Package 'MachineShop'

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Author Brian J Smith [aut, cre]

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

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 Machine

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

Response Values:

response Observed predict Predicted

Performance Assessment:

calibration Model calibration Confusion matrix confusion Parital dependence dependence diff Model performance differences lift Lift curves Model performance metrics performance metrics performance_curve Model performance curves varimp Variable importance

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Methods for resample estimation include

BootControl Simple bootstrap
BootOptimismControl Optimism-corrected bootstrap
CVControl Repeated K-fold cross-validation
CVOptimismControl Optimism-corrected cross-validation
OOBControl Out-of-bootstrap
SplitControl Split training-testing
TrainControl Training 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

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. Useful for calling model constructors with quoted parameter values that are defined in terms of nobs, nvars, or y.

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Usage

```
.(expr)
```

Arguments

expr

any syntactically valid R expression.

Value

The quoted (unevaluated) expression.

See Also

quote

Examples

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

AdaBagModel

Bagging with Classification Trees

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
)
```

AdaBoostModel 7

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.

Value

MLModel class object.

See Also

```
bagging, fit, resample
```

Examples

```
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.

8 AdaBoostModel

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 = 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.

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.

number of cross-validations.

doctor rogate now to use surrogates in the spitting

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

xval

Response Types: factor

Automatic Tuning of Grid Parameters: mfinal, maxdepth, coeflearn*

* included only in randomly sampled grid points

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

Value

MLModel class object.

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See Also

```
boosting, fit, resample
```

Examples

```
fit(Species ~ ., data = iris, model = AdaBoostModel(mfinal = 5))
```

as.MLModel

Coerce to an MLModel

Description

Function to coerce an MLModelFit object to an MLModel.

Usage

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

Arguments

x model fit result.

... arguments passed to other methods.

Value

MLModel class object.

BARTMachineModel

Bayesian Additive Regression Trees Model

Description

Builds a BART model for regression or classification.

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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 metric may be spedified 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

```
model_fit <- fit(sale_amount ~ ., data = ICHomes, model = BARTMachineModel)
varimp(model_fit, metric = "splits", num_replicates = 20, scale = FALSE)</pre>
```

BARTModel

Bayesian Additive Regression Trees Model

Description

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

Usage

```
BARTModel(
 K = NULL
  sparse = FALSE,
  theta = 0,
  omega = 1,
  a = 0.5,
 b = 1,
  rho = NULL,
  augment = FALSE,
  xinfo = NULL,
  usequants = FALSE,
  sigest = NA,
  sigdf = 3,
  sigquant = 0.9,
  lambda = NA,
  k = 2,
  power = 2,
  base = 0.95,
  tau.num = NULL,
  offset = NULL,
  ntree = NULL,
  numcut = 100,
```

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```
ndpost = 1000,
nskip = NULL,
keepevery = NULL,
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.

k 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 values for the NULL arguments and further model details can be found in the source links below.

BlackBoostModel 13

Value

MLModel class object.

See Also

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

Examples

```
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.

nu step size or shrinkage parameter between 0 and 1.
```

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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 protype of the test statistic to be applied for variable selection. teststat 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. minbucket minimum sum of weights in a terminal node. maxdepth maximum depth of the tree. saveinfo logical indicating whether to store information about variable selection in info slot of each partynode.

Details

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

Automatic Tuning of Grid Parameters: mstop, maxdepth

additional arguments to ctree_control.

Default values for the NULL arguments and further model details can be found in the source links below.

Value

MLModel class object.

See Also

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

Examples

```
library(MASS)
fit(type ~ ., data = Pima.tr, model = BlackBoostModel)
```

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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 of boosting iterations.

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 metric may be spedified 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

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

calibration

Model Calibration

Description

Calculate calibration estimates from observed and predicted responses.

Usage

```
calibration(
   x,
   y = NULL,
   breaks = 10,
   span = 0.75,
   dist = NULL,
   na.rm = TRUE,
   ...
)
```

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Arguments

X	observed responses or resample result containing observed and predicted responses.
У	predicted responses if not contained in x.
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.
dist	character string specifying a distribution with which to estimate observed survival means. Possible values are "empirical" for the Kaplan-Meier estimator, "exponential", "extreme", "gaussian", "loggaussian", "logistic", "loglogistic", "lognormal", "rayleigh", "t", or "weibull" (default).
na.rm	logical indicating whether to remove observed or predicted responses that are NA when calculating metrics.
	arguments passed to other methods.

Value

Calibration class object that inherits from data. frame.

See Also

```
c, plot
```

Examples

CForestModel

Conditional Random Forest Model

Description

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

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Usage

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

Arguments

teststat character specifying the type of the test statistic to be applied.

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.

ntree number of trees to grow in a forest.

mtry number of input variables randomly sampled as candidates at each node for

random forest like algorithms.

replace logical indicating whether sampling of observations is done with or without re-

placement.

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 Parameters:** mtry

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

Value

MLModel class object.

See Also

```
cforest, fit, resample
```

Examples

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

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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 'Resamples'
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.

Value

Object of the same class as the arguments.

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confusion

Confusion Matrix

Description

Calculate confusion matrices of predicted and observed responses.

Usage

```
confusion(
    x,
    y = 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.
cutoff	numeric (0, 1) threshold above which binary factor probabilities are classified as events and below which survival probabilities are classified. If NULL, then binary 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.

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 Resamples object.

See Also

```
c, plot, summary
```

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Examples

```
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 = NULL,
   k = 2,
   trace = FALSE,
   steps = 1000
)
```

Arguments

ties	character string specifying the method for tie handling.
	arguments passed to coxph.control.
direction	$mode\ of\ stepwise\ search,\ can\ be\ one\ of\ "both"\ (default),\ "backward",\ or\ "forward".$
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 values for the NULL arguments and further model details can be found in the source link 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.

#' @return 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.

Usage

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

Arguments

object model fit result.

data data frame containing all predictor variables. If not specified, the training data

will be used by default.

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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").

stats function, function name, or vector of these with which to compute response variable summary statistics over non-selected predictor variables.

Value

PartialDependence class object that inherits from data.frame.

See Also

plot

Examples

```
gbm_fit <- fit(Species ~ ., data = iris, model = GBMModel)
(pd <- dependence(gbm_fit, select = c(Petal.Length, Petal.Width)))
plot(pd)</pre>
```

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 'Resamples'
diff(x, ...)
```

Arguments

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

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Value

PerformanceDiff class object that inherits from Performance.

