Package ‘MachineShop’

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Author Brian J Smith [aut, cre]
Maintainer Brian J Smith <brian-j-smith@uiowa.edu>
Description Meta-package for statistical and machine learning with a unified interface for model fitting, prediction, performance assessment, and presentation of results. Approaches for model fitting and prediction of numerical, categorical, or censored time-to-event outcomes include traditional regression models, regularization methods, tree-based methods, support vector machines, neural networks, ensembles, data preprocessing, filtering, and model tuning and selection. Performance metrics are provided for model assessment and can be estimated with independent test sets, split sampling, cross-validation, or bootstrap resampling. Resample estimation can be executed in parallel for faster processing and nested in cases of model tuning and selection. Modeling results can be summarized with descriptive statistics; calibration curves; variable importance; partial dependence plots; confusion matrices; and ROC, lift, and other performance curves.
Depends R (>= 4.0.0)
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         'ML_BARTMachineModel.R' 'ML_BARTModel.R' 'ML_BlackBoostModel.R'
         'ML_C50Model.R' 'ML_CForestModel.R' 'ML_CoxModel.R'
         'ML_EarthModel.R' 'ML_FDAModel.R' 'ML_GAMBoostModel.R'
         'ML_GBMModel.R' 'ML_GLMBoostModel.R' 'ML_GLMModel.R'
         'ML_GLMNetModel.R' 'ML_KNNModel.R' 'ML_LARSModel.R'
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         'ML_POLRModel.R' 'ML_QDAModel.R' 'ML_RFSCModel.R'
         'ML_RPartModel.R' 'ML_RandomForestModel.R' 'ML_RangerModel.R'
         'ML_SVMModel.R' 'ML_StackedModel.R' 'ML_SuperModel.R'
         'ML_SurvRegModel.R' 'ML_TreeModel.R' 'ML_XGBModel.R'
         'MachineShop-package.R' 'ModelFrame.R' 'ModelRecipe.R'
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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.

**Details**

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

Training:

- `fit` Model fitting
- `resample` Resample estimation of model performance

Tuning Grids:

- `expand_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` Model calibration
- `confusion` Confusion matrix
- `dependence` Partial dependence
- `diff` Model performance differences
Methods for resample estimation include

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

Graphical and tabular summaries of modeling results can be obtained with

- `plot`
- `print`
- `summary`

Further information on package features is available with

- **metricinfo** Performance metric information
- **modelinfo** Model information
- **settings** Global settings

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

**Author(s)**

**Maintainer:** Brian J Smith <brian-j-smith@uiowa.edu>

**See Also**

Useful links:

- [https://brian-j-smith.github.io/MachineShop/](https://brian-j-smith.github.io/MachineShop/)
**AdaBagModel**

Bagging with Classification Trees

**Description**

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

**Usage**

```r
 AdaBagModel(
   mfinal = 100,
   minsplit = 20,
   minbucket = round(minsplit/3),
   cp = 0.01,
   maxcompete = 4,
   maxsurrogate = 5,
   usesurrogate = 2,
   xval = 10,
   surrogatetyle = 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.
- **cp**: complexity parameter.
- **maxcompete**: number of competitor splits retained in the output.
- **maxsurrogate**: number of surrogate splits retained in the output.
- **usesurrogate**: how to use surrogates in the splitting process.
- **xval**: number of cross-validations.
- **surrogatetyle**: 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.
AdaBoostModel

Value

MLModel class object.

See Also

bagging, fit, resample

Examples

## Requires prior installation of suggested package adabag to run

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

---

### AdaBoostModel

**Boosting with Classification Trees**

Description

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

Usage

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

Arguments

- `boos` if TRUE, then bootstrap samples are drawn from the training set using the observation weights at each iteration. If FALSE, then all observations are used with their weights.
- `mfinal` number of iterations for which boosting is run.
coeflearn learning algorithm.
minsplits minimum number of observations that must exist in a node in order for a split to be attempted.
minbucket minimum number of observations in any terminal node.

cp complexity parameter.
maxcompete number of competitor splits retained in the output.
maxsurrogate number of surrogate splits retained in the output.
usesurrogate how to use surrogates in the splitting process.
xval number of cross-validations.
surrogatestyle controls the selection of a best surrogate.
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))
Description

Function to coerce an object to MLModel.

Usage

```r
as.MLModel(x, ...)
```

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

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

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

Arguments

- `x` : model fit result, modeled input, or model specification from the `parsnip` package.
- `...` : 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.
BARTMachineModel

Usage

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

Arguments

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

details

Response types: binary factor, numeric

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

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

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

Value

MLModel class object.

See Also

bartMachine, fit, resample

Examples

```r
## Requires prior installation of suggested package bartMachine to run

model_fit <- fit(sale_amount ~ ., data = ICHomes, model = BARTMachineModel)
varimp(model_fit, method = "model", type = "splits", num_replicates = 20,
       scale = FALSE)
```

---

**BARTModel**  
*Bayesian Additive Regression Trees Model*

**Description**

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

**Usage**

