggested package gbm to run

TreeModel 137

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Classification and Regression Tree Models

Description

A tree is grown by binary recursive partitioning using the response in the specified formula and choosing splits from the terms of the right-hand-side.

Usage

```
TreeModel(
  mincut = 5,
  minsize = 10,
  mindev = 0.01,
  split = c("deviance", "gini"),
  k = numeric(),
  best = integer(),
  method = c("deviance", "misclass")
)
```

Arguments

mincut minimum number of observations to include in either child node.

minsize smallest allowed node size: a weighted quantity.

mindev within-node deviance must be at least this times that of the root node for the

node to be split.

split splitting criterion to use.

k scalar cost-complexity parameter defining a subtree to return.

best integer alternative to k requesting the number of terminal nodes of a subtree in

the cost-complexity sequence to return.

method character string denoting the measure of node heterogeneity used to guide cost-

complexity pruning.

Details

Response types: factor, numeric

Further model details can be found in the source link below.

Value

MLModel class object.

See Also

```
tree, prune.tree, fit, resample
```

TunedInput

Examples

```
## Requires prior installation of suggested package tree to run
fit(Species ~ ., data = iris, model = TreeModel)
```

TunedInput

Tuned Model Inputs

Description

Recipe tuning over a grid of parameter values.

Usage

```
TunedInput(object, ...)
## S3 method for class 'recipe'
TunedInput(
  object,
  grid = expand_steps(),
  control = MachineShop::settings("control"),
  metrics = NULL,
  cutoff = MachineShop::settings("cutoff"),
  stat = MachineShop::settings("stat.TrainingParams"),
  ...
)
```

Arguments

object	untrained recipe.
	arguments passed to other methods.
grid	RecipeGrid containing parameter values at which to evaluate a recipe, such as those returned by expand_steps.
control	control function, function name, or object defining the resampling method to be employed.
metrics	metric function, function name, or vector of these with which to calculate performance. If not specified, default metrics defined in the performance functions are used. Recipe selection is based on the first calculated metric.
cutoff	argument passed to the metrics functions.
stat	function or character string naming a function to compute a summary statistic on resampled metric values for recipe tuning.

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Value

TunedModelRecipe class object that inherits from TunedInput and recipe.

See Also

```
fit, resample, set_optim
```

Examples

```
library(recipes)
data(Boston, package = "MASS")

rec <- recipe(medv ~ ., data = Boston) %>%
    step_pca(all_numeric_predictors(), id = "pca")

grid <- expand_steps(
    pca = list(num_comp = 1:2)
)

fit(TunedInput(rec, grid = grid), model = GLMModel)</pre>
```

TunedModel

Tuned Model

Description

Model tuning over a grid of parameter values.

Usage

```
TunedModel(
  object,
  grid = MachineShop::settings("grid"),
  control = MachineShop::settings("control"),
  metrics = NULL,
  cutoff = MachineShop::settings("cutoff"),
  stat = MachineShop::settings("stat.TrainingParams")
)
```

Arguments

object

model function, function name, or object defining the model to be tuned.

grid

single integer or vector of integers whose positions or names match the parameters in the model's pre-defined tuning grid if one exists and which specify the number of values used to construct the grid; TuningGrid function, function name, or object; ParameterGrid object; or data frame containing parameter values at which to evaluate the model, such as that returned by expand_params.

TunedModel TunedModel

control	control function, function name, or object defining the resampling method to be employed.
metrics	metric function, function name, or vector of these with which to calculate performance. If not specified, default metrics defined in the performance functions are used. Model selection is based on the first calculated metric.
cutoff	argument passed to the metrics functions.
stat	function or character string naming a function to compute a summary statistic on resampled metric values for model tuning.

Details

The expand_modelgrid function enables manual extraction and viewing of grids created automatically when a TunedModel is fit.

Response types: factor, numeric, ordered, Surv

Value

TunedModel class object that inherits from MLModel.

See Also

```
fit, resample, set_optim
```

Examples

```
## Requires prior installation of suggested package gbm to run
## May require a long runtime
# Automatically generated grid
model_fit <- fit(sale_amount ~ ., data = ICHomes,</pre>
                 model = TunedModel(GBMModel))
varimp(model_fit)
(tuned_model <- as.MLModel(model_fit))</pre>
summary(tuned_model)
plot(tuned_model, type = "1")
# Randomly sampled grid points
fit(sale_amount ~ ., data = ICHomes,
   model = TunedModel(
      GBMModel,
      grid = TuningGrid(size = 1000, random = 5)
   ))
# User-specified grid
fit(sale_amount ~ ., data = ICHomes,
   model = TunedModel(
      GBMModel,
      grid = expand_params(
       n.trees = c(50, 100),
        interaction.depth = 1:2,
```

TuningGrid 141

```
n.minobsinnode = c(5, 10)
)
```

TuningGrid

Tuning Grid Control

Description

Defines control parameters for a tuning grid.