See Also

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

Examples

```
## 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)
plot(res_diff)</pre>
```

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.

EarthModel 25

Value

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

See Also

```
role_binom
```

Examples

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

EarthModel

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 = NULL,
  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.

26 expand_model

Details

Response Types: factor, numeric

Automatic Tuning of Grid Parameters: nprune, degree*

* included only in randomly sampled grid points

Default values for the NULL arguments and further model details can be found in the source link below.

In calls to varimp for EarthModel, argument metric may be specified as "gcv" (default) for the generalized cross-validation decrease over all subsets that include each predictor, as "rss" for the residual sums of squares decrease, or as "nsubsets" for the number of model subsets that include 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

```
earth, fit, resample
```

Examples

```
model_fit <- fit(Species ~ ., data = iris, model = EarthModel)
varimp(model_fit, metric = "nsubsets", 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(x, ..., random = FALSE)
```

Arguments

x model function, function name, or call.

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

which to expand x.

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

all points are to be returned.

expand_params 27

Value

list of expanded models.

See Also

SelectedModel

Examples

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 vectors or factors 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

28 expand_steps

Examples

```
library(MASS)
grid <- expand_params(
    n.trees = c(50, 100),
    interaction.depth = 1:2
)
fit(medv ~ ., data = Boston, model = TunedModel(GBMModel, grid = grid))</pre>
```

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

Examples

```
library(recipes)
library(MASS)

rec <- recipe(medv ~ ., data = Boston) %>%
    step_corr(all_numeric(), -all_outcomes(), id = "corr") %>%
    step_pca(all_numeric(), -all_outcomes(), id = "pca")
```

extract 29

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

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 = NULL,
   dimension = NULL,
   eps = .Machine$double.eps,
   method = .(mda::polyreg),
   ...
)

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

Arguments

df

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 method for FDAModel and to FDAModel for PDAModel.
lambda	shrinkage penalty coefficient.

alternative specification of lambda in terms of equivalent degrees of freedom.

fit 31

Details

```
Response Types: factor

Automatic Tuning of Grid Parameters

• FDAModel: nprune, degree*

• PDAModel: lambda
```

* included only in randomly sampled grid points

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 values for the NULL arguments and further model details can be found in the source links below.

Value

MLModel class object.

See Also

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

Examples

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

fit

Model Fitting

Description

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

Usage

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

32 fit

```
## S3 method for class 'recipe'
fit(x, model, ...)
## S3 method for class 'MLModel'
fit(x, ...)
## S3 method for class 'MLModelFunction'
fit(x, ...)
```

Arguments

X	input specifying a relationship between model predictor and response variables. Alternatively, a model function or call may be given first followed by the input specification.
	arguments passed to other methods.
data	data frame containing observed predictors and outcomes.
model	model function, function name, or call; ignored and can be omitted when fitting modeled inputs.
у	response variable.

Details

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

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
```

Examples

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

gbm_fit <- fit(Surv(time, status) ~ ., data = veteran, model = GBMModel)
varimp(gbm_fit)</pre>
```

GAMBoostModel 33

GAMBoostModel Gradient Boosting with Additive Models	e 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 process.

Details

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

Automatic Tuning of Grid Parameters: mstop

Default values for the NULL arguments and further model details can be found in the source links below.

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Value

MLModel class object.

See Also

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

Examples

```
library(MASS)
fit(type ~ ., data = Pima.tr, model = GAMBoostModel)
```

GBMMode1

Generalized Boosted Regression Model

Description

Fits generalized boosted regression models.

Usage

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

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.

GLMBoostModel 35

Details

```
Response Types: factor, numeric, PoissonVariate, Surv
```

Automatic Tuning of Grid Parameters: n.trees, interaction.depth, shrinkage*, n.minobsinnode* included only in randomly sampled grid points

Default values for the NULL arguments and further model details can be found in the source link below.

Value

MLModel class object.

See Also

```
gbm, fit, resample
```

Examples

```
fit(Species ~ ., 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.

Usage

```
GLMBoostModel(
  family = NULL,
  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.

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.
```

36 GLMModel

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 Parameters: mstop
```

Default values for the NULL arguments and further model details can be found in the source links below.

Value

MLModel class object.

See Also

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

Examples

```
library(MASS)
fit(type ~ ., data = Pima.tr, model = GLMBoostModel)
```

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 = NULL,
  k = 2,
```

GLMModel 37

```
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

GLMModel **Response Types:** BinomialVariate, factor, matrix, NegBinomialVariate, numeric, PoissonVariate

 ${\tt GLMStepAICModel} \ \, \textbf{Response Types:} \ \, \textbf{binary factor, BinomialVariate, NegBinomialVariate, numeric, PoissonVariate}$

Default values for the NULL arguments and further model details can be found in the source link 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)
```

38 GLMNetModel

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 = NULL,
  penalty.factor = .(rep(1, nvars)),
  standardize.response = FALSE,
  thresh = 1e-07,
  maxit = 1e+05,
  type.gaussian = .(ifelse(nvars < 500, "covariance", "naive")),
  type.logistic = c("Newton", "modified.Newton"),
  type.multinomial = c("ungrouped", "grouped")
)</pre>
```

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.

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Details

Response Types: BinomialVariate, factor, matrix, numeric, PoissonVariate, Surv **Automatic Tuning of Grid Parameters:** lambda, alpha

Default values for the NULL arguments and further model details can be found in the source link below.

