# Package 'MachineShop'

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Type Package

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

#### **Depends** R (>= 4.0.0)

- **Imports** abind, cli (>= 3.1.0), dials (>= 0.0.4), foreach, ggplot2 (>= 3.3.0), kernlab, magrittr, Matrix, methods, nnet, party, polspline, progress, recipes (>= 0.2.0), rlang, rsample (>= 0.1.0), Rsolnp, survival, tibble, utils
- Suggests adabag, BART, bartMachine, C50, cluster, doParallel, e1071, earth, elasticnet, generics, gbm, glmnet, gridExtra, Hmisc, kableExtra, kknn, knitr, lars, MASS, mboost, mda, ParBayesianOptimization, parsnip, partykit, pls, pso, randomForest, randomForestSRC, ranger, rBayesianOptimization, rmarkdown, rms, rpart, testthat, tree, xgboost

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BugReports https://github.com/brian-j-smith/MachineShop/issues

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MachineShop-package MachineShop: Machine Learning Models and Tools

#### Description

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

#### Details

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

Training:

fitModel fittingresampleResample estimation of model performance

**Tuning Grids:** 

expand_model	Model expansion over tuning parameters
expand_modelgrid	Model tuning grid expansion
expand_params	Model parameters expansion
expand_steps	Recipe step parameters expansion

**Response Values:** 

response	Observed
predict	Predicted

Performance Assessment:

calibration confusion dependence diff Model calibration Confusion matrix Parital dependence Model performance differences

lift	Lift curves
performance metrics	Model performance metrics
performance_curve	Model performance curves
rfe	Recursive feature elimination
varimp	Variable importance

Methods for resample estimation include

BootControl	Simple bootstrap
BootOptimismControl	Optimism-corrected bootstrap
CVControl	Repeated K-fold cross-validation
CVOptimismControl	Optimism-corrected cross-validation
00BControl	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 <brian-j-smith@uiowa.edu>

#### See Also

Useful links:

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

AdaBagModel

## Description

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

## Usage

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

## Arguments

mfinal	number of trees to use.
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.
ср	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.
maxdepth	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

## Requires prior installation of suggested package adabag to run

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

AdaBoostModel Ba

Boosting with Classification Trees

## Description

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

## Usage

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

```
)
```

boos	if TRUE, then bootstrap samples are drawn from the training set using the observation weights at each iteration. If FALSE, then all observations are used with their weights.
mfinal	number of iterations for which boosting is run.

#### AdaBoostModel

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.
ср	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.
maxdepth	maximum depth of any node of the final tree, with the root node counted as depth 0.

## Details

Response types: factor

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

\* excluded from grids by default

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

## Value

MLModel class object.

## See Also

boosting, fit, resample

## Examples

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

as.MLInput

## Description

Function to coerce an object to MLInput.

#### Usage

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

#### Arguments

х	model fit result or MachineShop model specification.
	arguments passed to other methods.

#### Value

MLInput class object.

as.MLModel

Coerce to an MLModel

#### Description

Function to coerce an object to MLModel.

## Usage

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

## Arguments

х	model fit result, MachineShop model specification, or parsnip model specifi-
	cation.
	arguments passed to other methods.

#### Value

MLModel class object.

## See Also

ParsnipModel

BARTMachineModel Bayesian Additive Regression Trees Model

## Description

Builds a BART model for regression or classification.

## 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,
    ...
)
```

num_trees	number of trees to be grown in the sum-of-trees model.
num_burn	number of MCMC samples to be discarded as "burn-in".
num_iter	number of MCMC samples to draw from the posterior distribution.
alpha, beta	base and power hyperparameters in tree prior for whether a node is nonterminal or not.
k	regression prior probability that $E(Y X)$ is contained in the interval $(y_{min}, y_{max})$ , based on a normal distribution.

q	quantile of the prior on the error variance at which the data-based estimate is placed.
nu	regression degrees of freedom for the inverse $sigma^2$ prior.
mh_prob_steps	vector of prior probabilities for proposing changes to the tree structures: (GROW, PRUNE, CHANGE).
verbose	logical indicating whether to print progress information about the algorithm.
	additional arguments to bartMachine.

## Details

Response types: binary factor, numeric

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

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

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

#### Value

MLModel class object.

#### See Also

bartMachine, fit, resample

#### Examples

## Requires prior installation of suggested package bartMachine to run

BARTModel

#### Description

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

## Usage

```
BARTModel(
 K = integer(),
  sparse = FALSE,
  theta = 0,
  omega = 1,
  a = 0.5,
  b = 1,
  rho = numeric(),
  augment = FALSE,
  xinfo = matrix(NA, 0, 0),
  usequants = FALSE,
  sigest = NA,
  sigdf = 3,
  sigquant = 0.9,
  lambda = NA,
  k = 2,
  power = 2,
  base = 0.95,
  tau.num = numeric(),
  offset = numeric(),
  ntree = integer(),
  numcut = 100,
  ndpost = 1000,
  nskip = integer(),
  keepevery = integer(),
 printevery = 1000
)
```

К	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 uniformly.
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 and further model details can be found in the source links below.

#### Value

MLModel class object.

## See Also

gbart, mbart, surv.bart, fit, resample

## Examples

## Requires prior installation of suggested package BART to run

fit(sale\_amount ~ ., data = ICHomes, model = BARTModel)

BlackBoostModel

## Description

Gradient boosting for optimizing arbitrary loss functions where regression trees are utilized as baselearners.

#### 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,
  . . .
)
```

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.
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.
teststat	type of the test statistic to be applied for variable selection.
testtype	how to compute the distribution of the test statistic.
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.
	additional arguments to ctree_control.

## Details

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

#### Automatic tuning of grid parameters: mstop, maxdepth

Default values 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

## Requires prior installation of suggested packages mboost and partykit to run

data(Pima.tr, package = "MASS")

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

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,
```

#### C50Model

```
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.	

#### Details

#### Response types: factor

## Automatic tuning of grid parameters: trials, rules, winnow

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

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

## Value

MLModel class object.

## See Also

C5.0, fit, resample

## Examples

```
## Requires prior installation of suggested package C50 to run
model_fit <- fit(Species ~ ., data = iris, model = C50Model)</pre>
```

varimp(model\_fit, method = "model", type = "splits", scale = FALSE)

calibration Model Calibration

#### Description

Calculate calibration estimates from observed and predicted responses.

#### Usage

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

#### Arguments

x	observed responses or resample result containing observed and predicted re- sponses.
У	predicted responses if not contained in x.
weights	numeric vector of non-negative case weights for the observed x responses [de-fault: equal weights].
breaks	value defining the response variable bins within which to calculate observed mean values. May be specified as a number of bins, a vector of breakpoints, or NULL to fit smooth curves with splines for predicted survival probabilities and with loess for others.
span	numeric parameter controlling the degree of loess smoothing.
distr	character string specifying a distribution with which to estimate the observed survival mean. Possible values are "empirical" for the Kaplan-Meier estima- tor, "exponential", "extreme", "gaussian", "loggaussian", "logistic", "loglogistic", "lognormal", "rayleigh", "t", or "weibull". Defaults to the distribution that was used in predicting mean survival times.

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## case\_weights

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

## Requires prior installation of suggested package gbm to run

library(survival)

case\_weights Extract Case Weights

#### Description

Extract the case weights from an object.

#### Usage

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

object	model fit result, ModelFrame, or recipe.
newdata	dataset from which to extract the weights if given; otherwise, object is used. The dataset should be given as a ModelFrame or as a data frame if object con-
	tains a ModelFrame or a recipe, respectively.

## Examples

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

CForestModel Conditional Random Forest Model

#### Description

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

#### Usage

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

#### Arguments

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.

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#### combine

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 parameter: 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)

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(...)
```

#### confusion

```
## S3 method for class 'ListOf'
c(...)
## S3 method for class 'PerformanceCurve'
c(...)
## S3 method for class 'Resample'
c(...)
## S4 method for signature 'SurvMatrix,SurvMatrix'
e1 + e2
```

## Arguments

	named or unnamed calibration, confusion, lift, performance curve, summary, or
	resample results. Curves must have been generated with the same performance
	metrics and resamples with the same resampling control.
e1, e2	objects.

## Value

Object of the same class as the arguments.

confusion	Confusion Matrix		
-----------	------------------	--	--

## Description

Calculate confusion matrices of predicted and observed responses.

## Usage

```
confusion(
    x,
    y = NULL,
    weights = NULL,
    cutoff = MachineShop::settings("cutoff"),
    na.rm = TRUE,
    ...
)
```

ConfusionMatrix(data = NA, ordered = FALSE)

#### confusion

## Arguments

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

## See Also

c, plot, summary

## Examples

## Requires prior installation of suggested package gbm to run

```
res <- resample(Species ~ ., data = iris, model = GBMModel)
(conf <- confusion(res))
plot(conf)</pre>
```

#### CoxModel

#### Description

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

#### Usage

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

## Arguments

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

#### Details

#### Response types: Surv

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

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

## dependence

## Value

MLModel class object.

## See Also

coxph, coxph.control, stepAIC, fit, resample

#### Examples

library(survival)

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

dependence

## Partial Dependence

## Description

Calculate partial dependence of a response on select predictor variables.

## Usage

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

object	model fit result.
data	data frame containing all predictor variables. If not specified, the training data will be used by default.
select	expression indicating predictor variables for which to compute partial depen- dence (see subset for syntax) [default: all].
interaction	logical indicating whether to calculate dependence on the interacted predictors.
n	number of predictor values at which to perform calculations.

intervals	character string specifying whether the n values are spaced uniformly ("uniform") or according to variable quantiles ("quantile").
distr, method	arguments passed to predict.
stats	function, function name, or vector of these with which to compute response variable summary statistics over non-selected predictor variables.
na.rm	logical indicating whether to exclude missing predicted response values from the calculation of summary statistics.

#### Value

PartialDependence class object that inherits from data.frame.

#### See Also

plot

#### Examples

## Requires prior installation of suggested package gbm to run

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

## Description

Functions that have been deprecated and will be removed in a future version of the package.

#### Usage