```r
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(),
nmtree = integer(),
umcut = 100,
ndpost = 1000,
nskip = integer(),
keepevery = integer(),
printevery = 1000
)

Arguments

K if provided, then coarsen the times of survival responses per the quantiles $1/K, 2/K, \ldots, K/K$ to reduce computational burden.

sparse logical indicating whether to perform variable selection based on a sparse Dirichlet 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: $0.5 <= a <= 1$ 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.
BlackBoostModel

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

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

BlackBoostModel  

*Gradient Boosting with Regression Trees*

Description

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

Usage

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

- **family**: optional `Family` object. Set automatically according to the class type of the response variable.
- **mstop**: number of initial boosting iterations.
- **nu**: step size or shrinkage parameter between 0 and 1.
- **risk**: method to use in computing the empirical risk for each boosting iteration.
- **stopintern**: logical indicating 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

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

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

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

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

**Usage**

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

**Arguments**

- **trials**: integer number of boosting iterations.
- **rules**: logical indicating whether to decompose the tree into a rule-based model.
- **subset**: logical indicating whether the model should evaluate groups of discrete predictors 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

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

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

---

### Calibration

**Model Calibration**

Calculate calibration estimates from observed and predicted responses.

Usage

```r
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 responses.

y  predicted responses if not contained in x.

weights  numeric vector of non-negative case weights for the observed x responses [default: equal weights].

breaks  value defining the response variable bins within which to calculate observed mean values. May be specified as a number of bins, a vector of breakpoints, or NULL to fit smooth curves with splines for predicted survival probabilities and with loess for others.

span  numeric parameter controlling the degree of loess smoothing.

distr  character string specifying a distribution with which to estimate the observed survival mean. Possible values are "empirical" for the Kaplan-Meier estimator, "exponential", "extreme", "gaussian", "loggaussian", "logistic", "loglogistic", "lognormal", "rayleigh", "t", or "weibull". Defaults to the distribution that was used in predicting mean survival times.

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)

control <- CVControl() %>% set_predict(times = c(90, 180, 360))
res <- resample(Surv(time, status) ~ ., data = veteran, model = GBMModel, 
               control = control)

cal <- calibration(res)
plot(cal)
case_weights

Extract Case Weights

Description

Extract the case weights from an object.

Usage

case_weights(object, newdata = NULL)

Arguments

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

Examples

## Training and test sets
inds <- sample(nrow(ICHomes), nrow(ICHomes) * 2 / 3)
trainset <- ICHomes[inds, ]
testset <- ICHomes[-inds, ]

## ModelFrame case weights
trainmf <- ModelFrame(sale_amount ~ . - built, data = trainset, weights = built)
testmf <- ModelFrame(formula(trainmf), data = testset, weights = built)
mf_fit <- fit(trainmf, model = GLMModel)
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)
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**

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

**Arguments**

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

**Details**

**Response types:** factor, numeric, Surv

**Automatic tuning of grid parameter:** `mtry`

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

**Value**

MLModel class object.
combine

See Also
cforest, fit, resample

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

combine

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

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

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

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

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

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

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

## 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**

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

`ConfusionMatrix(data = NA, ordered = FALSE)`

**Arguments**

- **x**  
  factor of observed responses or resample result containing observed and predicted responses.

- **y**  
  predicted responses if not contained in x.

- **weights**  
  numeric vector of non-negative case weights for the observed x responses [default: equal weights].

- **cutoff**  
  numeric (0, 1) threshold above which binary factor probabilities are classified as events and below which survival probabilities are classified. If NULL, then factor responses are summed directly over predicted class probabilities, whereas a default cutoff of 0.5 is used for survival probabilities. Class probability summations and survival will appear as decimal numbers that can be interpreted as expected counts.

- **na.rm**  
  logical indicating whether to remove observed or predicted responses that are NA when calculating metrics.

- **...**  
  arguments passed to other methods.

- **data**  
  square matrix, or object that can be converted to one, of cross-classified predicted and observed values in the rows and columns, respectively.

- **ordered**  
  logical indicating whether the confusion matrix row and columns should be regarded as ordered.
CoxModel

Value

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

See Also

c.plot, summary

Examples

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

CoxModel

Proportional Hazards Regression Model

Description

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

Usage

```r
CoxModel(ties = c("efron", "breslow", "exact"), ...)
```  

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

Arguments

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

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; \( k = .(\log(\text{nobs})) \) 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 [default: exp(1)]. Transformed p-values are automatically scaled in the calculation of variable importance to range from 0 to 100. To obtain unscaled importance values, set scale = FALSE.

#' @return

MLModel class object.

See Also

coxph, coxph.control, stepAIC, fit, resample

Examples

library(survival)

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

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"),

dependence

distr = character(),
method = character(),
stats = MachineShop::settings("stats.PartialDependence"),
na.rm = TRUE
)

Arguments

object      model fit result.
data        data frame containing all predictor variables. If not specified, the training data
             will be used by default.
select      expression indicating predictor variables for which to compute partial 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