Value

MLModel class object.

See Also

```
glmnet, fit, resample
```

Examples

```
fit(sale_amount ~ ., data = ICHomes, model = GLMNetModel(lambda = 0.01))
```

Grid

Tuning Grid Control

Description

Defines control parameters for a tuning grid.

Usage

```
Grid(length = 3, random = FALSE)
```

Arguments

length number of values to be generated for each model parameter in the tuning grid.

random number of unique grid points to sample at random, Inf for all random points, or

TALOF COUNTY OF THE POINTS TO SUMPLY AND THE POINTS, OF

FALSE for all fixed points.

Value

Grid class object.

See Also

TunedModel

Examples

```
TunedModel(GBMModel, grid = Grid(10, random = 5))
```

40 inputs

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

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.

KNNModel 41

formula Traditional model formula
matrix Design matrix of predictors

ModelFrame Model frame

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

NegBinomialVariate

numeric ordered

PoissonVariate

Surv

Recipe Roles role_binom

role_surv

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

ModeledInput Input with a prespecified model
SelectedInput Input selection from a candidate set
TunedInput Input tuning over a parameter grid

See Also

fit, resample

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,
```

42 LARSModel

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*

* included only in randomly sampled grid points

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

Value

MLModel class object.

See Also

```
kknn, fit, resample
```

Examples

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

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.

LARSModel 43

Usage

```
LARSModel(
  type = c("lasso", "lar", "forward.stagewise", "stepwise"),
  trace = FALSE,
  normalize = TRUE,
  intercept = TRUE,
  step = NULL,
  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 Parameters: step

Default values for the NULL arguments and further model details can be found in the source link below.

Value

MLModel class object.

See Also

```
lars, fit, resample
```

Examples

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

44 LDAModel

LDAMode1

Linear Discriminant Analysis Model

Description

Performs linear discriminant analysis.

Usage

```
LDAModel(
  prior = NULL,
  tol = 1e-04,
  method = c("moment", "mle", "mve", "t"),
  nu = 5,
  dimen = NULL,
  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 Parameters: 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 values for the NULL arguments and further model details can be found in the source links below.

Value

MLModel class object.

See Also

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

lift 45

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, na.rm = TRUE, ...)
```

Arguments

X	observed responses or resample result containing observed and predicted responses.
у	predicted responses if not contained in x.
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
```

Examples

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

46 MDAModel

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

Mixture Discriminant Analysis Model

Description

Performs mixture discriminant analysis.

MDAModel 47

Usage

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

Arguments

subclasses	numeric value or vector of subclasses per class.
sub.df	effective degrees of freedom of the centroids per class if subclass centroid shrinkage is performed.
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.
method	regression function used in optimal scaling. The default of linear regression is provided by polyreg from the mda package. For penalized mixture discriminant models, 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.
trace	logical indicating whether iteration information is printed.
	additional arguments to mda.start and method.

Details

Response Types: factor

Automatic Tuning of Grid Parameters: 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 values for the NULL arguments and further model details can be found in the source links below.

Value

MLModel class object.

48 metricinfo

See Also

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

Examples

```
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 function.

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)))
```

metrics 49

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

metrics

Performance Metrics

Description

Compute measures of agreement between observed and predicted responses.

Usage

```
accuracy(
 observed,
 predicted = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
auc(
 observed,
 predicted = NULL,
 metrics = c(MachineShop::tpr, MachineShop::fpr),
 stat = MachineShop::settings("stat.Curve"),
)
brier(observed, predicted = NULL, ...)
cindex(observed, predicted = NULL, ...)
cross_entropy(observed, predicted = NULL, ...)
f_score(
 observed,
 predicted = NULL,
 cutoff = MachineShop::settings("cutoff"),
 beta = 1,
)
fnr(observed, predicted = NULL, cutoff = MachineShop::settings("cutoff"), ...)
fpr(observed, predicted = NULL, cutoff = MachineShop::settings("cutoff"), ...)
kappa2(
```

50 metrics

```
observed,
 predicted = NULL,
  cutoff = MachineShop::settings("cutoff"),
)
npv(observed, predicted = NULL, cutoff = MachineShop::settings("cutoff"), ...)
ppv(observed, predicted = NULL, cutoff = MachineShop::settings("cutoff"), ...)
pr_auc(observed, predicted = NULL, ...)
precision(
 observed,
 predicted = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
recall(
 observed,
 predicted = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
roc_auc(observed, predicted = NULL, ...)
roc_index(
 observed,
 predicted = NULL,
 cutoff = MachineShop::settings("cutoff"),
 f = function(sensitivity, specificity) (sensitivity + specificity)/2,
)
rpp(observed, predicted = NULL, cutoff = MachineShop::settings("cutoff"), ...)
sensitivity(
 observed,
 predicted = NULL,
 cutoff = MachineShop::settings("cutoff"),
)
specificity(
 observed,
 predicted = NULL,
```

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```
cutoff = MachineShop::settings("cutoff"),
...
)

tnr(observed, predicted = NULL, cutoff = MachineShop::settings("cutoff"), ...)

tpr(observed, predicted = NULL, cutoff = MachineShop::settings("cutoff"), ...)

weighted_kappa2(observed, predicted = NULL, power = 1, ...)

gini(observed, predicted = NULL, ...)

mae(observed, predicted = NULL, ...)

mse(observed, predicted = NULL, ...)

r2(observed, predicted = NULL, dist = NULL, ...)

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

rmse(observed, predicted = 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.

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

events and below which survival probabilities are classified.

. . . arguments passed to or from other methods.

metrics list of two performance metrics for the calculation [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].

f 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.

dist character string specifying a distribution with which to estimate the 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"

(default).

52 MLControl

See Also

metricinfo, performance

MLControl

Resampling Controls

Description

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

Usage

```
BootControl(samples = 25, ...)
BootOptimismControl(samples = 25, ...)