```
ModeledInput(...)
```

rpp(...)

## Arguments

... arguments passed to non-deprecated equivalent.

#### Details

```
Use ModelSpecification() instead of ModeledInput().
Use ppr() instead of rpp().
```

#### Description

Pairwise model differences in resampled performance metrics.

## Usage

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

#### Arguments

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

## Value

PerformanceDiff class object that inherits from Performance.

#### See Also

t.test, plot, summary

## Examples

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

```
## Survival response example
library(survival)
fo <- Surv(time, status) ~ .
control <- CVControl()
gbm_res1 <- resample(fo, data = veteran, GBMModel(n.trees = 25), control)
gbm_res2 <- resample(fo, data = veteran, GBMModel(n.trees = 50), control)
gbm_res3 <- resample(fo, data = veteran, GBMModel(n.trees = 100), control)
res <- c(GBM1 = gbm_res1, GBM2 = gbm_res2, GBM3 = gbm_res3)
res_diff <- diff(res)</pre>
```

diff

```
summary(res_diff)
plot(res_diff)
```

DiscreteVariate Discrete Variate Constructors

#### Description

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

#### Usage

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

```
PoissonVariate(x = integer())
```

#### Arguments

х	numeric vector.
size	number or numeric vector of binomial trials.
min, max	minimum and maximum bounds for discrete numbers.

### Value

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

#### See Also

#### role\_binom

## Examples

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

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EarthModel

## Description

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

#### Usage

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

#### Arguments

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

#### Details

Response types: factor, numeric

Automatic tuning of grid parameters: nprune, degree\*

\* excluded from grids by default

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

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

## Value

MLModel class object.

## See Also

earth, fit, resample

## Examples

## Requires prior installation of suggested package earth to run

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

expand\_model

Model Expansion Over Tuning Parameters

## Description

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

## Usage

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

## Arguments

object	model function, function name, or object; or another object that can be coerced to a model.
	named vectors or factors or a list of these containing the parameter values over which to expand object.
random	number of points to be randomly sampled from the parameter grid or FALSE if all points are to be returned.

#### Value

list of expanded models.

#### See Also

SelectedModel

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## expand\_modelgrid

#### Examples

expand\_modelgrid Model Tuning Grid Expansion

## Description

Expand a model grid of tuning parameter values.

#### Usage

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

#### Arguments

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

## Details

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

## Value

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

#### See Also

#### TunedModel

## Examples

expand\_params Model Pa

Model Parameters Expansion

## Description

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

#### Usage

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

## Arguments

	named data frames or vectors or a list of these containing the parameter values over which to create the grid.
random	number of points to be randomly sampled from the parameter grid or FALSE if all points are to be returned.

#### Value

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

#### See Also

#### TunedModel

## Examples

```
## Requires prior installation of suggested package gbm to run
data(Boston, package = "MASS")
grid <- expand_params(
    n.trees = c(50, 100),
    interaction.depth = 1:2
)
fit(medv ~ ., data = Boston, model = TunedModel(GBMModel, grid = grid))
```

expand\_steps

## 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

extract

#### Description

Operators acting on data structures to extract elements.

#### Usage

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

## Arguments

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

FDAModel

Flexible and Penalized Discriminant Analysis Models

## Description

Performs flexible discriminant analysis.

## Usage

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

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

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 <b>mda</b> package. For penalized discriminant analysis, gen.ridge is appropriate. Other possibilities are mars for multivari- ate 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.
df	alternative specification of lambda in terms of equivalent degrees of freedom.

# Details

Response types: factor

```
Automatic tuning of grid parameters: • FDAModel: nprune, degree*
```

• PDAModel: lambda

\* excluded from grids by default

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

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

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

# Value

MLModel class object.

## See Also

fda, predict.fda, fit, resample

## Examples

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

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

fit

Model Fitting

### Description

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

# Usage

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

## Arguments

formula, dataformula defining the model predictor and response variables and a data frame containing them.modelmodel function, function name, or object; or another object that can be coerced to a model. A model can be given first followed by any of the variable spec- ifications, and the argument can be omitted altogether in the case of modeled inputs.x, ymatrix and object containing predictor and response variables.inputinput object defining and containing the model predictor and response variables.		arguments passed from the generic function to its methods and from the MLModel and MLModelFunction methods to others. The first argument of each fit method is positional and, as such, must be given first in calls to them.
<ul> <li>to a model. A model can be given first followed by any of the variable specifications, and the argument can be omitted altogether in the case of modeled inputs.</li> <li>x, y matrix and object containing predictor and response variables.</li> </ul>	formula, data	
	model	to a model. A model can be given first followed by any of the variable spec- ifications, and the argument can be omitted altogether in the case of modeled
input input object defining and containing the model predictor and response variables.	х, у	matrix and object containing predictor and response variables.
	input	input object defining and containing the model predictor and response variables.
object model specification.	object	model specification.

# 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.

## **GAMBoostModel**

## See Also

as.MLModel, response, predict, varimp

### Examples

## Requires prior installation of suggested package gbm to run

```
## Survival response example
library(survival)
gbm_fit <- fit(Surv(time, status) ~ ., data = veteran, model = GBMModel)
varimp(gbm_fit)</pre>
```

GAMBoostModel

Gradient Boosting with Additive Models

#### Description

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

# Usage

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

## Arguments

family	optional Family object. Set automatically according to the class type of the response variable.
baselearner	character specifying the component-wise base learner to be used.
dfbase	gobal degrees of freedom for P-spline base learners ("bbs").
mstop	number of initial boosting iterations.
nu	step size or shrinkage parameter between 0 and 1.
risk	method to use in computing the empirical risk for each boosting iteration.

stopintern	logical inidicating whether the boosting algorithm stops internally when the out- of-bag risk increases at a subsequent iteration.
trace	logical indicating whether status information is printed during the fitting pro-
	cess.

# Details

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

## Automatic tuning of grid parameter: mstop

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

## Value

MLModel class object.

## See Also

gamboost, Family, baselearners, fit, resample

## Examples

## Requires prior installation of suggested package mboost to run

data(Pima.tr, package = "MASS")

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

GBMModel

Generalized Boosted Regression Model

## Description

Fits generalized boosted regression models.

### Usage

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

## **GLMBoostModel**

## 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 parame- ters needed. Set automatically according to the class type of the response vari- able.	
n.trees interaction.dep	n.trees total number of trees to fit. .nteraction.depth	
	maximum depth of variable interactions.	
n.minobsinnode	minimum number of observations in the trees terminal nodes.	
shrinkage	shrinkage parameter applied to each tree in the expansion.	
bag.fraction	fraction of the training set observations randomly selected to propose the next tree in the expansion.	

# Details

Response types: factor, numeric, PoissonVariate, Surv

Automatic tuning of grid parameters: n.trees, interaction.depth, shrinkage\*, n.minobsinnode\* \* excluded from grids by default

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

## Value

MLModel class object.

## See Also

gbm, fit, resample

## Examples

## Requires prior installation of suggested package gbm to run

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.
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 parameter: mstop

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

## Value

MLModel class object.

## See Also

glmboost, Family, fit, resample

# Examples

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

GLMModel

## Description

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

## Usage

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

# Arguments

family	optional error distribution and link function to be used in the model. Set auto- matically according to the class type of the response variable.
quasi	logical indicator for over-dispersion of binomial and Poisson families; i.e., dis- persion 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

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

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

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

## Value

MLModel class object.

#### See Also

glm, glm.control, stepAIC, fit, resample

#### Examples

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

GLMNetModel GLM Lasso or Elasticnet Model

## Description

Fit a generalized linear model via penalized maximum likelihood.

#### Usage

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

## **GLMNetModel**

## Arguments

family	optional response type. Set automatically according to the class type of the response variable.	
alpha	elasticnet mixing parameter.	
lambda	regularization parameter. The default value $lambda = 0$ performs no regular- ization and should be increased to avoid model fitting issues if the number of predictor variables is greater than the number of observations.	
standardize	logical flag for predictor variable standardization, prior to model fitting.	
intercept	logical indicating whether to fit intercepts.	
penalty.factor	vector of penalty factors to be applied to each coefficient.	
standardize.response		
	logical indicating whether to standardize "mgaussian" response variables.	
thresh	convergence threshold for coordinate descent.	
maxit	maximum number of passes over the data for all lambda values.	
type.gaussian	algorithm type for guassian models.	
type.logistic	algorithm type for logistic models.	
type.multinomial		
	algorithm type for multinomial models.	

# Details

Response types: BinomialVariate, factor, matrix, numeric, PoissonVariate, Surv

## Automatic tuning of grid parameters: lambda, alpha

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

#### Value

MLModel class object.

### See Also

glmnet, fit, resample

## Examples

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

#### ICHomes

#### 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

formula	Traditional model formula
matrix	Design matrix of predictors
ModelFrame	Model frame
ModelSpecification	Model specification
recipe	Preprocessing recipe roles and steps

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

<b>Response Functions</b>	BinomialVariate 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.

ModelSpecification	Model specification
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,
    distance = 2,
    scale = TRUE,
    kernel = c("optimal", "biweight", "cos", "epanechnikov", "gaussian", "inv", "rank",
        "rectangular", "triangular", "triweight")
)
```

# Arguments

k	numer of neigbors considered.
distance	Minkowski distance parameter.
scale	logical indicating whether to scale predictors to have equal standard deviations.
kernel	kernel to use.

# Details

Response types: factor, numeric, ordinal

## Automatic tuning of grid parameters: k, distance\*, kernel\*

\* excluded from grids by default

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

## Value

MLModel class object.