Usage

```
TuningGrid(size = 3, random = FALSE)
```

Arguments

size

single integer or vector of integers whose positions or names match the parameters in a model's tuning grid and which specify the number of values used to

construct the grid.

random

number of unique points to sample at random from the grid defined by size. If size is a single unnamed integer, then random = Inf will include all values of all grid parameters in the constructed grid, whereas random = FALSE will include

all values of default grid parameters.

Details

Returned TuningGrid objects may be supplied to TunedModel for automated construction of model tuning grids. These grids can be extracted manually and viewed with the expand_modelgrid function.

Value

TuningGrid class object.

See Also

```
TunedModel, expand_modelgrid
```

Examples

```
TunedModel(XGBTreeModel, grid = TuningGrid(10, random = 5))
```

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unMLModelFit

Revert an MLModelFit Object

Description

Function to revert an MLModelFit object to its original class.

Usage

```
unMLModelFit(object)
```

Arguments

object

model fit result.

Value

The supplied object with its MLModelFit classes and fields removed.

varimp

Variable Importance

Description

Calculate measures of relative importance for model predictor variables.

Usage

```
varimp(
  object,
  method = c("permute", "model"),
  scale = TRUE,
  sort = c("decreasing", "increasing", "asis"),
  ...
)
```

Arguments

object

model fit result.

 ${\tt method}$

character string specifying the calculation of variable importance as permutation-base ("permute") or model-specific ("model"). If model-specific importance is specified but not defined, the permutation-based method will be used instead with its default values (below). Permutation-based variable importance is defined as the relative change in model predictive performances between datasets with and without permuted values for the associated variable (Fisher et al. 2019).

varimp 143

scale logical value or vector indicating whether importance values are scaled to a maximum of 100.

character string specifying the sort order of importance values to be "decreasing", "increasing", or as predictors appear in the model formula ("asis").

arguments passed to model-specific or permutation-based variable importance functions. These include the following arguments and default values for method = "permute".

- select = NULL expression indicating predictor variables for which to compute variable importance (see subset for syntax) [default: all].
- samples = 1 number of times to permute the values of each variable. Larger numbers of samples decrease variability in the estimates at the expense of increased computation time.
- prop = numeric() proportion of observations to sample without replacement
 at each round of variable permutations [default: all]. Subsampling of ob servations can decrease computation time.
- size = integer() number of observations to sample at each round of permutations [default: all].
- times = numeric() numeric vector of follow-up times at which to predict survival probabilities or NULL for predicted survival means.
- metric = NULL metric function or function name with which to calculate performance. If not specified, the first applicable default metric from the performance functions is used.
- compare = c("-", "/") character specifying the relative change to compute in comparing model predictive performances between datasets with and without permuted values. The choices are difference ("-") and ratio ("/").
- stats = MachineShop::settings("stat.TrainingParams") function, function name, or vector of these with which to compute summary statistics on the set of variable importance values from the permuted datasets.
- na.rm = TRUE logical indicating whether to exclude missing variable importance values from the calculation of summary statistics.
- progress = TRUE logical indicating whether to display iterative progress during computation.

Details

The varimp function supports calculation of variable importance with the permutation-based method of Fisher et al. (2019) or with model-based methods where defined. Permutation-based importance is the default and has the advantages of being available for any model, any performance metric defined for the associated response variable type, and any predictor variable in the original training dataset. Conversely, model-specific importance is not defined for some models and will fall back to the permutation method in such cases; is generally limited to metrics implemented in the source packages of models; and may be computed on derived, rather than original, predictor variables. These disadvantages can make comparisons of model-specific importance across different classes of models infeasible. A downside of the permutation-based approach is increased computation time. To counter this, the permutation algorithm can be run in parallel simply by loading a parallel backend for the **foreach** package %dopar% function, such as **doParallel** or **doSNOW**.

. . .

sort

Permutation variable importance is interpreted as the contribution of a predictor variable to the predictive performance of a model as measured by the performance metric used in the calculation. Importance of a predictor is conditional on and, with the default scaling, relative to the values of all other predictors in the analysis.

Value

VariableImportance class object.

References

Fisher, A., Rudin, C., & Dominici, F. (2019). All models are wrong, but many are useful: Learning a variable's importance by studying an entire class of prediction models simultaneously. *Journal of Machine Learning Research*, 20, 1-81.

See Also

plot

Examples

```
## Requires prior installation of suggested package gbm to run
## Survival response example
library(survival)

gbm_fit <- fit(Surv(time, status) ~ ., data = veteran, model = GBMModel)
(vi <- varimp(gbm_fit))
plot(vi)</pre>
```

XGBMode1

Extreme Gradient Boosting Models

Description

Fits models with an efficient implementation of the gradient boosting framework from Chen & Guestrin.