CVControl(folds = 10, repeats = 1, ...)

CVOptimismControl(folds = 10, repeats = 1, ...)

OOBControl(samples = 25, ...)

SplitControl(prop = 2/3, ...)

TrainControl(
   times = NULL,
   dist = NULL,
   method = NULL,
   seed = sample(.Machine$integer.max, 1), ...
)
```

Arguments

```
samples number of bootstrap samples.
... arguments passed to MLControl.

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).

times, dist, method arguments passed to predict.

seed integer to set the seed at the start of resampling.
```

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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 seperate trianing 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).

The base MLControl constructor initializes a set of control parameters that are common to all resampling methods.

Value

MLControl class object.

References

Efron B and Tibshirani RJ (1993). An Introduction to the Bootstrap. Monographs on Statistics and Applied Probability 57. Boca Raton, Florida, USA: Chapman & Hall/CRC.

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

Harrell FE, Lee KL, and Mark DB (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 Proceedings of the 14th International Joint Conference on Artificial Intelligence - Volume 2, 1137-43. IJCAI'95. San Francisco, CA, USA: Morgan Kaufmann Publishers Inc.

Davison AC and Hinkley DV (1997). Bootstrap Methods and Their Application. New York, NY, USA: Cambridge University Press.

Hastie T, Tibshirani R, and Friedman J (2009). The Elements of Statistical Learning: Data Mining, Inference, and Prediction, Second Edition. Springer Series in Statistics. New York, NY, USA: 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.

54 MLMetric

See Also

```
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()
```

 ${\tt MLMetric}$

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 () 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.

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Value

MLMetric class object.

See Also

metrics

Examples

MLModel

MLModel Class Constructor

Description

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

Usage

```
MLModel(
  name = "MLModel",
  label = name,
  packages = character(),
  response_types = character(),
  predictor_encoding = c(NA, "model.matrix", "terms"),
  params = list(),
  grid = function(x, length, random, ...) NULL,
  fit = function(formula, data, weights, ...) stop("no fit function"),
  predict = function(object, newdata, times, ...) stop("no predict function"),
  varimp = function(object, ...) NULL,
  ...
)
```

Arguments

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

label optional character descriptor for the model.

packages character vector of packages required to use the model.

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response_types character vector of response variable types to which the model can be fit. Supported types are "binary", = "BinomialVariate", "DiscreteVariate", "factor", "matrix", "NegBinomialVariate", "numeric", "ordered", "PoissonVariate", and "Surv". predictor_encoding character string indicating whether the model is fit with predictor variables encoded as a "model.matrix", a data.frame containing the originally specified model "terms", or unspecified (default). list of user-specified model parameters to be passed to the fit function. params tuning grid function whose first agument x is a ModelFrame of the model fit data grid and formula, followed by a length to use in generating sequences of parameter values, a number of grid points to sample at random, and 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. variable importance function whose arguments are the object returned by fit, varimp optional arguments passed from calls to varimp, and an ellipsis.

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 passed from other methods.

Argument data in the fit function may be converted to a data frame with the as.data.frame function as needed. The 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 vector or column matrix of probabilities for the second level of binary factors or a matrix whose columns contain the probabilities for factors with more than two levels.

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.

Value

MLModel class object.

See Also

models, fit, resample

ModeledInput 57

Examples

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

ModeledInput

ModeledInput Classes

Description

Class for storing a model input and specification pair for MachineShop model fitting.

Usage

```
ModeledInput(x, ...)
## S3 method for class 'formula'
ModeledInput(x, data, model, ...)
## S3 method for class 'matrix'
ModeledInput(x, y, model, ...)
## S3 method for class 'ModelFrame'
ModeledInput(x, model, ...)
## S3 method for class 'recipe'
ModeledInput(x, model, ...)
## S3 method for class 'MLModel'
ModeledInput(x, ...)
## S3 method for class 'MLModelFunction'
ModeledInput(x, ...)
```

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Arguments

Х	input specifying a relationship between model predictor and response variables. Alternatively, a model function or call may be given first followed by the input specification.
	arguments passed to other methods.
data	data frame or an object that can be converted to one.
model	model function, function name, or call.
У	response variable.

Value

ModeledFrame or ModeledRecipe class object that inherits from ModelFrame or recipe.

See Also

```
fit, resample, SelectedInput
```

Examples

```
## Modeled model frame
mod_mf <- ModeledInput(sale_amount ~ ., data = ICHomes, model = GLMModel)
fit(mod_mf)

## Modeled recipe
library(recipes)

rec <- recipe(sale_amount ~ ., data = ICHomes)
mod_rec <- ModeledInput(rec, model = GLMModel)
fit(mod_rec)</pre>
```

ModelFrame

ModelFrame Class

Description

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

Usage

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

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```
x,
y = NULL,
na.rm = TRUE,
offsets = NULL,
weights = NULL,
strata = NULL,
...
)
```

Arguments

Χ	model formula or matrix of predictor variables.
	arguments passed to other methods.
data	data frame or an object that can be converted to one.
na.rm	logical indicating whether to remove cases with NA values for any of the model variables.
weights	vector of case weights [default: equal].
strata	vector of resampling stratification levels [default: none].
у	response variable.
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

modelinfo

Display Model Information

Description

Display information about models supplied by the MachineShop package.

60 models

Usage

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

Arguments

. . .

model functions, function names, or calls; 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.

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 variable importance is defined for the model.

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

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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	_	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	
PDAModel	f		
PLSModel	f	n	
POLRMode1	O		
QDAModel	f		
RandomForestModel	f	n	
RangerModel	f	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	

NaiveBayesModel

XGBMode1	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.

StackedModel Stacked regression SuperModel Super learner

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

See Also

modelinfo, fit, resample

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.

Details

Response Types: factor

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

Value

MLModel class object.

NNetModel 63

See Also

```
naiveBayes, fit, resample
```

Examples

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

NNetModel

Neural Network Model

Description

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

Usage

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

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.