## See Also

kknn, fit, resample

# Examples

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

LARSModel

# Description

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

## Usage

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

### Arguments

type	model type.
trace	logical indicating whether status information is printed during the fitting pro-
	cess.
normalize	whether to standardize each variable to have unit L2 norm.
intercept	whether to include an intercept in the model.
step	algorithm step number to use for prediction. May be a decimal number indicat- ing a fractional distance between steps. If specified, the maximum number of algorithm steps will be ceiling(step); otherwise, step will be set equal to the source package default maximum [default: max.steps].
use.Gram	whether to precompute the Gram matrix.

# Details

Response types: numeric

# Automatic tuning of grid parameter: step

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

## Value

MLModel class object.

## See Also

lars, fit, resample

## Examples

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

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

```
LDAModel
```

Linear Discriminant Analysis Model

# Description

Performs linear discriminant analysis.

# Usage

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

# Arguments

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

## Details

Response types: factor

#### Automatic tuning of grid parameter: dimen

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

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

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

# lift

# Value

MLModel class object.

# See Also

lda, predict.lda, fit, resample

## Examples

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

lift

# Model Lift Curves

# Description

Calculate lift curves from observed and predicted responses.

## Usage

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

# Arguments

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

# Value

LiftCurve class object that inherits from PerformanceCurve.

# See Also

c, plot, summary

## Examples

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

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

LMModel

Linear Models

# Description

Fits linear models.

### Usage

LMModel()

### Details

Response types: factor, matrix, numeric

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

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

## Value

MLModel class object.

### See Also

lm, fit, resample

## Examples

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

MDAModel

# Description

Performs mixture discriminant analysis.

# Usage

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

## Arguments

subclasses	numeric value or vector of subclasses per class.
sub.df	effective degrees of freedom of the centroids per class if subclass centroid shrink- age 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 <b>mda</b> package. For penalized mixture discrimi- nant models, gen.ridge is appropriate. Other possibilities are mars for multi- variate 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 parameter: subclasses

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

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

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

#### Value

MLModel class object.

# See Also

mda, predict.mda, fit, resample

## Examples

## Requires prior installation of suggested package mda to run

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

metricinfo

### Display Performance Metric Information

## Description

Display information about metrics provided by the MachineShop package.

### Usage

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

#### Arguments

•••

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

#### Value

List of named metric elements each containing the following components:

label character descriptor for the metric.

- **maximize** logical indicating whether higher values of the metric correspond to better predictive performance.
- **arguments** closure with the argument names and corresponding default values of the metric function.
- **response\_types** data frame of the observed and predicted response variable types supported by the metric.

### metrics

## Examples

```
## All metrics
metricinfo()
## Metrics by observed and predicted response types
names(metricinfo(factor(0)))
names(metricinfo(factor(0), factor(0)))
names(metricinfo(factor(0), matrix(0)))
names(metricinfo(factor(0), numeric(0)))
## Metric-specific information
metricinfo(auc)
```

metrics

#### Performance Metrics

## Description

Compute measures of agreement between observed and predicted responses.

#### Usage

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

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

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

metrics

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

```
method = c("mse", "pearson", "spearman"),
distr = character(),
...
)
rmse(observed, predicted = NULL, weights = NULL, ...)
rmsle(observed, predicted = NULL, weights = NULL, ...)
```

## Arguments

observed	observed responses; or confusion, performance curve, or resample result con- taining observed and predicted responses.
predicted	predicted responses if not contained in observed.
weights	numeric vector of non-negative case weights for the observed responses [default: equal weights].
cutoff	numeric (0, 1) threshold above which binary factor probabilities are classified as events and below which survival probabilities are classified. If NULL, then confusion matrix-based metrics are computed on predicted class probabilities if given.
	arguments passed to or from other methods.
multiclass	character string specifying the method for computing generalized area under the performance curve for multiclass factor responses. Options are to average over areas for each pair of classes ("pairs") or for each class versus all others ("all").
metrics	vector of two metric functions or function names that define a curve under which to calculate area [default: ROC metrics].
stat	function or character string naming a function to compute a summary statistic at each cutoff value of resampled metrics in performance curves, or NULL for resample-specific metrics.
beta	relative importance of recall to precision in the calculation of $f\_score$ [default: F1 score].
fun	function to calculate a desired sensitivity-specificity tradeoff.
power	power to which positional distances of off-diagonals from the main diagonal in confusion matrices are raised to calculate weighted_kappa2.
method	character string specifying whether to compute r2 as the coefficient of determi- nation ("mse") or as the square of "pearson" or "spearman" correlation.
distr	character string specifying a distribution with which to estimate the observed survival mean in the total sum of square component of r2. Possible values are "empirical" for the Kaplan-Meier estimator, "exponential", "extreme", "gaussian", "loggaussian", "logistic", "loglogistic", "lognormal", "rayleigh", "t", or "weibull". Defaults to the distribution that was used in predicting mean survival times.

### References

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

### See Also

metricinfo, performance

MLControl

**Resampling Controls** 

#### Description

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

## Usage

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

## **MLControl**

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

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

## Arguments

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

#### Details

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

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

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

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

00BControl constructs an MLControl object for out-of-bootstrap resampling in which models are fit with bootstrap resampled training sets and used to predict the unsampled cases.

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

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

#### Value

Object that inherits from the MLControl class.

#### References

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

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

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

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

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

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

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

### See Also

set\_monitor, set\_predict, set\_strata, resample, SelectedInput, SelectedModel, TunedInput, TunedModel

### Examples

```
## Bootstrapping with 100 samples
BootControl(samples = 100)
## Optimism-corrected bootstrapping with 100 samples
BootOptimismControl(samples = 100)
## Cross-validation with 5 repeats of 10 folds
CVControl(folds = 10, repeats = 5)
## Optimism-corrected cross-validation with 5 repeats of 10 folds
CVOptimismControl(folds = 10, repeats = 5)
## Out-of-bootstrap validation with 100 samples
OOBControl(samples = 100)
## Split sample validation with 2/3 training and 1/3 testing
SplitControl(prop = 2/3)
## Training set evaluation
```

TrainControl()

MLMetric

# Description

Create a performance metric for use with the MachineShop package.

# Usage

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

# Arguments

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

## Value

MLMetric class object.

## See Also

metrics

## Examples

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

MLModel

## Description

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

# Usage

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

MLModelFunction(object, ...)

### Arguments

name	character name of the object to which the model is assigned.	
label	optional character descriptor for the model.	
packages	character vector of package names upon which the model depends. Each name may be optionally followed by a comment in parentheses specifying a version requirement. The comment should contain a comparison operator, whitespace and a valid version number, e.g. "xgboost ( $>= 1.3.0$ )".	
response_types	character vector of response variable types to which the model can be fit. Supported types are "binary", = "BinomialVariate", "DiscreteVariate", "factor", "matrix", "NegBinomialVariate", "numeric", "ordered", "PoissonVariate", and "Surv".	
weights	logical value or vector of the same length as response_types indicating whether case weights are supported for the responses.	
predictor_encoding		
	character string indicating whether the model is fit with predictor variables en- coded as a "model.frame", a "model.matrix", or unspecified (default).	
params	list of user-specified model parameters to be passed to the fit function.	

## MLModel

gridinfo	tibble of information for construction of tuning grids consisting of a character column param with the names of parameters in the grid, a list column get_values with functions to generate grid points for the corresponding parameters, and an optional logical column default indicating which parameters to include by default in regular grids. Values functions may optionally include arguments n and data for the number of grid points to generate and a ModelFrame of the model fit data and formula, respectively; and must include an ellipsis ().
fit	model fitting function whose arguments are a formula, a ModelFrame named data, case weights, and an ellipsis.
predict	model prediction function whose arguments are the object returned by fit, a ModelFrame named newdata of predictor variables, optional vector of times at which to predict survival, and an ellipsis.
varimp	variable importance function whose arguments are the object returned by fit, optional arguments passed from calls to varimp, and an ellipsis.
	arguments passed to other methods.
object	function that returns an MLModel object when called without any supplied argument values.

## Details

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

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

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

matrix matrix of predicted responses.

numeric vector or column matrix of predicted responses.

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

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

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

## Value

An MLModel or MLModelFunction class object.

## See Also

models, fit, resample

## Examples

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

ModelFrame ModelFrame Class

#### Description

ModelFrame(...)

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

### Usage

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

# ModelFrame

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

# Arguments

	arguments passed from the generic function to its methods. The first argument of each ModelFrame method is positional and, as such, must be given first in calls to them.
formula, data	formula defining the model predictor and response variables and a data frame containing them. In the associated method, arguments groups, strata, and weights will be evaluated as expressions, whose objects are searched for first in the accompanying data environment and, if not found there, next in the calling environment.
groups	vector of values defining groupings of cases to keep together when folds are constructed for cross-validation [default: none].
strata	vector of values to use in conducting stratified resample estimation of model performance [default: none].
weights	numeric vector of non-negative case weights for the y response variable [default: equal weights].
na.rm	logical indicating whether to remove cases with NA values for any of the model variables.
х, у	matrix and object containing predictor and response variables.
offsets	numeric vector, matrix, or data frame of values to be added with a fixed coefficient of 1 to linear predictors in compatible regression models.

## Value

ModelFrame class object that inherits from data.frame.

# See Also

fit, resample, response, SelectedInput

## Examples

modelinfo

### Description

Display information about models supplied by the MachineShop package.

#### Usage

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

#### Arguments

```
. . .
```

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

## Value

List of named model elements each containing the following components:

label character descriptor for the model.

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

response\_types character vector of response variable types supported by the model.

- **weights** logical value or vector of the same length as response\_types indicating whether case weights are supported for the responses.
- **arguments** closure with the argument names and corresponding default values of the model function.
- **grid** logical indicating whether automatic generation of tuning parameter grids is implemented for the model.
- varimp logical indicating whether model-specific variable importance is defined.