```r
#gbm_fit <- fit(Species ~ ., data = iris, model = GBMModel)
(gbm_fit <- dependence(gbm_fit, select = c(Petal.Length, Petal.Width)))
plot(pd)
```
### Deprecated Functions

**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()`.

---

### Model Performance Differences

**Description**

Pairwise model differences in resampled performance metrics.

**Usage**

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

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

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

**Arguments**

- `x` model performance or resample result.
- `...` arguments passed to other methods.
**DiscreteVariate**

**Value**

PerformanceDiff class object that inherits from Performance.

**See Also**

t.test, plot, summary

**Examples**

```r
## Requires prior installation of suggested package gbm to run
## Survival response example
library(survival)
fo <- Surv(time, status) ~ .
control <- CVControl()

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

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

---

**DiscreteVariate Constructors**

**Description**

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

**Usage**

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

- **x**: numeric vector.
- **size**: number or numeric vector of binomial trials.
- **min, max**: minimum and maximum bounds for discrete numbers.

Value

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

See Also

role_binom

Examples

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

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.
expand_model

nfolds number of cross-validation folds.
ncross number of cross-validations if nfolds > 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

```r
## 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)
```

---

**expand_model**

**Model Expansion Over Tuning Parameters**

Description

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

Usage

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

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, ...)

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

Examples

```r
## Requires prior installation of suggested package gbm to run
data(Boston, package = "MASS")

models <- expand_model(GBMModel, n.trees = c(50, 100), interaction.depth = 1:2)

fit(medv ~ ., data = Boston, model = SelectedModel(models))
```
expand_modelgrid

## 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.

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

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

object  
  model specification.

### Details

The expand_modelgrid function enables manual extraction and viewing of grids created automati-

cally 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

### See Also

TunedModel
Examples

```r
expand_modelgrid(TunedModel(GBMModel, grid = 5))

expand_modelgrid(TunedModel(GLMNetModel, grid = c(alpha = 5, lambda = 10)),
                 sale_amount ~ ., data = ICHomes)

gbm_grid <- ParameterGrid(
  n.trees = dials::trees(),
  interaction.depth = dials::tree_depth(),
  size = 5
)
expand_modelgrid(TunedModel(GBMModel, grid = gbm_grid))

rf_grid <- ParameterGrid(
  mtry = dials::mtry(),
  nodesize = dials::max_nodes(),
  size = c(3, 5)
)
expand_modelgrid(TunedModel(RandomForestModel, grid = rf_grid),
                 sale_amount ~ ., data = ICHomes)
```

---

**expand_params**  
*Model Parameters Expansion*

**Description**

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

**Usage**

```r
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

```r
## 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

**Recipe Step Parameters Expansion**

**Description**

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

**Usage**

```r
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

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

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

expand_steps(
  corr = list(threshold = c(0.8, 0.9),
              method = c("pearson", "spearman")),
  pca = list(num_comp = 1:3)
)
```

extract

Extract Elements of an Object

Description

Operators acting on data structures to extract elements.

Usage

```r
## 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

**x**  
object from which to extract elements.

**i, j, ...**  
indices specifying elements to extract.

**drop**  
logical indicating that the result be returned as an object coerced to the lowest dimension possible if TRUE or with the original dimensions and class otherwise.

---

**FDAModel**  
*Flexible and Penalized Discriminant Analysis Models*

---

**Description**

Performs flexible discriminant analysis.

**Usage**

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

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

### Arguments

**theta**  
optional matrix of class scores, typically with number of columns less than one minus the number of classes.
dimension dimension of the discriminant subspace, less than the number of classes, to use for prediction.

eps numeric threshold for small singular values for excluding discriminant variables.

method regression function used in optimal scaling. The default of linear regression is provided by polyreg from the mda package. For penalized discriminant analysis, gen.ridge is appropriate. Other possibilities are mars for multivariate adaptive regression splines and bruto for adaptive backfitting of additive splines. Use the . operator to quote specified functions.

... additional arguments to 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)
**Description**

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

**Usage**

```r
fitted(...)
```

## S3 method for class 'formula'
```r
fitted(formula, data, model, ...)
```

## S3 method for class 'matrix'
```r
fitted(x, y, model, ...)
```

## S3 method for class 'ModelFrame'
```r
fitted(input, model = NULL, ...)
```

## S3 method for class 'recipe'
```r
fitted(input, model = NULL, ...)
```

## S3 method for class 'ModelSpecification'
```r
fitted(object, ...)
```

## S3 method for class 'MLModel'
```r
fitted(model, ...)
```

## S3 method for class 'MLModelFunction'
```r
fitted(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 fitted method is positional and, as such, must be given first in calls to them.

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

model model function, function name, or object; or another object that can be coerced to a model. A model can be given first followed by any of the variable specifications, and the argument can be omitted altogether in the case of modeled inputs.

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

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

object model specification.
Details

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

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

Value

MLModelFit class object.