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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 values for the NULL arguments and further model details can be found in the source link below.

Value

MLModel class object.

See Also

```
nnet, fit, resample
```

Examples

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

 ${\tt ParameterGrid}$

Tuning Parameters Grid

Description

Defines a tuning grid from a set of parameters.

Usage

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

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Arguments

named param objects as defined in the dials package.
 length single number or vector of numbers of parameter values to use in constructing a regular grid if random = FALSE; ignored otherwise.
 random number of unique grid points to sample at random or FALSE for all points from a regular grid defined by length.
 x list of named param objects or a parameters object.

Value

ParameterGrid class object that inherits from parameters and Grid.

See Also

TunedModel

Examples

```
## GBMModel tuning parameters
library(dials)

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

performance

Model Performance Metrics

Description

Compute measures of model performance.

Usage

```
performance(x, ...)

## S3 method for class 'BinomialVariate'
performance(
    x,
    y,
    metrics = MachineShop::settings("metrics.numeric"),
    na.rm = TRUE,
    ...
```

66 performance

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

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Arguments

X	observed responses; or confusion or resample result containing observed and predicted responses.
•••	arguments passed from the Resamples method to the response type-specific methods or from the method for ConfusionList to ConfusionMatrix.
у	predicted responses if not contained in x.
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.

See Also

```
plot, summary
```

Examples

```
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, type = "prob")
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.

68 performance_curve

Usage

```
performance_curve(x, ...)

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

## S3 method for class 'Resamples'
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.
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
```

Examples

```
library(MASS)
res <- resample(type ~ ., data = Pima.tr, model = GBMModel)
## ROC curve
roc <- performance_curve(res)
plot(roc)</pre>
```

plot 69

auc(roc)

plot

Model Performance Plots

Description

Plot measures of model performance and predictor variable importance.

Usage

```
## 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(
  х,
  find = NULL,
 diagonal = TRUE,
  stat = MachineShop::settings("stat.Curve"),
)
## S3 method for class 'MLModel'
plot(
 Х,
 metrics = NULL,
 stat = MachineShop::settings("stat.train"),
  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.Resamples"),
```

70 plot

```
type = c("boxplot", "density", "errorbar", "violin"),
)
## S3 method for class 'PerformanceCurve'
plot(
  х,
  type = c("tradeoffs", "cutoffs"),
  diagonal = FALSE,
  stat = MachineShop::settings("stat.Curve"),
)
## S3 method for class 'Resamples'
plot(
  Х,
 metrics = NULL,
  stat = MachineShop::settings("stat.Resamples"),
  type = c("boxplot", "density", "errorbar", "violin"),
)
## S3 method for class 'VarImp'
plot(x, n = NULL, ...)
```

Arguments

x calibration, confusion, lift, trained model fit, partial dependence, performance,

performance curve, resample, 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 Resamples model ordering. 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.

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 [default: all].

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Examples

```
## 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.

Value

MLModel class object.

See Also

```
mvr, fit, resample
```

72 POLRModel

Examples

```
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
```

Examples

predict 73

Model Prediction

Description

Predict outcomes with a fitted model.

Usage

```
## S3 method for class 'MLModelFit'
predict(
  object,
  newdata = NULL,
  times = NULL,
  type = c("response", "prob"),
  cutoff = MachineShop::settings("cutoff"),
  dist = NULL,
  method = NULL,
  ...
)
```

Arguments

object	model fit result.
newdata	optional data frame with which to obtain predictions. If not specified, the training 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 scale ("response") or on a probability distribution scale ("prob").
cutoff	numeric (0, 1) threshold above which binary factor probabilities are classified as events and below which survival probabilities are classified.
dist	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", "efron" (default), or "fleming-harrington".
	arguments passed to model-specific prediction functions.

See Also

74 print

Examples

```
## 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("max.print"), ...)
## S3 method for class 'Calibration'
print(x, n = MachineShop::settings("max.print"), ...)
## S3 method for class 'ListOf'
print(x, n = MachineShop::settings("max.print"), ...)
## S3 method for class 'MLModel'
print(x, n = MachineShop::settings("max.print"), ...)
## S3 method for class 'ModelFrame'
print(x, n = MachineShop::settings("max.print"), ...)
## S3 method for class 'ModeledInput'
print(x, n = MachineShop::settings("max.print"), ...)
## S3 method for class 'Performance'
print(x, n = MachineShop::settings("max.print"), ...)
## S3 method for class 'PerformanceCurve'
print(x, n = MachineShop::settings("max.print"), ...)
## S3 method for class 'RecipeGrid'
print(x, n = MachineShop::settings("max.print"), ...)
## S3 method for class 'Resamples'
print(x, n = MachineShop::settings("max.print"), ...)
```

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```
## S3 method for class 'SelectedInput'
print(x, n = MachineShop::settings("max.print"), ...)
## S3 method for class 'SurvMatrix'
print(x, n = MachineShop::settings("max.print"), ...)
## S3 method for class 'TrainBit'
print(x, n = MachineShop::settings("max.print"), ...)
## S3 method for class 'TunedInput'
print(x, n = MachineShop::settings("max.print"), ...)
## S3 method for class 'VarImp'
print(x, n = MachineShop::settings("max.print"), ...)
```

Arguments

x object to print.n integer number of models or data frame rows to show.... arguments passed to other methods.

QDAModel

Quadratic Discriminant Analysis Model

Description

Performs quadratic discriminant analysis.

Usage

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

Arguments

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".

type of parameter estimation to use for prediction.

76 RandomForestModel

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 values for the NULL arguments and further model details can be found in the source links below.

Value

MLModel class object.