## Examples

```
## All models
modelinfo()
## Models by response types
names(modelinfo(factor(0)))
names(modelinfo(factor(0), numeric(0)))
## Model-specific information
```

models

## Description

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

Function	Categorical	Continuous	Survival
AdaBagModel	f		
AdaBoostModel	f		
BARTModel	f	n	S
BARTMachineModel	b	n	
BlackBoostModel	b	n	S
C50Model	f		
CForestModel	f	n	S
CoxModel			S
CoxStepAICModel			S
EarthModel	f	n	
FDAModel	f		
GAMBoostModel	b	n	S
GBMModel	f	n	S
GLMBoostModel	b	n	S
GLMModel	f	m,n	
GLMStepAICModel	b	n	
GLMNetModel	f	m,n	S
KNNModel	f,o	n	
LARSMode1		n	
LDAModel	f		
LMModel	f	m,n	
MDAModel	f		
NaiveBayesModel	f		
NNetModel	f	n	
ParsnipModel	f	m,n	S
PDAModel	f		
PLSModel	f	n	
POLRMode1	0		
QDAModel	f		
RandomForestModel	f	n	
RangerModel	f	n	S
RFSRCMode1	f	m,n	S
RFSRCFastModel	f	m,n	S
RPartModel	f	n	S
SurvRegMode1			S
SurvRegStepAICModel			S
SVMModel	f	n	
SVMANOVAModel	f	n	

	c		
SVMBesselModel	1	n	
SVMLaplaceModel	f	n	
SVMLinearModel	f	n	
SVMPolyModel	f	n	
SVMRadialModel	f	n	
SVMSplineModel	f	n	
SVMTanhModel	f	n	
TreeModel	f	n	
XGBModel	f	n	S
XGBDARTModel	f	n	S
XGBLinearModel	f	n	S
XGBTreeModel	f	n	S

Categorical: b = binary, f = factor, o = ordered Continuous: m = matrix, n = numeric Survival: S = Surv

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

ModelSpecification	Model specification
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

ModelSpecification Model Specification

# Description

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

# Usage

```
ModelSpecification(...)
## Default S3 method:
ModelSpecification(
    input,
    model = NULL,
```

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

## Arguments

	arguments passed from the generic function to its methods. The first argument of each ModelSpecification method is positional and, as such, must be given first in calls to them.
input	input object defining and containing the model predictor and response variables.
model	model function, function name, or object; or another object that can be coerced to a model. The argument can be omitted altogether in the case of modeled inputs.
control	control function, function name, or object defining the resampling method to be employed. If NULL or if the model specification contains any ModeledInput, SelectedInput, or SelectedModel objects, then object-specific control struc- tures and training parameters are used for selection and tuning, as usual, and objects are trained sequentially with nested resampling. Otherwise,
	• tuning of input and model objects is performed simultaneously over a global grid of their parameter values, and
	• the specified control method and training parameters below override those of any included TunedInput or TunedModel.
metrics	metric function, function name, or vector of these with which to calculate per- formance. If not specified, default metrics defined in the performance functions are used. Model selection is based on the first calculated metric.
cutoff	argument passed to the metrics functions.
stat	function or character string naming a function to compute a summary statistic on resampled metric values for model tuning.
formula, data	formula defining the model predictor and response variables and a data frame containing them.
х,у	matrix and object containing predictor and response variables.

### Value

ModelSpecification class object.

## See Also

fit, resample, set\_monitor, set\_optim

# Examples

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

NaiveBayesModel Naive Bayes Classifier Model

### Description

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

### Usage

NaiveBayesModel(laplace = 0)

## Arguments

laplace positive numeric controlling Laplace smoothing.

## Details

### Response types: factor

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

## Value

MLModel class object.

## See Also

naiveBayes, fit, resample

### NNetModel

## Examples

## Requires prior installation of suggested package e1071 to run

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

NNetModel

Neural Network Model

## Description

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

## Usage

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

## 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 fit- ting.
censored	a variant on softmax, in which non-zero targets mean possible classes.
skip	switch to add skip-layer connections from input to output.
rang	Initial random weights on [-rang, rang].
decay	parameter for weight decay.

maxit	maximum number of iterations.
trace	switch for tracing optimization.
MaxNWts	maximum allowable number of weights.
abstol	stop if the fit criterion falls below abstol, indicating an essentially perfect fit.
reltol	stop if the optimizer is unable to reduce the fit criterion by a factor of at least 1 - reltol.

## Details

Response types: factor, numeric

Automatic tuning of grid parameters: size, decay

Default values 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)

ParameterGrid Tuning Parameters Grid

### Description

Defines a tuning grid from a set of parameters.

## Usage

```
ParameterGrid(...)
```

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

## ParsnipModel

## Arguments

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

## Value

ParameterGrid class object that inherits from parameters and TuningGrid.

## See Also

TunedModel

## Examples

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

ParsnipModel Parsnip Model

## Description

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

### Usage

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

## Arguments

object	model specification from the <b>parsnip</b> package.
	tuning parameters with which to update object.

### Value

ParsnipModel class object that inherits from MLModel.

#### See Also

as.MLModel, fit, resample

#### Examples

```
## Requires prior installation of suggested package parsnip to run
prsp_model <- parsnip::linear_reg(engine = "glmnet")
model <- ParsnipModel(prsp_model, penalty = 1, mixture = 1)
model
model_fit <- fit(sale_amount ~ ., data = ICHomes, model = model)
predict(model_fit)</pre>
```

performance

## Model Performance Metrics

## Description

Compute measures of model performance.

#### Usage

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

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

#### Arguments

observed responses; or confusion, trained model fit, resample, or rfe result.
arguments passed from the Resample method to the response type-specific meth- ods or from the method for ConfusionList to ConfusionMatrix. Elliptical ar- guments in the response type-specific methods are passed to metrics supplied as a single MLMetric function and are ignored otherwise.
predicted responses if not contained in x.
numeric vector of non-negative case weights for the observed x responses [default: equal weights].
metric function, function name, or vector of these with which to calculate per- formance.
logical indicating whether to remove observed or predicted responses that are NA when calculating metrics.
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

## Requires prior installation of suggested package gbm to run

```
res <- resample(Species ~ ., data = iris, model = GBMModel)
(perf <- performance(res))
summary(perf)
plot(perf)
## Survival response example
library(survival)
gbm_fit <- fit(Surv(time, status) ~ ., data = veteran, model = GBMModel)
obs <- response(gbm_fit, newdata = veteran)
pred <- predict(gbm_fit, newdata = veteran)
performance(obs, pred)</pre>
```

#### performance\_curve

#### 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.

## Usage

```
performance_curve(x, ...)
## Default S3 method:
performance_curve(
  х,
 у,
 weights = NULL,
 metrics = c(MachineShop::tpr, MachineShop::fpr),
 na.rm = TRUE,
  . . .
)
## S3 method for class 'Resample'
performance_curve(
  х,
 metrics = c(MachineShop::tpr, MachineShop::fpr),
 na.rm = TRUE,
  . . .
)
```

## Arguments

x	observed responses or resample result containing observed and predicted re- sponses.
•••	arguments passed to other methods.
У	predicted responses if not contained in x.
weights	numeric vector of non-negative case weights for the observed x responses [de-fault: equal weights].
metrics	list of two performance metrics for the analysis [default: ROC metrics]. Preci- sion 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

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## Examples

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

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 = numeric(),
 diagonal = TRUE,
  stat = MachineShop::settings("stat.Curve"),
  • • •
)
## S3 method for class 'MLModel'
plot(
  х,
 metrics = NULL,
  stat = MachineShop::settings("stat.TrainingParams"),
```

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

# Arguments

x	calibration, confusion, lift, trained model fit, partial dependence, performance, performance curve, resample, rfe, or variable importance result.
type	type of plot to construct.
se	logical indicating whether to include standard error bars.
	arguments passed to other methods.
find	numeric true positive rate at which to display reference lines identifying the corresponding rates of positive predictions.
diagonal	logical indicating whether to include a diagonal reference line.
stat	function or character string naming a function to compute a summary statistic on resampled metrics for trained MLModel line plots and Resample model ordering. The original ordering is preserved if a value of NULL is given. For LiftCurve and PerformanceCurve classes, plots are of resampled metrics aggregated by the statistic if given or of resample-specific metrics if NULL.
metrics	vector of numeric indexes or character names of performance metrics to plot.
stats	vector of numeric indexes or character names of partial dependence summary statistics to plot.
n	number of most important variables to include in the plot.

# Examples

## Requires prior installation of suggested package gbm to run
## Factor response example
fo <- Species ~ . control <- CVControl()
gbm_fit <- fit(fo, data = iris, model = GBMModel, control = control) plot(varimp(gbm_fit))
<pre>gbm_res1 &lt;- resample(fo, iris, GBMModel(n.trees = 25), control) gbm_res2 &lt;- resample(fo, iris, GBMModel(n.trees = 50), control) gbm_res3 &lt;- resample(fo, iris, GBMModel(n.trees = 100), control) plot(gbm_res3)</pre>
res <- c(GBM1 = gbm_res1, GBM2 = gbm_res2, GBM3 = gbm_res3) plot(res)

PLSModel

## 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

## Examples

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

POLRModel

#### 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

## Description

Predict outcomes with a fitted model.

## Usage

```
## S3 method for class 'MLModelFit'
predict(
    object,
    newdata = NULL,
    times = numeric(),
    type = c("response", "default", "numeric", "prob"),
    cutoff = MachineShop::settings("cutoff"),
    distr = character(),
    method = character(),
    ...
)
## S4 method for signature 'MLModelFit'
```