See Also

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

Examples

```r
## 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)
```

---

**GAMBoostModel**

*Gradient Boosting with Additive Models*

**Description**

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

**Usage**

```r
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**: global 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 indicating 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

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

Examples

```r
## 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
)

Arguments

distribution  optional character string specifying the name of the distribution to use or list with a component name specifying the distribution and any additional parameters needed. Set automatically according to the class type of the response variable.

n.trees  total number of trees to fit.

interaction.depth  maximum depth of variable interactions.

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

shrinkage  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
GLMBoostModel

Examples

```r
## 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

```r
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 indicating 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.
GLMModel

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

Generalized Linear Model

Description

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

Usage

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

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

Arguments

family  optional error distribution and link function to be used in the model. Set automatically according to the class type of the response variable.

quasi   logical indicator for over-dispersion of binomial and Poisson families; i.e., dispersion parameters not fixed at one.
GLMNetModel

... 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 [default: 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)
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")
)

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 regularization 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.
**ICHomes**

**See Also**

`glmnet`, `fit`, `resample`

**Examples**

```r
## Requires prior installation of suggested package glmnet to run

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

---

**ICHomes**

**Iowa City Home Sales Dataset**

**Description**

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

**Usage**

ICHomes

**Format**

A data frame with 753 observations of 17 variables:

- `sale_amount` sale amount in dollars.
- `sale_year` sale year.
- `sale_month` sale month.
- `built` year in which the home was built.
- `style` home style (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.
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.

<table>
<thead>
<tr>
<th>Description</th>
<th></th>
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</thead>
<tbody>
<tr>
<td>Model inputs</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>inputs</th>
<th>Model Inputs</th>
</tr>
</thead>
<tbody>
<tr>
<td>formula</td>
<td>Traditional model formula</td>
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<tr>
<td>matrix</td>
<td>Design matrix of predictors</td>
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<tr>
<td>ModelFrame</td>
<td>Model frame</td>
</tr>
<tr>
<td>ModelSpecification</td>
<td>Model specification</td>
</tr>
<tr>
<td>recipe</td>
<td>Preprocessing recipe roles and steps</td>
</tr>
</tbody>
</table>

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

**Response Functions**

- 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.

<table>
<thead>
<tr>
<th>inputs</th>
<th>Model Specification</th>
<th>ModeledInput</th>
<th>SelectedInput</th>
<th>TunedInput</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>Model specification</td>
<td>Input with a prespecified model</td>
<td>Input selection from a candidate set</td>
<td>Input tuning over a parameter grid</td>
</tr>
</tbody>
</table>

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**: number of neighbors 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

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

## LARSModel

Least Angle Regression, Lasso and Infinitesimal Forward Stagewise Models

### Description

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

### Usage

```r
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 process.
- **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 indicating 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)
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.

Value

MLModel class object.

See Also

`lda, predict.lda, fit, resample`

Examples

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

---

**lift**  
Model Lift Curves

Description

Calculate lift curves from observed and predicted responses.

Usage

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

Arguments

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

Value

LiftCurve class object that inherits from PerformanceCurve.
LMMModel

See Also
c, plot, summary

Examples

```r
## 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)
```

---

**LMMModel**

*Linear Models*

**Description**

Fits linear models.

**Usage**

LMMModel()

**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 [default: `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**

```r
fit(sale_amount ~ ., data = ICHomes, model = LMMModel)
```
**MDA Model**

**Mixture Discriminant Analysis Model**

**Description**

Performs mixture discriminant analysis.

**Usage**

```r
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 shrinkage is performed.
- `tot.df`: specification of the total degrees of freedom as an alternative to `sub.df`.
- `dimension`: dimension of the discriminant subspace to use for prediction.
- `eps`: numeric threshold for automatically truncating the dimension.
- `iter`: limit on the total number of iterations.
- `method`: regression function used in optimal scaling. The default of linear regression is provided by `polyreg` from the `mda` package. For penalized mixture discriminant models, `gen.ridge` is appropriate. Other possibilities are `mars` for multivariate adaptive regression splines and `bruto` for adaptive backfitting of additive splines. Use the `.` operator to quote specified functions.
- `trace`: logical indicating whether iteration information is printed.
- `...`: additional arguments to `mda.start` and `method`.

**Details**

- **Response types**: factor
- **Automatic tuning of grid 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.
### metricinfo

**Value**

MLModel class object.

**See Also**

mda, predict.mda.fit, resample

**Examples**

```r
## Requires prior installation of suggested package mda to run

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

---

**Description**

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

**Usage**

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

**Arguments**

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

**Value**

List of named metric elements each containing the following components:

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

## All metrics
metricinfo()

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

## Metric-specific information
metricinfo(auc)

---

<table>
<thead>
<tr>
<th>metrics</th>
<th>Performance Metrics</th>
</tr>
</thead>
</table>

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,
  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(
metrics

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, ...)