See Also

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

Examples

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

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 = NULL
)
```

Arguments

ntree number of trees to grow.

mtry 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.

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

RangerModel 77

Details

```
\textbf{Response Types:} \  \, \textbf{factor}, \textbf{numeric}
```

Automatic Tuning of Grid Parameters: mtry, nodesize*

* included only in randomly sampled grid points

Default values for the NULL arguments and further model details can be found in the source link below.

Value

MLModel class object.

See Also

```
randomForest, fit, resample
```

Examples

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

RangerModel

Fast Random Forest Model

Description

Fast implementation of random forests or recursive partitioning.

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

78 RangerModel

Arguments

num.trees number of trees.

mtry number of variables to possibly split at in each node.

importance variable importance mode.

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.

minprop lower quantile of covariate distribution to be considered for splitting in the

"maxstat" rule.

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.

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*

* included only in randomly sampled grid points

Default values for the NULL arguments and further model details can be found in the source link below.

Value

MLModel class object.

See Also

ranger, fit, resample

recipe_roles 79

Examples

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

recipe_roles

Set Recipe Roles

Description

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

Usage

```
role_binom(recipe, x, size)
role_case(recipe, 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 ${\tt BinomialVariate}$ outcome.
stratum	variable for stratified resampling of cases.
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

80 resample

Examples

```
library(survival)
library(recipes)

rec <- recipe(time + status ~ ., data = veteran) %>%
    role_surv(time = time, event = status) %>%
    role_case(stratum = status)

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

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(x, ...)

## S3 method for class 'formula'
resample(x, data, model, control = MachineShop::settings("control"), ...)

## S3 method for class 'matrix'
resample(x, y, model, control = MachineShop::settings("control"), ...)

## S3 method for class 'ModelFrame'
resample(x, model, control = MachineShop::settings("control"), ...)

## S3 method for class 'recipe'
resample(x, model, control = MachineShop::settings("control"), ...)

## S3 method for class 'MLModel'
resample(x, ...)

## S3 method for class 'MLModelFunction'
resample(x, ...)
```

Arguments

Х

input specifying a relationship between model predictor and response variables. Alternatively, a model function or call may be given first followed by the input specification and control value.

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	arguments passed to other methods.
data	data frame containing observed predictors and outcomes.
model	model function, function name, or call; ignored and can be omitted when resampling modeled inputs.
control	control function, function name, or call defining the resampling method to be employed.
у	response variable.

Details

Stratified resampling is performed for the formula method according to values of the response variable; i.e. categorical levels for factor, continuous for numeric, and event status Surv.

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

Variables in recipe specifications may be designated as case strata with the role_case function. Resampling will be unstratified otherwise.

Value

Resamples class object.

See Also

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

Examples

```
## 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>
```

82 RPartModel

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 'recipe'
response(object, newdata = NULL, ...)
```

Arguments

```
object model fit result, ModelFrame, or recipe.
... arguments passed to other methods.

newdata data frame from which to extract the response variable values if given; otherwise, object is used.
```

Examples

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

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

RPartModel

Recursive Partitioning and Regression Tree Models

Description

Fit an rpart model.

RPartModel 83

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 Parameters: cp
```

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

Value

MLModel class object.

See Also

```
rpart, fit, resample
```

Examples

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

84 SelectedInput

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

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

Arguments

• • •	inputs specifying 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 or an object that can be converted to one.
control	control function, function name, or call 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.
stat	function or character string naming a function to compute a summary statistic on resampled metric values for recipe selection.
cutoff	argument passed to the metrics functions.
У	response variable.
X	list of inputs followed by arguments passed to their method function.

Value

 ${\tt Selected Model Frame\ or\ Selected Model Recipe\ class\ object\ that\ inherits\ from\ Selected Input\ and\ Model Frame\ or\ recipe.}$

See Also

```
fit, resample
```

Examples

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

fit(sel_mf, model = GLMModel)

## Selected recipe
library(recipes)
library(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)</pre>
```

86 SelectedModel

```
fit(sel_rec, model = GLMModel)
```

SelectedModel

Selected Model

Description

Model selection from a candidate set.

Usage

```
SelectedModel(
    ...,
    control = MachineShop::settings("control"),
    metrics = NULL,
    stat = MachineShop::settings("stat.train"),
    cutoff = MachineShop::settings("cutoff")
)
```

Arguments

• • •	model functions, function names, calls, or vectors of these to serve as the candidate set from which to select, such as that returned by expand_model.
control	control function, function name, or call 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.
stat	function or character string naming a function to compute a summary statistic on resampled metric values for model selection.
cutoff	argument passed to the metrics functions.

Details

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

Value

 ${\tt Selected Model\ class\ object\ that\ inherits\ from\ MLModel}.$

See Also

```
fit, resample
```

settings 87

Examples

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 call 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].

- dist.Surv character string specifying distributional approximations to estimated survival curves for predicting survival means. Choices are "empirical" for the Kaplan-Meier estimator, "exponential", or "weibull" (default).
- dist.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", or "weibull".
- grid number of parameter-specific values to generate automatically for tuning of models that have pre-defined grids or a Grid function, function name, or call [default: 3].
- max.print number of models or data rows to show with print methods or Inf to show all [default: 10].

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method. Empirical Surv character string specifying the empirical method of estimating baseline survival curves for Cox proportional hazards-based models. Choices are "breslow", "efron" (default), or "fleming-harrington".

- 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")].
- metrics.factor function, function name, or vector of these with which to calculate performance
 metrics for factor responses [default: c(Brier = "brier", Accuracy = "accuracy", Kappa =
 "kappa2", `Weighted Kappa` = "weighted_kappa2", `ROC AUC` = "roc_auc", Sensitivity
 = "sensitivity", Specificity = "specificity")].
- 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")].
- progress.resample logical indicating whether to display a progress bar during resampling [default: TRUE]. Displayed only if a computing cluster is not registered or is registered with the **doSNOW** package.
- require names of installed packages to load during parallel execution of resampling algorithms [default: c("MachineShop", "survival", "recipes")].
- 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.Resamples function or character string naming a function to compute one summary statistic to control the ordering of models in plots [default: "base::mean"].
- stat.train 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.Resamples 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")].
- verbose.resample logical indicating whether to enable verbose messages when resampling [default: FALSE].

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Examples

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

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

## View one setting
settings("control")

## View multiple settings
settings("control", "grid")

## Restore the previous settings
settings(presets)</pre>
```

StackedModel

Stacked Regression Model

Description

Fit a stacked regression model from multiple base learners.