```
predict(object, ...)
```

## Arguments

object	model fit result.
newdata	optional data frame with which to obtain predictions. If not specified, the train- ing data will be used by default.
times	numeric vector of follow-up times at which to predict survival events/probabilities or NULL for predicted survival means.
type	specifies prediction on the original outcome ("response"), numeric ("numeric"), or probability ("prob") scale; or model-specific default predictions ("default").
cutoff	numeric (0, 1) threshold above which binary factor probabilities are classified as events and below which survival probabilities are classified.
distr	character string specifying distributional approximations to estimated survival curves. Possible values are "empirical", "exponential", "rayleigh", or "weibull"; with defaults of "empirical" for predicted survival events/probabilities and "weibull" for predicted survival means.
method	character string specifying the empirical method of estimating baseline survival curves for Cox proportional hazards-based models. Choices are "breslow" or "efron" (default).
	arguments passed from the S4 to the S3 method.

#### See Also

confusion, performance, metrics

#### Examples

## Requires prior installation of suggested package gbm to run

## Survival response example
library(survival)

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

print

Print MachineShop Objects

#### Description

Print methods for objects defined in the MachineShop package.

#### Usage

```
## S3 method for class 'BinomialVariate'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'Calibration'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'DiscreteVariate'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'ListOf'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'MLControl'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'MLControl'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'MLMetric'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'MLMetric'
print(x, n = MachineShop::settings("print_max"), ...)
## S3 method for class 'MLModel'
print(x, n = MachineShop::settings("print_max"), id = FALSE, ...)
## S3 method for class 'MLModelFunction'
```

### print

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

### Arguments

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

QDAModel

#### Description

Performs quadratic discriminant analysis.

## Usage

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

## Arguments

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

## Details

#### Response types: factor

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

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

Default values 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)

quote

## Description

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

#### Usage

.(expr)

### Arguments

expr any syntactically valid R expression.

## Details

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

nobs number of observations in data to be fit.

nvars number of predictor variables.

y the response variable.

#### Value

The quoted (unevaluated) expression.

#### See Also

quote

## Examples

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

RandomForestModel Random Forest Model

### Description

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

## Usage

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

### Arguments

ntree	number of trees to grow.
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.

### Details

Response types: factor, numeric

Automatic tuning of grid parameters: mtry, nodesize\*

\* excluded from grids by default

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

## Value

MLModel class object.

## See Also

randomForest, fit, resample

## RangerModel

## Examples

## Requires prior installation of suggested package randomForest to run

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

RangerModel

#### Fast Random Forest Model

#### Description

Fast implementation of random forests or recursive partitioning.

## Usage

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

#### Arguments

num.trees	number of trees.	
mtry	number of variables to possibly split at in each node.	
importance	variable importance mode.	
<pre>min.node.size</pre>	minimum node size.	
replace	logical indicating whether to sample with replacement.	
sample.fraction		
	fraction of observations to sample.	
splitrule	splitting rule.	

num.random.spli	ts	
	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.va	riables	
	character vector with variable names to be always selected in addition to the mtry variables tried for splitting.	
respect.unorder	ed.factors	
	handling of unordered factor covariates.	
scale.permutati	on.importance	
	scale permutation importance by standard error.	
verbose	show computation status and estimated runtime.	

### Details

Response types: factor, numeric, Surv

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

\* excluded from grids by default

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

## Value

MLModel class object.

### See Also

ranger, fit, resample

## Examples

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

recipe\_roles

## Description

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

## Usage

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

## Arguments

recipe	existing recipe object.
x, size	number of counts and trials for the specification of a BinomialVariate outcome.
group	variable defining groupings of cases to keep together when folds are constructed for cross-validation [default: none].
stratum	variable to use in conducting stratified resample estimation of model perfor- mance.
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 specifica- tion 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

#### resample

#### Examples

```
library(survival)
library(recipes)

df <- within(veteran, {
   y <- Surv(time, status)
   remove(time, status)
})
rec <- recipe(y ~ ., data = df) %>%
   role_case(stratum = y)
(res <- resample(rec, model = CoxModel))
summary(res)</pre>
```

resample

#### Resample Estimation of Model Performance

#### Description

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

### Usage

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

#### resample

#### Arguments

	arguments passed from the MLModel and MLModelFunction methods to others and from the others to ModelSpecification. The first argument of each resample method is positional and, as such, must be given first in calls to them.
formula, data	formula defining the model predictor and response variables and a data frame containing them.
model	model function, function name, or object; or another object that can be coerced to a model. A model can be given first followed by any of the variable spec- ifications, and the argument can be omitted altogether in the case of modeled inputs.
х, у	matrix and object containing predictor and response variables.
input	input object defining and containing the model predictor and response variables.
object	model input or specification.
control	control function, function name, or object defining the resampling method to be employed.

### Details

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

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

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

### Value

Resample class object.

#### See Also

c, metrics, performance, plot, summary

#### Examples

## Requires prior installation of suggested package gbm to run

```
## Factor response example
```

fo <- Species ~ .
control <- CVControl()</pre>

```
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>
```

response

## Extract Response Variable

#### Description

Extract the response variable from an object.

## Usage

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

#### Arguments

object	model fit, input, or specification containing predictor and response variables.
	arguments passed to other methods.
newdata	data frame from which to extract the response variable values if given; other wise, object is used.

## Examples

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

rfe

### **Recursive Feature Elimination**

#### Description

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

#### Usage

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

```
progress = FALSE,
...
)
## S3 method for class 'MLModel'
rfe(model, ...)
## S3 method for class 'MLModelFunction'
rfe(model, ...)
```

# Arguments

	arguments passed from the MLModel and MLModelFunction methods to others and from the others to ModelSpecification. The first argument of each rfe method is positional and, as such, must be given first in calls to them.
formula, data	formula defining the model predictor and response variables and a data frame containing them.
model	model function, function name, or object; or another object that can be coerced to a model. A model can be given first followed by any of the variable spec- ifications, and the argument can be omitted altogether in the case of modeled inputs.
х,у	matrix and object containing predictor and response variables.
input	input object defining and containing the model predictor and response variables.
object	model input or specification.
select	expression indicating predictor variables that can be eliminated (see <pre>subset</pre> for <pre>syntax) [default: all].</pre>
control	control function, function name, or object defining the resampling method to be employed.
props	numeric vector of the proportions of most important predictor variables to retain in fitted models or an integer number of equal spaced proportions to generate automatically; ignored if sizes are given.
sizes	integer vector of the set sizes of most important predictor variables to retain.
random	logical indicating whether to eliminate variables at random with probabilities proportional to their importance.
recompute	logical indicating whether to recompute variable importance after eliminating each set of variables.
optimize	character string specifying a search through all props to identify the globally optimal model ("global") or a search that stops after identifying the first locally optimal model ("local").
samples	numeric vector or list giving the number of permutation samples for each of the rfe and varimp algorithms. One or both of the values may be specified as named arguments or in the order in which their defaults appear. Larger numbers of samples decrease variability in estimated model performances and variable importances at the expense of increased computation time. Samples are more expensive computationally for rfe than for varimp.

### RFSRCModel

metrics	metric function, function name, or vector of these with which to calculate per- formance. If not specified, default metrics defined in the performance functions are used.
stat	functions or character strings naming functions to compute summary statistics on resampled metric values and permuted samples. One or both of the values may be specified as named arguments or in the order in which their defaults appear.
progress	logical indicating whether to display iterative progress during elimination.

## Value

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

## See Also

performance, plot, summary, varimp

#### Examples

## Requires prior installation of suggested package gbm to run

```
(res <- rfe(sale_amount ~ ., data = ICHomes, model = GBMModel))
summary(res)
summary(performance(res))
plot(res, type = "line")</pre>
```

RFSRCMode1

Fast Random Forest (SRC) Model

## Description

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

#### Usage

```
RFSRCModel(
   ntree = 1000,
   mtry = integer(),
   nodesize = integer(),
   nodedepth = integer(),
   splitrule = character(),
   nsplit = 10,
```

```
block.size = integer(),
  samptype = c("swor", "swr"),
  membership = FALSE,
  sampsize = if (samptype == "swor") function(x) 0.632 * x else function(x) x,
  nimpute = 1,
  ntime = integer(),
  proximity = c(FALSE, TRUE, "inbag", "oob", "all"),
  distance = c(FALSE, TRUE, "inbag", "oob", "all"),
forest.wt = c(FALSE, TRUE, "inbag", "oob", "all"),
  xvar.wt = numeric(),
  split.wt = numeric(),
  var.used = c(FALSE, "all.trees", "by.tree"),
  split.depth = c(FALSE, "all.trees", "by.tree"),
  do.trace = FALSE,
  statistics = FALSE
)
RFSRCFastModel(
  ntree = 500,
  sampsize = function(x) min(0.632 * x, max(x^0.75, 150)),
  ntime = 50,
  terminal.qualts = FALSE,
  . . .
)
```

## Arguments

ntree	number of trees.
mtry	number of variables randomly selected as candidates for splitting a node.
nodesize	minumum size of terminal nodes.
nodedepth	maximum depth to which a tree should be grown.
splitrule	splitting rule (see rfsrc).
nsplit	non-negative integer value for number of random splits to consider for each candidate splitting variable.
block.size	interval number of trees at which to compute the cumulative error rate.
samptype	whether bootstrap sampling is with or without replacement.
membership	logical indicating whether to return terminal node membership.
sampsize	function specifying the bootstrap size.
nimpute	number of iterations of the missing data imputation algorithm.
ntime	integer number of time points to constrain ensemble calculations for survival outcomes.
proximity	whether and how to return proximity of cases as measured by the frequency of sharing the same terminal nodes.
distance	whether and how to return distance between cases as measured by the ratio of the sum of edges from each case to the root node.

#### RFSRCModel

forest.wt	whether and how to return the forest weight matrix.	
xvar.wt	vector of non-negative weights representing the probability of selecting a variable for splitting.	
split.wt	vector of non-negative weights used for multiplying the split statistic for a variable.	
var.used	whether and how to return variables used for splitting.	
split.depth	whether and how to return minimal depth for each variable.	
do.trace	number of seconds between updates to the user on approximate time to comple- tion.	
statistics	logical indicating whether to return split statistics.	
terminal.qualts		
	logical indicating whether to return terminal node membership information.	
	arguments passed to RFSRCModel.	

## Details

Response types: factor, matrix, numeric, Surv

Automatic tuning of grid parameters: mtry, nodesize

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

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

### Value

MLModel class object.

#### See Also

rfsrc, rfsrc.fast, fit, resample

#### Examples

## Requires prior installation of suggested package randomForestSRC to run

model\_fit <- fit(sale\_amount ~ ., data = ICHomes, model = RFSRCModel)
varimp(model\_fit, method = "model", type = "random", scale = TRUE)</pre>

RPartModel

## Description

Fit an rpart model.

## 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.
ср	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.
maxdepth	maximum depth of any node of the final tree, with the root node counted as depth 0.

### Details

Response types: factor, numeric, Surv

## Automatic tuning of grid parameter: cp

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

### Value

MLModel class object.

## SelectedInput

#### See Also

rpart, fit, resample

### Examples

## Requires prior installation of suggested packages rpart and partykit to run

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

SelectedInput Selected Model Inputs

### Description

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

#### Usage

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

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