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, ...)

roc_index(
    observed,
    predicted = NULL,
    weights = NULL,
    cutoff = MachineShop::settings("cutoff"),
    fun = function(sensitivity, specificity) (sensitivity + specificity)/2,
    ...
)

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

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

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

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

weighted_kappa2(observed, predicted = NULL, weights = NULL, power = 1, ...)
gini(observed, predicted = NULL, weights = NULL, ...)
mae(observed, predicted = NULL, weights = NULL, ...)
mse(observed, predicted = NULL, weights = NULL, ...)
msle(observed, predicted = NULL, weights = NULL, ...)
r2(observed, predicted = NULL, weights = NULL, 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 containing 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.
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.
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.

See Also
metricinfo, performance
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)
)

OOBControl(
samples = 25,
weights = TRUE,
seed = sample(.Machine$integer.max, 1)
)

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

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

**Arguments**

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

**Details**

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


CVControl constructs an MLControl object for repeated K-fold cross-validation (Kohavi 1995). In this procedure, the full data set is repeatedly partitioned into K-folds. Within a partitioning, prediction is performed on each of the K folds with models fit on all remaining folds.
CVOptimismControl constructs an MLControl object for optimism-corrected cross-validation resampling (Davison and Hinkley 1997, eq. 6.48).

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

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

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

Value

Object that inherits from the MLControl class.

References


See Also

*set_monitor, set_predict, set_strata, resample, SelectedInput, SelectedModel, TunedInput, TunedModel*

Examples

```r
## 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 Class Constructor**

**Description**

Create a performance metric for use with the *MachineShop* package.

**Usage**

```r
MLMetric(object, name = "MLMetric", label = name, maximize = TRUE)
MLMetric(object) <- value
```

**Arguments**

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

**Value**

`MLMetric` class object.

**See Also**

`metrics`
MLModel

MLModel Class Constructor

Description

Create a model for use with the MachineShop package.

Usage

MLModel(
  name = "MLModel",
  label = name,
  packages = character(),
  response_types = character(),
  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,
  ...
)

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".

Examples

f2_score <- function(observed, predicted, ...) {
  f_score(observed, predicted, beta = 2, ...)
}

MLMetric(f2_score) <- list(name = "f2_score",
                           label = "F Score (beta = 2)",
                           maximize = TRUE)
weights logical value or vector of the same length as response_types indicating whether case weights are supported for the responses.

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

params list of user-specified model parameters to be passed to the fit function.

gridinfo tibble of information for construction of tuning grids consisting of a character column param with the names of parameters in the grid, a list column get_values with functions to generate grid points for the corresponding parameters, and an optional logical column default indicating which parameters to include by default in regular grids. Values functions may optionally include arguments n and data for the number of grid points to generate and a ModelFrame of the model fit data and formula, respectively; and must include an ellipsis (...).

fit model fitting function whose arguments are a formula, a ModelFrame named data, case weights, and an ellipsis.

predict model prediction function whose arguments are the object returned by fit, a ModelFrame named newdata of predictor variables, optional vector of times at which to predict survival, and an ellipsis.

varimp variable importance function whose arguments are the object returned by fit, optional arguments passed from calls to varimp, and an ellipsis.

... arguments passed to other methods.

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 vector or column matrix of probabilities for the second level of binary factors or a matrix whose columns contain the probabilities for factors with more than two levels.

matrix matrix of predicted responses.

numeric vector or column matrix of predicted responses.

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

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

Value

MLModel class object.

See Also

models, fit, resample
Examples

## Logistic regression model
LogisticModel <- MLModel(
  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)
summary(res)

ModelFrame

ModelFrame Class

Description

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

Usage

ModelFrame(...)

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

## S3 method for class 'matrix'
ModelFrame(
  x,
  ...
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.