Usage

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

Arguments

... model functions, function names, calls, or vector of these to serve as base learn-

ers.

control control function, function name, or call 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.

90 step_kmeans

See Also

```
fit, resample
```

Examples

```
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, ...)
tunable.step_kmeans(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.

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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 EW (1965). Cluster analysis of multivariate data: efficiency vs interpretability of classifications. Biometrics 21, 768–769.

Hartigan JA and Wong MA (1979). A K-means clustering algorithm. Applied Statistics 28, 100–108.

Lloyd SP (1957, 1982). Least squares quantization in PCM. Technical Note, Bell Laboratories. Published in 1982 in IEEE Transactions on Information Theory 28, 128–137.

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

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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.

```
step_kmedoids(
  recipe,
  . . . ,
 k = 5,
  center = TRUE,
  scale = TRUE,
 method = c("pam", "clara"),
 metric = "euclidean",
 optimize = FALSE,
  num_samp = 50,
  samp\_size = 40 + 2 * k,
  replace = TRUE,
  prefix = "KMedoids",
  role = "predictor",
  skip = FALSE,
 id = recipes::rand_id("kmedoids")
)
tunable.step_kmedoids(x, ...)
```

step_kmedoids 93

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-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 clustering 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.

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.

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References

Kaufman L and Rousseeuw PJ (1990). Finding Groups in Data: An Introduction to Cluster Analysis. Wiley: New York.

Reynolds A, Richards G, de la Iglesia B and 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

```
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

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.

```
step_lincomp(
  recipe,
    ...,
  transform,
  num_comp = 5,
  options = list(),
  center = TRUE,
  scale = TRUE,
  replace = TRUE,
  prefix = "LinComp",
  role = "predictor",
```

step_lincomp 95

```
skip = FALSE,
  id = recipes::rand_id("lincomp")
)
## S3 method for class 'step_lincomp'
tidy(x, ...)
tunable.step_lincomp(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.

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 orig-

inal 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.

96 step_sbf

See Also

```
recipe, prep, bake
```

Examples

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.

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

step_sbf 97

```
## S3 method for class 'step_sbf'
tidy(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.
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.
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.

Value

Х

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.

step_sbf object.

See Also

```
recipe, prep, bake
```

98 step_spca

Examples

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.

```
step_spca(
  recipe,
    ...,
  num_comp = 5,
  sparsity = 0,
  num_var = NULL,
  shrinkage = 1e-06,
  center = TRUE,
  scale = TRUE,
  max_iter = 200,
  tol = 0.001,
  replace = TRUE,
  prefix = "SPCA",
  role = "predictor",
  skip = FALSE,
```

step_spca 99

```
id = recipes::rand_id("spca")
)
tunable.step_spca(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.

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.

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.

shrinkage numeric shrinkage (quadratic) penalty for the components to improve condition-

ing; larger values produce more shrinkage of component loadings toward zero.

center, scale logicals indicating whether to mean center and standard deviation scale the orig-

inal 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.

100 summary

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 and Tibshirani R (2006). Sparse principal component analysis. Journal of Computational and Graphical Statistics, 15(2):265–286.

See Also

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

Examples

```
library(recipes)

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.

```
## $3 method for class 'ConfusionList'
summary(object, ...)
## $3 method for class 'ConfusionMatrix'
summary(object, ...)
## $3 method for class 'MLModel'
```

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

Arguments

object	confusion, lift, trained model fit, performance, performance curve, or resample 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.
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

```
## Factor response example
fo <- Species ~ .
control <- CVControl()</pre>
```

102 SuperModel

```
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

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, calls, or vector of these to serve as base learn-

ers.

model model function, function name, or call defining the super model.

control control function, function name, or call 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 Lann, M.J., Hubbard A.E. (2007) *Super Learner*. Statistical Applications in Genetics and Molecular Biology, 6(1).

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See Also

```
fit, resample
```

Examples

```
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 = NULL)
SurvProbs(data = NA, times = NULL)
```

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.

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
```

104 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 = NULL,
 parms = NULL,
)
SurvRegStepAICModel(
 dist = c("weibull", "exponential", "gaussian", "logistic", "lognormal",
    "logloglogistic"),
  scale = NULL,
 parms = NULL,
 direction = c("both", "backward", "forward"),
  scope = NULL,
 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 values for the NULL arguments and further model details can be found in the source link below.

Value

MLModel class object.

See Also

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

Examples

```
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.

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

106 SVMModel

```
SVMBesselModel(sigma = 1, order = 1, degree = 1, ...)
SVMLaplaceModel(sigma = NULL, ...)
SVMLinearModel(...)
SVMPolyModel(degree = 1, scale = 1, offset = 1, ...)
SVMRadialModel(sigma = NULL, ...)
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.

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.

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.

Details

Response Types: factor, numeric

Automatic Tuning of Grid Parameters • SVMANOVAModel: C, degree

• SVMBesselModel: C, order, degree

• SVMLaplaceModel: C, sigma

• SVMLinearModel: C

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```
SVMPolyModel: C, degree, scaleSVMRadialModel: C, sigma
```

Arguments kernel and kpar are automatically set by the kernel-specific constructor functions. Default values for the NULL arguments and further model details can be found in the source 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 p-value adjustment for multiple statistical comparisons as implemented by p. adjust.
    arguments passed to other methods.
```

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 contined in the third dimension.

108 TreeModel

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>
```

TreeModel

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 = NULL,
  best = NULL,
  method = c("deviance", "misclass")
)
```

complexity pruning.