```
SelectedInput(x, ...)
```

### Arguments

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

#### Value

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

### SelectedModel

#### 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)
data(Boston, package = "MASS")
rec1 <- recipe(medv ~ crim + zn + indus + chas + nox + rm, data = Boston)
rec2 <- recipe(medv ~ chas + nox + rm + age + dis + rad + tax, data = Boston)
sel_rec <- SelectedInput(rec1, rec2)
fit(sel_rec, model = GLMModel)
```

SelectedModel Selected Model

## Description

Model selection from a candidate set.

#### Usage

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

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

## Arguments

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

### Details

Response types: factor, numeric, ordered, Surv

#### Value

SelectedModel or SelectedModelSpecification class object that inherits from MLModel or ModelSpecification, respectively.

## See Also

fit, resample

## Examples

## Requires prior installation of suggested package gbm and glmnet to run

```
model_fit <- fit(
   sale_amount ~ ., data = ICHomes,
   model = SelectedModel(GBMModel, GLMNetModel, SVMRadialModel)
)
(selected_model <- as.MLModel(model_fit))
summary(selected_model)</pre>
```

settings

#### Description

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

#### Usage

settings(...)

#### Arguments

• • •

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

#### Value

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

### Settings

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

- cutoff numeric (0, 1) threshold above which binary factor probabilities are classified as events and below which survival probabilities are classified [default: 0.5].
- distr.SurvMeans character string specifying distributional approximations to estimated survival curves for predicting survival means. Choices are "empirical" for the Kaplan-Meier estimator, "exponential", "rayleigh", or "weibull" (default).
- distr.SurvProbs character string specifying distributional approximations to estimated survival curves for predicting survival events/probabilities. Choices are "empirical" (default) for the Kaplan-Meier estimator, "exponential", "rayleigh", or "weibull".
- grid size argument to TuningGrid indicating the number of parameter-specific values to generate automatically for tuning of models that have pre-defined grids or a TuningGrid function, function name, or object [default: 3].
- method.EmpiricalSurv character string specifying the empirical method of estimating baseline survival curves for Cox proportional hazards-based models. Choices are "breslow" or "efron" (default).
- metrics.ConfusionMatrix function, function name, or vector of these with which to calculate performance metrics for confusion matrices [default: c(Accuracy = "accuracy", Kappa = "kappa2", `Weighted Kappa` = "weighted\_kappa2", Sensitivity = "sensitivity", Specificity = "specificity")].

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

#### 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")</pre>
```

#### set\_monitor

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

set\_monitor

Training Parameters Monitoring Control

#### Description

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

#### Usage

```
set_monitor(object, ...)
## S3 method for class 'MLControl'
set_monitor(object, progress = TRUE, verbose = FALSE, ...)
## S3 method for class 'MLOptimization'
set_monitor(object, progress = FALSE, verbose = FALSE, ...)
## S3 method for class 'ModelSpecification'
```

```
set_monitor(object, which = c("all", "control", "optim"), ...)
```

## Arguments

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

#### Value

Argument object updated with the supplied parameters.

# See Also

resample, set\_optim, set\_predict, set\_strata

#### Examples

CVControl() %>% set\_monitor(verbose = TRUE)

set\_optim

#### Tuning Parameter Optimization

#### Description

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

## Usage

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

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

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

# Arguments

object	input or model object.
	arguments passed to the TrainingParams method of set_optim_grid from its other methods.
num_init	number of grid points to sample for the initialization of Bayesian optimization.
times	maximum number of times to repeat the optimization step. Multiple sets of model parameters are evaluated automatically at each step of the BFGS algorithm to compute a finite-difference approximation to the gradient.
each	number of times to sample and evaluate model parameters at each optimization step. This is the swarm size in particle swarm optimization, which defaults to $floor(10 + 2 * sqrt(length(bounds)))$ .
acquisition	character string specifying the acquisition function as "ucb" (upper confidence bound), "ei" (expected improvement), "eips" (expected improvement per sec- ond), or "poi" (probability of improvement).
kappa, conf	upper confidence bound ("ucb") quantile or its probability to balance exploita- tion against exploration. Argument kappa takes precedence if both are given and multiplies the predictive standard deviation added to the predictive mean in the acquisition function. Larger values encourage exploration of the model parameter space.
epsilon	improvement methods ("ei", "eips", and "poi") parameter to balance exploitation against exploration. Values should be between -0.1 and 0.1 with larger ones encouraging exploration.
control	list of control parameters passed to bayesOpt by set_optim_bayes with pack- age "ParBayesianOptimization", to BayesianOptimization by set_optim_bayes with package "rBayesianOptimization", to optim by set_optim_bfgs and set_optim_sann, and to psoptim by set_optim_pso.
packages	R package or packages to use for the optimization method, or an empty vector if none are needed. The first package in set_optim_bayes is used unless otherwise specified by the user.
random	number of points to sample for a random grid search, or FALSE for an exhaustive grid search. Used when a grid search is specified or as the fallback method for non-numeric model parameters present during other optimization methods.
progress	logical indicating whether to display iterative progress during optimization.
verbose	numeric or logical value specifying the level of progress detail to print, with 0 (FALSE) indicating none and 1 (TRUE) or higher indicating increasing amounts of detail.

fun	user-defined optimization function to which the arguments below are passed in order. An ellipsis can be included in the function definition when using only a subset of the arguments and ignoring others. A tibble returned by the func- tion with the same number of rows as model evaluations will be included in a TrainingStep summary of optimization results; other types of return values will be ignored.
	<b>optim</b> function that takes a numeric vector or list of named model parameters as the first argument, optionally accepts the maximum number of iterations as argument max_iter, and returns a scalar measure of performance to be maximized. Parameter names are available from the grid and bounds ar- guments described below. If the function cannot be evaluated at a given set of parameter values, then -Inf is returned.
	grid data frame containing a tuning grid of all model parameters.
	<b>bounds</b> named list of lower and upper bounds for each finite numeric model parameter in grid. The types (integer or double) of the original parameter values are preserved in the bounds.
	<b>params</b> list of optimization parameters as supplied to set_optim_method.
	<b>monitor</b> list of the progress and verbose values.
label	character descriptor for the optimization method.
params	list of user-specified model parameters to be passed to fun.

#### Details

The optimization functions implement the following methods.

- set\_optim\_bayes Bayesian optimization with a Gaussian process model (Snoek et al. 2012).
- set\_optim\_bfgs limited-memory modification of quasi-Newton BFGS optimization (Byrd et al. 1995).
- set\_optim\_grid exhaustive or random grid search.
- set\_optim\_pso particle swarm optimization (Bratton and Kennedy 2007, Zambrano-Bigiarini et al. 2013).
- set\_optim\_sann simulated annealing (Belisle 1992). This method depends critically on the control parameter settings. It is not a general-purpose method but can be very useful in getting to good parameter values on a very rough optimization surface.
- set\_optim\_method user-defined optimization function.

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

#### Value

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

#### References

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

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

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

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

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

# See Also

BayesianOptimization, bayesOpt, optim, psoptim, set\_monitor, set\_predict, set\_strata

## Examples

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

set\_predict Resampling Prediction Control

## Description

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

#### Usage

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

#### Arguments

 object
 control object.

 times, distr, method
 arguments passed to predict.

 ...
 arguments passed to other methods.

#### set\_strata

#### Value

Argument object updated with the supplied parameters.

#### See Also

resample, set\_monitor, set\_optim, set\_strata

#### Examples

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

set\_strata Resampling Stratification Control

## Description

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

#### Usage

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

#### Arguments

object	control object.
breaks	number of quantile bins desired for stratification of numeric data during resam- pling.
nunique	number of unique values at or below which numeric data are stratified as cate- gorical.
prop	minimum proportion of data in each strata.
size	minimum number of values in each strata.
	arguments passed to other methods.

#### Details

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

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Value

Argument object updated with the supplied parameters.

# See Also

resample, set\_monitor, set\_optim, set\_predict

# Examples

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

StackedModel Stacked Regression Model

## Description

Fit a stacked regression model from multiple base learners.

#### Usage

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

# Arguments

	model functions, function names, objects; other objects that can be coerced to models; or vector of these to serve as base learners.
control	control function, function name, or object defining the resampling method to be employed for the estimation of base learner weights.
weights	optional fixed base learner weights.

# Details

Response types: factor, numeric, ordered, Surv

# Value

StackedModel class object that inherits from MLModel.

#### References

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

#### step\_kmeans

#### See Also

fit, resample

## Examples

## Requires prior installation of suggested packages gbm and glmnet to run