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

offsets numeric vector, matrix, or data frame of values to be added with a fixed coefficient of 1 to linear predictors in compatible regression models.

Value

ModelFrame class object that inherits from data.frame.

See Also

fit, resample, response, SelectedInput

Examples

## Requires prior installation of suggested package gbm to run

mf <- ModelFrame(ncases / (ncases + ncontrols) ~ agegp + tobgp + alcgp,  
  data = esoph, weights = ncases + ncontrols)  
gbm_fit <- fit(mf, model = GBMModel)  
varimp(gbm_fit)
Display Model Information

Description
Display information about models supplied by the MachineShop package.

Usage
modelinfo(...)

Arguments

... model functions, function names, or objects; observed responses for which to
display information. If none are specified, information is returned on all avail-
able 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 func-
tion.
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
modelinfo(GBMModel)
### 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.

<table>
<thead>
<tr>
<th>Function</th>
<th>Categorical</th>
<th>Continuous</th>
<th>Survival</th>
</tr>
</thead>
<tbody>
<tr>
<td>AdaBagModel</td>
<td>f</td>
<td></td>
<td></td>
</tr>
<tr>
<td>AdaBoostModel</td>
<td>f</td>
<td></td>
<td></td>
</tr>
<tr>
<td>BARTModel</td>
<td>f</td>
<td>n</td>
<td>S</td>
</tr>
<tr>
<td>BARTMachineModel</td>
<td>b</td>
<td>n</td>
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</tr>
<tr>
<td>BlackBoostModel</td>
<td>b</td>
<td>n</td>
<td>S</td>
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<tr>
<td>C50Model</td>
<td>f</td>
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<tr>
<td>CForestModel</td>
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<td>n</td>
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<tr>
<td>CoxModel</td>
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<td>S</td>
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<tr>
<td>CoxStepAICModel</td>
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<td></td>
<td>S</td>
</tr>
<tr>
<td>EarthModel</td>
<td>f</td>
<td>n</td>
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</tr>
<tr>
<td>FDAModel</td>
<td>f</td>
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<tr>
<td>GAMBoostModel</td>
<td>b</td>
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<tr>
<td>GBMModel</td>
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<tr>
<td>GLMBoostModel</td>
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<tr>
<td>GLMMModel</td>
<td>f</td>
<td>m,n</td>
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<tr>
<td>GLMStepAICModel</td>
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<tr>
<td>GLMNetModel</td>
<td>f</td>
<td>m,n</td>
<td>S</td>
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<tr>
<td>KNNModel</td>
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<td>n</td>
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<tr>
<td>LARSMModel</td>
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<td>n</td>
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<tr>
<td>LDAModel</td>
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<tr>
<td>LMMModel</td>
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<tr>
<td>MDAModel</td>
<td>f</td>
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</tr>
<tr>
<td>NaiveBayesModel</td>
<td>f</td>
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<tr>
<td>NNetModel</td>
<td>f</td>
<td></td>
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<tr>
<td>ParsnipModel</td>
<td>f</td>
<td>m,n</td>
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<tr>
<td>PDAModel</td>
<td>f</td>
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<tr>
<td>PLSModel</td>
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<tr>
<td>POLRModel</td>
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<tr>
<td>QDAModel</td>
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<tr>
<td>RandomForestModel</td>
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<tr>
<td>RangerModel</td>
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<tr>
<td>RFSRCModel</td>
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<tr>
<td>RFSRCFastModel</td>
<td>f</td>
<td>m,n</td>
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<tr>
<td>RPartModel</td>
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<tr>
<td>SurvRegModel</td>
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<tr>
<td>SurvRegStepAICModel</td>
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<td>S</td>
</tr>
<tr>
<td>SVMModel</td>
<td>f</td>
<td>n</td>
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</tr>
<tr>
<td>SVMANOVAModel</td>
<td>f</td>
<td>n</td>
<td></td>
</tr>
</tbody>
</table>
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
- StackedModel
- SuperModel
- SelectedModel
- TunedModel

See Also
modelinfo, fit, resample

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

Usage
ModelSpecification(...)
```r
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. Specification of a resampling method results in the following characteristics.
    1. Tuning of input and model objects is performed simultaneously over a global grid of their parameter values.
    2. The specification’s `control` method and training parameters below override those of any included `TunedInput` or `TunedModel`.
    3. `ModeledInput`, `SelectedInput`, and `SelectedModel` objects are not allowed in the `input` or `model` arguments.