Usage

```
XGBModel(
  nrounds = 100,
  ...,
  objective = character(),
  aft_loss_distribution = "normal",
  base_score = 0.5,
  verbose = 0,
```

```
print_every_n = 1
XGBDARTModel(
  eta = 0.3,
  gamma = 0,
 max_depth = 6,
 min_child_weight = 1,
 max_delta_step = .(0.7 * is(y, "PoissonVariate")),
  subsample = 1,
  colsample_bytree = 1,
  colsample_bylevel = 1,
  colsample_bynode = 1,
  alpha = 0,
  lambda = 1,
  tree_method = "auto",
  scale_pos_weight = 1,
  refresh_leaf = 1,
  grow_policy = "depthwise",
 max_leaves = 0,
 max_bin = 256,
  num_parallel_tree = 1,
  sample_type = "uniform",
  normalize_type = "tree",
  rate_drop = 0,
 one_drop = 0,
  skip_drop = 0,
)
XGBLinearModel(
  alpha = 0,
  lambda = 0,
  updater = "shotgun",
  feature_selector = "cyclic",
  top_k = 0,
)
XGBTreeModel(
  eta = 0.3,
  gamma = 0,
 max_depth = 6,
 min_child_weight = 1,
 max_delta_step = .(0.7 * is(y, "PoissonVariate")),
  subsample = 1,
  colsample_bytree = 1,
  colsample_bylevel = 1,
```

```
colsample_bynode = 1,
alpha = 0,
lambda = 1,
tree_method = "auto",
scale_pos_weight = 1,
refresh_leaf = 1,
grow_policy = "depthwise",
max_leaves = 0,
max_bin = 256,
num_parallel_tree = 1,
...
)
```

Arguments

subsample

nrounds number of boosting iterations. model parameters as described below and in the XGBoost documentation and arguments passed to XGBModel from the other constructors. objective optional character string defining the learning task and objective. Set automatically if not specified according to the following values available for supported response variable types. factor: "multi:softprob", "binary:logistic" (2 levels only) numeric: "reg:squarederror", "reg:logistic", "reg:gamma", "reg:tweedie", "rank:pairwise", "rank:ndcg", "rank:map" PoissonVariate: "count:poisson" Surv: "survival:aft", "survival:cox" The first values listed are the defaults for the corresponding response types. aft_loss_distribution character string specifying a distribution for the accelerated failure time objective ("survival:aft") as "extreme", "logistic", or "normal". base_score initial prediction score of all observations, global bias. numeric value controlling the amount of output printed during model fitting, verbose such that 0 = none, 1 = performance information, and 2 = additional information. print_every_n numeric value designating the fitting iterations at at which to print output when verbose > 0. shrinkage of variable weights at each iteration to prevent overfitting. eta minimum loss reduction required to split a tree node. gamma max_depth maximum tree depth. min_child_weight minimum sum of observation weights required of nodes. max_delta_step, tree_method, scale_pos_weight, updater, refresh_leaf, grow_policy, max_leaves, max_bin, num_parallel_tree other tree booster parameters.

subsample ratio of the training observations.

```
colsample_bytree, colsample_bylevel, colsample_bynode
```

subsample ratio of variables for each tree, level, or split.

alpha, lambda L1 and L2 regularization terms for variable weights.

sample_type, normalize_type

type of sampling and normalization algorithms.

rate_drop rate at which to drop trees during the dropout procedure.

one_drop integer indicating whether to drop at least one tree during the dropout procedure.

skip_drop probability of skipping the dropout procedure during a boosting iteration.

feature_selector, top_k

character string specifying the feature selection and ordering method, and number of top variables to select in the "greedy" and "thrifty" feature selectors.

Details

Response types: factor, numeric, PoissonVariate, Surv

Automatic tuning of grid parameters: • XGBModel: NULL

- XGBDARTModel: nrounds, eta*, gamma*, max_depth, min_child_weight*, subsample*, colsample_bytree*, rate_drop*, skip_drop*
- XGBLinearModel: nrounds, alpha, lambda
- XGBTreeModel: nrounds, eta*, gamma*, max_depth, min_child_weight*, subsample*, colsample_bytree*

The booster-specific constructor functions XGBDARTModel, XGBLinearModel, and XGBTreeModel are special cases of XGBModel which automatically set the XGBoost booster parameter. These are called directly in typical usage unless XGBModel is needed to specify a more general model.

Default argument values and further model details can be found in the source See Also link below.

In calls to varimp for XGBTreeModel, argument type may be specified as "Gain" (default) for the fractional contribution of each predictor to the total gain of its splits, as "Cover" for the number of observations related to each predictor, or as "Frequency" for the percentage of times each predictor is used in the trees. Variable importance is automatically scaled to range from 0 to 100. To obtain unscaled importance values, set scale = FALSE. See example below.

Value

MLModel class object.

See Also

```
xgboost, fit, resample
```

Examples

```
## Requires prior installation of suggested package xgboost to run
model_fit <- fit(
   Species ~ ., data = iris, model = XGBTreeModel(nthread = 1)</pre>
```

^{*} excluded from grids by default

```
varimp(model_fit, method = "model", type = "Frequency", scale = FALSE)
```

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