```
model <- StackedModel(GBMModel, SVMRadialModel, GLMNetModel(lambda = 0.01))
model_fit <- fit(sale_amount ~ ., data = ICHomes, model = model)
predict(model_fit, newdata = ICHomes)</pre>
```

step\_kmeans

K-Means Clustering Variable Reduction

#### Description

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

# Usage

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

#### 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.
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.
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.
character string specifying the clustering algorithm to use.
maximum number of algorithm iterations allowed.
number of random cluster centers generated for starting the Hartigan-Wong al- gorithm.
logical indicating whether to replace the original variables.
character string prefix added to a sequence of zero-padded integers to generate names for the resulting new variables.
analysis role that added step variables should be assigned. By default, they are designated as model predictors.
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.
unique character string to identify the step.
step_kmeans object.

# Details

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

#### Value

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

#### References

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

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

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

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

#### See Also

kmeans, recipe, prep, bake

#### Examples

```
library(recipes)
```

```
rec <- recipe(rating ~ ., data = attitude)
kmeans_rec <- rec %>%
   step_kmeans(all_predictors(), k = 3)
kmeans_prep <- prep(kmeans_rec, training = attitude)
kmeans_data <- bake(kmeans_prep, attitude)
pairs(kmeans_data, lower.panel = NULL)
tidy(kmeans_rec, number = 1)</pre>
```

```
tidy(kmeans_prep, number = 1)
```

step\_kmedoids

K-Medoids Clustering Variable Selection

#### Description

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

## Usage

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

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

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

# Arguments

recipe	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 <b>cluster</b> 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.

## References

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

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

#### See Also

pam, clara, recipe, prep, bake

#### Examples

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.

# Usage

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

# Arguments

recipe	recipe object to which the step will be added.
	one or more selector functions to choose which variables will be used to compute the components. See selections for more details. These are not currently used by the tidy method.
transform	function whose first argument x is a matrix of variables with which to compute linear combinations and second argument step is the current step. The func- tion 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.
х	step_lincomp object.

# Value

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

## See Also

recipe, prep, bake

#### Examples

step\_sbf

Variable Selection by Filtering

#### Description

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

# Usage

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

## S3 method for class 'step\_sbf'
tidy(x, ...)

# Arguments

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.

#### step\_spca

x step\_sbf object.

#### Value

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

## See Also

recipe, prep, bake

## Examples

```
library(recipes)
glm_filter <- function(x, y, step) {
  model_fit <- glm(y ~ ., data = data.frame(y, x))
  p_value <- drop1(model_fit, test = "F")[-1, "Pr(>F)"]
  p_value < step$threshold
}
rec <- recipe(rating ~ ., data = attitude)
sbf_rec <- rec %>%
  step_sbf(all_numeric_predictors(),
        filter = glm_filter, options = list(threshold = 0.05))
sbf_prep <- prep(sbf_rec, training = attitude)
sbf_data <- bake(sbf_prep, attitude)
pairs(sbf_data, lower.panel = NULL)
tidy(sbf_rec, number = 1)
tidy(sbf_prep, number = 1)</pre>
```

step\_spca

Sparse Principal Components Analysis Variable Reduction

# Description

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

#### Usage

step\_spca(
 recipe,
 ...,

```
num_comp = 5,
sparsity = 0,
num_var = integer(),
shrinkage = 1e-06,
center = TRUE,
scale = TRUE,
max_iter = 200,
tol = 0.001,
replace = TRUE,
prefix = "SPCA",
role = "predictor",
skip = FALSE,
id = recipes::rand_id("spca")
)
```

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

# Arguments

recipe	recipe object to which the step will be added.
	one or more selector functions to choose which variables will be used to compute the components. See selections for more details. These are not currently used by the tidy method.
num_comp	number of components to derive. The value of num_comp will be constrained to a minimum of 1 and maximum of the number of original variables when prep is run.
sparsity, num_v	ar
	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.
х	step_spca object.

## Details

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

## Value

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

#### References

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

#### See Also

spca, recipe, prep, bake

#### Examples

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

#### Description

Summary statistics for resampled model performance metrics.

## Usage

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

# SuperModel

#### Arguments

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

# Value

An object of summary statistics.

# Examples

## Requires prior installation of suggested package gbm to run

```
## Factor response example
fo <- Species ~ .
control <- CVControl()
gbm_res1 <- resample(fo, iris, GBMModel(n.trees = 25), control)
gbm_res2 <- resample(fo, iris, GBMModel(n.trees = 50), control)
gbm_res3 <- resample(fo, iris, GBMModel(n.trees = 100), control)
summary(gbm_res3)
res <- c(GBM1 = gbm_res1, GBM2 = gbm_res2, GBM3 = gbm_res3)
summary(res)</pre>
```

SuperModel

Super Learner Model

## Description

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

# Usage

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

#### Arguments

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

# Details

Response types: factor, numeric, ordered, Surv

# Value

SuperModel class object that inherits from MLModel.

## References

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

#### See Also

fit, resample

#### Examples

## Requires prior installation of suggested packages gbm and glmnet to run

```
model <- SuperModel(GBMModel, SVMRadialModel, GLMNetModel(lambda = 0.01))
model_fit <- fit(sale_amount ~ ., data = ICHomes, model = model)
predict(model_fit, newdata = ICHomes)</pre>
```

SurvMatrix

## Description

Create a matrix of survival events or probabilites.

## Usage

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

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

# Arguments

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

# Value

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

## See Also

performance, metrics

SurvRegModel

Parametric Survival Model

# Description

Fits the accelerated failure time family of parametric survival models.

# Usage

```
SurvRegModel(
  dist = c("weibull", "exponential", "gaussian", "logistic", "lognormal",
      "loglogistic"),
   scale = 0,
   parms = list(),
   ...
```

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

## Arguments

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

# Details

# Response types: Surv

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

# Value

MLModel class object.

# See Also

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

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)

## **SVMM**odel

## Examples

## Requires prior installation of suggested packages rms and Hmisc to run

library(survival)

fit(Surv(time, status) ~ ., data = veteran, model = SurvRegModel)

SVMModel

Support Vector Machine Models

## Description

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

#### Usage

```
SVMModel(
  scaled = TRUE,
  type = character(),
 kernel = c("rbfdot", "polydot", "vanilladot", "tanhdot", "laplacedot", "besseldot",
    "anovadot", "splinedot"),
 kpar = "automatic",
 C = 1,
 nu = 0.2,
  epsilon = 0.1,
  cache = 40,
  tol = 0.001,
  shrinking = TRUE
)
SVMANOVAModel(sigma = 1, degree = 1, ...)
SVMBesselModel(sigma = 1, order = 1, degree = 1, ...)
SVMLaplaceModel(sigma = numeric(), ...)
SVMLinearModel(...)
SVMPolyModel(degree = 1, scale = 1, offset = 1, ...)
SVMRadialModel(sigma = numeric(), ...)
```

```
SVMSplineModel(...)
```

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

# Arguments

scaled	logical vector indicating the variables to be scaled.
type	type of support vector machine.
kernel	kernel function used in training and predicting.
kpar	list of hyper-parameters (kernel parameters).
С	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 from the other constructors.
order	order of the Bessel function to be used as a kernel.
scale	scaling parameter of the polynomial and hyperbolic tangent kernels as a conve- nient way of normalizing patterns without the need to modify the data itself.
offset	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
- SVMPolyModel: C, degree, scale
- SVMRadialModel: C, sigma

Arguments kernel and kpar are automatically set by the kernel-specific constructor functions. Default values and further model details can be found in the source link below.

# Value

MLModel class object.

# See Also

ksvm, fit, resample

#### t.test

#### 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

х	performance difference result.
adjust	p-value adjustment for multiple statistical comparisons as implemented by p.adjust.
	arguments passed to other methods.

#### Details

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

$$t = \frac{x_R}{\sqrt{Fs_R^2/R}}$$

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

#### Value

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

## References

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

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

## Examples

## Requires prior installation of suggested package gbm to run

```
## 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 = numeric(),
  best = integer(),
  method = c("deviance", "misclass")
)
```

# TunedInput

# Arguments

mincut	minimum number of observations to include in either child node.
minsize	smallest allowed node size: a weighted quantity.
mindev	within-node deviance must be at least this times that of the root node for the node to be split.
split	splitting criterion to use.
k	scalar cost-complexity parameter defining a subtree to return.
best	integer alternative to k requesting the number of terminal nodes of a subtree in the cost-complexity sequence to return.
method	character string denoting the measure of node heterogeneity used to guide cost- complexity pruning.

# Details

Response types: factor, numeric

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

## Value

MLModel class object.

# See Also

tree, prune.tree, fit, resample

# Examples

## Requires prior installation of suggested package tree to run

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

TunedInput

Tuned Model Inputs

# Description

Recipe tuning over a grid of parameter values.

# Usage

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

# Arguments

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

# Value

TunedModelRecipe class object that inherits from TunedInput and recipe.

## See Also

fit, resample, set\_optim

# Examples

```
library(recipes)
data(Boston, package = "MASS")
rec <- recipe(medv ~ ., data = Boston) %>%
   step_pca(all_numeric_predictors(), id = "pca")
grid <- expand_steps(
   pca = list(num_comp = 1:2)
)</pre>
```

# TunedModel

```
fit(TunedInput(rec, grid = grid), model = GLMModel)
```

TunedModel

# Tuned Model

# Description

Model tuning over a grid of parameter values.

## Usage