Alternatively, a value of `NULL` may be specified so that any package input or model object is allowed, object-specific control structures and training parameters are used for selection and tuning, and objects are trained sequentially with nested resampling rather than simultaneously with a global grid.

- **metrics**
  - `metric` function, function name, or vector of these with which to calculate performance. If not specified, default metrics defined in the `performance` functions are used. Model selection is based on the first calculated metric.

- **cutoff**
  - argument passed to the `metrics` functions.

- **stat**
  - function or character string naming a function to compute a summary statistic on resampled metric values for model tuning.
NaiveBayesModel

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

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

Value

ModelSpecification class object.

See Also

fit, resample, set_monitor, set_optim

Examples

## Requires prior installation of suggested package gbm to run

```r
modelspec <- ModelSpecification(
  sale_amount ~ ., data = ICHomes, model = GBMModel
)
fit(modelspec)
```

---

NaiveBayesModel  Naive Bayes Classifier Model

Description

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

Usage

NaiveBayesModel(laplace = 0)

Arguments

laplace positive numeric controlling Laplace smoothing.

Details

Response types: factor

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

Value

MLModel class object.
### NNetModel

**Neural Network Model**

*Description*

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

*Usage*

```r
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 fitting.
- **censored**: a variant on softmax, in which non-zero targets mean possible classes.

*See Also*

naiveBayes, fit, resample

*Examples*

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

**skip**
switch to add skip-layer connections from input to output.

**rang**
Initial random weights on \([-\text{rang}, \text{rang}]\).

**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 \(1 - \text{reltol}\).

**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**

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

---

### ParameterGrid

**Tuning Parameters Grid**

**Description**

Defines a tuning grid from a set of parameters.

**Usage**

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

Value

ParameterGrid class object that inherits from parameters and TuningGrid.

See Also

TunedModel

Examples

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

Description

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

Usage

ParsnipModel(object, ...)

Arguments

object model specification from the parsnip package.
...

tuning parameters with which to update object.

Value

ParsnipModel class object that inherits from MLModel.
See Also

as.MLModel, fit, resample

Examples

```r
## 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_fit <- fit(sale_amount ~ ., data = ICHomes, model = model)
predict(model_fit)
```

---

### performance

#### Model Performance Metrics

**Description**

Compute measures of model performance.

**Usage**

```r
performance(x, ...)
```

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

```r
## S3 method for class 'factor'
performance(
  x,
  y,
  weights = NULL,
  metrics = MachineShop::settings("metrics.factor"),
  cutoff = MachineShop::settings("cutoff"),
  na.rm = TRUE,
  ...
)```
## S3 method for class 'matrix'
performance(
  x,
  y,
  weights = NULL,
  metrics = MachineShop::settings("metrics.matrix"),
  na.rm = TRUE,
  ...
)

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

## S3 method for class 'Surv'
performance(
  x,
  y,
  weights = NULL,
  metrics = MachineShop::settings("metrics.Surv"),
  cutoff = MachineShop::settings("cutoff"),
  na.rm = TRUE,
  ...
)

## S3 method for class 'ConfusionList'
performance(x, ...)

## S3 method for class 'ConfusionMatrix'
performance(x, metrics = MachineShop::settings("metrics.ConfusionMatrix"), ...)

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

## S3 method for class 'Resample'
performance(x, ...)

## S3 method for class 'TrainingStep'
performance(x, ...)

Arguments

- **x**: observed responses; or confusion, trained model fit, resample, or rfe result.
- **y**: predicted responses if not contained in x.
- **weights**: numeric vector of non-negative case weights for the observed x responses [default: equal weights].
- **metrics**: metric function, function name, or vector of these with which to calculate performance.
- **na.rm**: logical indicating whether to remove observed or predicted responses that are NA when calculating metrics.
- **cutoff**: numeric (0, 1) threshold above which binary factor probabilities are classified as events and below which survival probabilities are classified.

See Also

plot, summary

Examples

```r
## 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)
```
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(
  x,
  y,
  weights = NULL,
  metrics = c(MachineShop::tpr, MachineShop::fpr),
  na.rm = TRUE,
  ...
)
```

### S3 method for class `Resample`
```
performance_curve(
  x,
  metrics = c(MachineShop::tpr, MachineShop::fpr),
  na.rm = TRUE,
  ...
)
```

Arguments

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

Value

PerformanceCurve class object that inherits from `data.frame`.

See Also

- `auc`, `c.plot`, `summary`
Examples

```r
## 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)
```

---

**Description**

Plot measures of model performance and predictor variable importance.

**Usage**

```r
## 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(
  x,
  find = numeric(),
  diagonal = TRUE,
  stat = MachineShop::settings("stat.Curve"),
  ...
)

## S3 method for class 'MLModel'
plot(
  x,
  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(
  x,
  metrics = NULL,
  stat = MachineShop::settings("stat.Resample"),
  type = c("boxplot", "density", "errorbar", "violin"),
  ...
)

### S3 method for class 'PerformanceCurve'
plot(
  x,
  type = c("tradeoffs", "cutoffs"),
  diagonal = FALSE,
  stat = MachineShop::settings("stat.Curve"),
  ...
)

### S3 method for class 'Resample'
plot(
  x,
  metrics = NULL,
  stat = MachineShop::settings("stat.Resample"),
  type = c("boxplot", "density", "errorbar", "violin"),
  ...
)

### S3 method for class 'TrainingStep'
plot(
  x,
  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

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

## Factor response example

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

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

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

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

Partial Least Squares Model

Description

Function to perform partial least squares regression.

Usage

PLSModel(ncomp = 1, scale = FALSE)

Arguments

ncomp number of components to include in the model.
scale logical indicating whether to scale the predictors by the sample standard deviation.

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

Ordered Logistic or Probit Regression Model

Description

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

Usage

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

Arguments

method

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

Details

Response types: ordered

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

In calls to varimp for POLRModel, numeric argument base may be specified for the (negative) logarithmic transformation of p-values [default: 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

data(Boston, package = "MASS")

df <- within(Boston,
               medv <- cut(medv,
                            breaks = c(0, 10, 15, 20, 25, 50),
                            ordered = TRUE))

fit(medv ~ ., data = df, model = POLRModel)
predict

Model Prediction

Description
Predict outcomes with a fitted model.

Usage

```r
## 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(),
  ...
)
```

Arguments

- `object` model fit result.
- `newdata` optional data frame with which to obtain predictions. If not specified, the training data will be used by default.
- `times` numeric vector of follow-up times at which to predict survival events/probabilities or NULL for predicted survival means.
- `type` specifies prediction on the original outcome ("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 to model-specific prediction functions.