Arguments

mincut minimum number of observations to include in either child node. smallest allowed node size: a weighted quantity. minsize 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 costTunedInput 109

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
```

Examples

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

TunedInput

Tuned Model Inputs

Description

Recipe tuning over a grid of parameter values.

Usage

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

Arguments

```
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.

110 TunedModel

control	control function, function name, or call 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.
stat	function or character string naming a function to compute a summary statistic on resampled metric values for recipe tuning.
cutoff	argument passed to the metrics functions.

Value

TunedModelRecipe class object that inherits from TunedInput and recipe.

See Also

```
fit, resample
```

Examples

```
library(recipes)
library(MASS)

rec <- recipe(medv ~ ., data = Boston) %>%
    step_pca(all_numeric(), -all_outcomes(), 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.

```
TunedModel(
  model,
  grid = MachineShop::settings("grid"),
  fixed = NULL,
  control = MachineShop::settings("control"),
  metrics = NULL,
  stat = MachineShop::settings("stat.train"),
  cutoff = MachineShop::settings("cutoff")
)
```

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Arguments

model	model function, function name, or call defining the model to be tuned.
grid	data frame containing parameter values at which to evaluate a single model supplied to models, such as that returned by expand_params; the number of parameter-specific values to generate automatically if the model has a pre-defined grid; or a call to Grid or ParameterGrid.
fixed	list of fixed parameter values to combine with those in grid.
control	control function, function name, or call 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.
stat	function or character string naming a function to compute a summary statistic on resampled metric values for model tuning.
cutoff	argument passed to the metrics functions.

Details

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

Value

TunedModel class object that inherits from MLModel.

See Also

```
fit, resample
```

Examples

```
# 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 = "l")
# Randomly sampled grid points
fit(sale_amount ~ ., data = ICHomes,
    model = TunedModel(GBMModel, grid = Grid(length = 1000, random = 5)))
# User-specified grid
fit(sale\_amount \sim ., data = ICHomes,
    model = TunedModel(GBMModel,
                       grid = expand_params(n.trees = c(50, 100),
                                             interaction.depth = 1:2,
                                             n.minobsinnode = c(5, 10)))
```

varimp

Variable Importance

Description

Calculate measures of the relative importance of predictors in a model.

Usage

```
varimp(object, scale = TRUE, ...)
```

Arguments

object model fit result.

scale logical indicating whether importance measures should be scaled to range from

0 to 100.

... arguments passed to model-specific variable importance functions.

Value

VarImp class object.

See Also

plot

Examples

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

gbm_fit <- fit(Surv(time, status) ~ ., data = veteran, model = GBMModel)
(vi <- varimp(gbm_fit))
plot(vi)</pre>
```

XGBModel

Extreme Gradient Boosting Models

Description

Fits models within an efficient implementation of the gradient boosting framework from Chen & Guestrin.

```
XGBModel(params = list(), nrounds = 1, verbose = 0, print_every_n = 1)
XGBDARTModel(
  objective = NULL,
  aft_loss_distribution = "normal",
  aft_loss_distribution_scale = 1,
  base_score = 0.5,
  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,
  lambda = 1,
  alpha = 0,
  tree_method = "auto",
  sketch_eps = 0.03,
  scale_pos_weight = 1,
  refresh_leaf = 1,
  process_type = "default",
  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(
  objective = NULL,
  aft_loss_distribution = "normal",
  aft_loss_distribution_scale = 1,
  base_score = 0.5,
  lambda = 0,
  alpha = 0,
  updater = "shotgun",
  feature_selector = "cyclic",
  top_k = 0,
)
```

```
XGBTreeModel(
  objective = NULL,
  aft_loss_distribution = "normal",
  aft_loss_distribution_scale = 1,
 base_score = 0.5,
  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,
  lambda = 1,
  alpha = 0,
  tree_method = "auto",
  sketch_eps = 0.03,
  scale_pos_weight = 1,
  refresh_leaf = 1,
  process_type = "default",
  grow_policy = "depthwise",
 max_leaves = 0,
 max_bin = 256,
 num_parallel_tree = 1,
)
```

Arguments

```
list of model parameters as described in the XGBoost documentation.
params
nrounds
                  maximum number of boosting iterations.
verbose
                  numeric value controlling the amount of output printed during model fitting,
                  such that 0 = \text{none}, 1 = \text{performance information}, and 2 = \text{additional information}.
                  numeric value designating the fitting iterations at at which to print output when
print_every_n
                  verbose > 0.
objective
                  character string specifying the learning task and objective. Possible values for
                  supported response variable types are as follows.
                  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:cox", "survival:aft"
                  The first values listed are the defaults for the corresponding response types.
```

```
aft_loss_distribution

character string specifying the distribution for the accelerated failure time objective ("survival:aft") as "normal", "logistic", or "extreme".

aft_loss_distribution_scale

numeric scaling parameter for the accelerated failure time distribution.

base_score

initial numeric prediction score of all instances, global bias.

eta, gamma, max_depth, min_child_weight, max_delta_step, subsample, colsample_bytree, colsample_bylevel see params reference.

... arguments passed to XGBModel.
```

Details

Response Types: factor, numeric, PoissonVariate, Surv

Automatic Tuning of Grid Parameters • XGBDARTModel: nrounds, max_depth, eta, gamma*, min_child_weight*, subsample, colsample_bytree, rate_drop, skip_drop

- XGBLinearModel: nrounds, lambda, alpha
- XGBTreeModel: nrounds, max_depth, eta, gamma*, min_child_weight*, subsample, colsample_bytree

Default values for the NULL arguments and further model details can be found in the source link below.

In calls to varimp for XGBTreeModel, argument metric may be spedified 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

```
model_fit <- fit(Species ~ ., data = iris, model = XGBTreeModel)
varimp(model_fit, metric = "Frequency", scale = FALSE)</pre>
```

^{*} included only in randomly sampled grid points

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