```
TunedModel(
   object,
   grid = MachineShop::settings("grid"),
   control = MachineShop::settings("control"),
   metrics = NULL,
   cutoff = MachineShop::settings("cutoff"),
   stat = MachineShop::settings("stat.TrainingParams")
)
```

## Arguments

object	model function, function name, or object defining the model to be tuned.
grid	single integer or vector of integers whose positions or names match the param- eters in the model's pre-defined tuning grid if one exists and which specify the number of values used to construct the grid; TuningGrid function, function name, or object; ParameterGrid object; or data frame containing parameter values at which to evaluate the model, such as that returned by expand_params.
control	control function, function name, or object defining the resampling method to be employed.
metrics	metric function, function name, or vector of these with which to calculate per- formance. If not specified, default metrics defined in the performance functions are used. Model selection is based on the first calculated metric.
cutoff	argument passed to the metrics functions.
stat	function or character string naming a function to compute a summary statistic on resampled metric values for model tuning.

# Details

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

Response types: factor, numeric, ordered, Surv

# TuningGrid

# Value

TunedModel class object that inherits from MLModel.

# See Also

fit, resample, set\_optim

# Examples

```
## Requires prior installation of suggested package gbm to run
## May require a long runtime
# Automatically generated grid
model_fit <- fit(sale_amount ~ ., data = ICHomes,</pre>
                 model = TunedModel(GBMModel))
varimp(model_fit)
(tuned_model <- as.MLModel(model_fit))</pre>
summary(tuned_model)
plot(tuned_model, type = "1")
# Randomly sampled grid points
fit(sale_amount ~ ., data = ICHomes,
    model = TunedModel(
      GBMModel,
      grid = TuningGrid(size = 1000, random = 5)
   ))
# User-specified grid
fit(sale_amount ~ ., data = ICHomes,
   model = TunedModel(
      GBMModel,
      grid = expand_params(
       n.trees = c(50, 100),
        interaction.depth = 1:2,
        n.minobsinnode = c(5, 10)
      )
   ))
```

TuningGrid

Tuning Grid Control

#### Description

Defines control parameters for a tuning grid.

## unMLModelFit

# Usage

TuningGrid(size = 3, random = FALSE)

# Arguments

size	single integer or vector of integers whose positions or names match the param- eters in a model's tuning grid and which specify the number of values used to construct the grid.
random	number of unique points to sample at random from the grid defined by size. If size is a single unnamed integer, then random = Inf will include all values of all grid parameters in the constructed grid, whereas random = FALSE will include all values of default grid parameters.

# Details

Returned TuningGrid objects may be supplied to TunedModel for automated construction of model tuning grids. These grids can be extracted manually and viewed with the expand\_modelgrid function.

# Value

TuningGrid class object.

#### See Also

TunedModel, expand\_modelgrid

# Examples

TunedModel(XGBTreeModel, grid = TuningGrid(10, random = 5))

unMLModelFit Revert an MLModelFit Object

# Description

Function to revert an MLModelFit object to its original class.

# Usage

```
unMLModelFit(object)
```

#### Arguments

object model fit result.

# 142

# Value

The supplied object with its MLModelFit classes and fields removed.

varimp

Variable Importance

# Description

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

# Usage

```
varimp(object, method = c("permute", "model"), scale = TRUE, ...)
```

# Arguments

object	model fit result.
method	character string specifying the calculation of variable importance as permutation- base ("permute") or model-specific ("model"). If model-specific importance is specified but not defined, the permutation-based method will be used instead with its default values (below). Permutation-based variable importance is de- fined as the relative change in model predictive performances between datasets with and without permuted values for the associated variable (Fisher et al. 2019).
scale	logical indicating whether importance values should be scaled to a maximum of 100.
	arguments passed to model-specific or permutation-based variable importance functions. These include the following arguments and default values for method = "permute".
	<pre>select = NULL expression indicating predictor variables for which to compute     variable importance (see subset for syntax) [default: all].</pre>
	<pre>samples = 1 number of times to permute the values of each variable. Larger numbers of samples decrease variability in the estimates at the expense of increased computation time.</pre>
	<pre>prop = numeric() proportion of observations to sample without replacement at each round of variable permutations [default: all]. Subsampling of ob- servations can decrease computation time.</pre>
	<pre>size = integer() number of observations to sample at each round of permu- tations [default: all].</pre>
	<pre>times = numeric() numeric vector of follow-up times at which to predict sur- vival probabilities or NULL for predicted survival means.</pre>
	<pre>metric = NULL metric function or function name with which to calculate per- formance. If not specified, the first applicable default metric from the per- formance functions is used.</pre>

- compare = c("-", "/") character specifying the relative change to compute in comparing model predictive performances between datasets with and without permuted values. The choices are difference ("-") and ratio ("/").
- stats = MachineShop::settings("stat.TrainingParams") function, function name, or vector of these with which to compute summary statistics on the set of variable importance values from the permuted datasets.
- na.rm = TRUE logical indicating whether to exclude missing variable importance values from the calculation of summary statistics.
- progress = TRUE logical indicating whether to display iterative progress during computation.

#### Value

VariableImportance class object.

#### References

Fisher, A., Rudin, C., & Dominici, F. (2019). All models are wrong, but many are useful: Learning a variable's importance by studying an entire class of prediction models simultaneously. *Journal of Machine Learning Research*, 20, 1-81.

#### See Also

plot

#### Examples

## Requires prior installation of suggested package gbm to run

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

XGBModel

Extreme Gradient Boosting Models

#### Description

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

# Usage

```
XGBModel(
  nrounds = 100,
  . . . ,
  objective = character(),
  aft_loss_distribution = "normal",
  aft_loss_distribution_scale = 1,
  base_score = 0.5,
  verbose = 0,
  print_every_n = 1
)
XGBDARTModel(
  eta = 0.3,
  gamma = 0,
 max_depth = 6,
 min_child_weight = 1,
 max_delta_step = .(0.7 * is(y, "PoissonVariate")),
  subsample = 1,
  colsample_bytree = 1,
  colsample_bylevel = 1,
  colsample_bynode = 1,
  alpha = 0,
  lambda = 1,
  tree_method = "auto",
  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(
  alpha = 0,
  lambda = 0,
  updater = "shotgun",
  feature_selector = "cyclic",
  top_k = 0,
  . . .
```

# )

```
XGBTreeModel(
 eta = 0.3,
 gamma = 0,
 max_depth = 6,
 min_child_weight = 1,
 max_delta_step = .(0.7 * is(y, "PoissonVariate")),
  subsample = 1,
  colsample_bytree = 1,
  colsample_bylevel = 1,
  colsample_bynode = 1,
  alpha = 0,
  lambda = 1,
  tree_method = "auto",
  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

nrounds	number of boosting iterations.	
	model parameters as described below and in the XGBoost documentation and arguments passed to XGBModel from the other constructors.	
objective	optional character string defining the learning task and objective. Set automat- ically if not specified according to the following values available for supported response variable types.	
	<pre>factor: "multi:softprob", "binary:logistic" (2 levels only)</pre>	
	<pre>numeric: "reg:squarederror", "reg:logistic", "reg:gamma", "reg:tweedie",</pre>	
	PoissonVariate: "count:poisson"	
	<pre>Surv: "survival:aft", "survival:cox"</pre>	
	The first values listed are the defaults for the corresponding response types.	
aft_loss_distribution		
	character string specifying a distribution for the accelerated failure time objec- tive ("survival:aft") as "extreme", "logistic", or "normal".	
aft_loss_distribution_scale		
	numeric scaling parameter for the accelerated failure time distribution.	
base_score	initial prediction score of all observations, global bias.	

verbose	numeric value controlling the amount of output printed during model fitting,
	such that $0 = $ none, $1 = $ performance information, and $2 = $ additional information.
print_every_n	numeric value designating the fitting iterations at at which to print output when verbose $> 0$ .
eta	shrinkage of variable weights at each iteration to prevent overfitting.
gamma	minimum loss reduction required to split a tree node.
max_depth	maximum tree depth.
min_child_weight	
	minimum sum of observation weights required of nodes.
<pre>max_delta_step,</pre>	, tree_method, sketch_eps, scale_pos_weight, updater, refresh_leaf, process_type, grow_po other tree booster parameters.
subsample	subsample ratio of the training observations.
colsample_bytree, colsample_bylevel, colsample_bynode	
	subsample ratio of variables for each tree, level, or split.
alpha, lambda	L1 and L2 regularization terms for variable weights.
<pre>sample_type, normalize_type</pre>	
	type of sampling and normalization algorithms.
rate_drop	rate at which to drop trees during the dropout procedure.
one_drop	integer indicating whether to drop at least one tree during the dropout procedure.
skip_drop	probability of skipping the dropout procedure during a boosting iteration.
feature_selector, top_k	
	character string specifying the feature selection and ordering method, and num- ber of top variables to select in the "greedy" and "thrifty" feature selectors.

# Details

Response types: factor, numeric, PoissonVariate, Surv

Automatic tuning of grid parameters: • XGBDARTModel: nrounds, eta\*, gamma\*, max\_depth, min\_child\_weight\*, subsample\*, colsample\_bytree\*, rate\_drop\*, skip\_drop\*

- XGBLinearModel: nrounds, alpha, lambda
- XGBTreeModel: nrounds, eta\*, gamma\*, max\_depth, min\_child\_weight\*, subsample\*, colsample\_bytree\*

\* excluded from grids by default

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

In calls to varimp for XGBTreeModel, argument type may be specified as "Gain" (default) for the fractional contribution of each predictor to the total gain of its splits, as "Cover" for the number of observations related to each predictor, or as "Frequency" for the percentage of times each predictor is used in the trees. Variable importance is automatically scaled to range from 0 to 100. To obtain unscaled importance values, set scale = FALSE. See example below.

# Value

MLModel class object.

# XGBModel

# See Also

xgboost, fit, resample

# Examples

## Requires prior installation of suggested package xgboost to run

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

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