See Also

- `confusion`
- `performance`
- `metrics`
## Requires prior installation of suggested package gbm to run

## Survival response example

```r
library(survival)

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

---

### Description

Print methods for objects defined in the `MachineShop` package.

### Usage

```r
## 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 'MLMetric'
print(x, ...)

## S3 method for class 'MLModel'
print(x, n = MachineShop::settings("print_max"), id = FALSE, ...)

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

## S3 method for class 'ModelFrame'
print(x, n = MachineShop::settings("print_max"), id = FALSE, data = TRUE, ...)
```
## S3 method for class 'ModelRecipe'
print(x, n = MachineShop::settings("print_max"), id = FALSE, data = TRUE, ...)

## S3 method for class 'ModelSpecification'
print(x, n = MachineShop::settings("print_max"), id = FALSE, ...)

## S3 method for class 'Performance'
print(x, n = MachineShop::settings("print_max"), ...)

## S3 method for class 'PerformanceCurve'
print(x, n = MachineShop::settings("print_max"), ...)

## S3 method for class 'RecipeGrid'
print(x, n = MachineShop::settings("print_max"), ...)

## S3 method for class 'Resample'
print(x, n = MachineShop::settings("print_max"), ...)

## S3 method for class 'SurvMatrix'
print(x, n = MachineShop::settings("print_max"), ...)

## S3 method for class 'SurvTimes'
print(x, n = MachineShop::settings("print_max"), ...)

## S3 method for class 'TrainingStep'
print(x, n = MachineShop::settings("print_max"), ...)

## S3 method for class 'VariableImportance'
print(x, n = MachineShop::settings("print_max"), ...)

### 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.

- **level**
  - 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.

- **id**
  - logical indicating whether to show object identifiers.

- **data**
  - logical indicating whether to show model data.

---

**QDAModel**

**Quadratic Discriminant Analysis Model**
Description

Performs quadratic discriminant analysis.

Usage

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

Arguments

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

Details

Response types: factor

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

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

Default 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  

**Quote Operator**

Description

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

Usage

\[ .(\text{expr}) \]

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

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

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
Examples

```r
## 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

```r
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.
- **min.node.size**: minimum node size.
- **replace**: logical indicating whether to sample with replacement.
- **sample.fraction**: fraction of observations to sample.
- **splitrule**: splitting rule.
num.random.splits

number of random splits to consider for each candidate splitting variable in the "extratrees" rule.

alpha

significance threshold to allow splitting in the "maxstat" rule.

minprop

lower quantile of covariate distribution to be considered for splitting in the "maxstat" rule.

split.select.weights

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

always.split.variables

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

respect.unordered.factors

handling of unordered factor covariates.

scale.permutation.importance

scale permutation importance by standard error.

verbose

show computation status and estimated runtime.

Details

Response types: factor, numeric, Surv

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

* 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

Set Recipe Roles

Description

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

Usage

role_binom(recipe, x, size)

role_case(recipe, 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 performance.
- **weight**: numeric variable of case weights for model fitting.
- **replace**: logical indicating whether to replace existing roles.
- **offset**: numeric variable to be added to a linear predictor, such as in a generalized linear model, with known coefficient 1 rather than an estimated coefficient.
- **time, event**: numeric follow up time and 0-1 numeric or logical event indicator for specification of a Surv outcome. If the event indicator is omitted, all cases are assumed to have events.

Value

An updated recipe object.

See Also

- recipe
Examples

```r
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)
```

---

**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**

```r
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, ...)
```
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 specifications, and the argument can be omitted altogether in the case of modeled inputs.

x, y 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()
response <- 

rm_list <- c(GBM1 = gbm_res1, GBM2 = gbm_res2, GBM3 = gbm_res3)
summary(res)
plot(res)

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; otherwise, object is used.
Examples

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

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

---

**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**

```r
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,
  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 specifications, and the argument can be omitted altogether in the case of modeled inputs.

- **x, y**  
  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.

- **props**  
  numeric vector of the proportions of most important predictor variables to retain in fitted models or an integer number of equal spaced proportions to generate automatically; ignored if sizes are given.

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

- **random**  
  logical indicating whether to eliminate variables at random with probabilities proportional to their importance.

- **recompute**  
  logical indicating whether to recompute variable importance after eliminating each set of variables.

- **optimize**  
  character string specifying a search through all props to identify the globally optimal model ("global") or a search that stops after identifying the first locally optimal model ("local").

- **samples**  
  numeric vector or list giving the number of permutation samples for each of the rfe and varimp algorithms. One or both of the values may be specified as named arguments or in the order in which their defaults appear. Larger numbers of samples decrease variability in estimated model performances and variable importances at the expense of increased computation time. Samples are more expensive computationally for rfe than for varimp.

- **metrics**  
  metric function, function name, or vector of these with which to calculate performance. If not specified, default metrics defined in the performance functions are used.
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

```r
## 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")
```

## Fast Random Forest (SRC) Model

### Description

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

### Usage

```r
RFSRCModel(
  ntree = 1000,
  mtry = integer(),
  nodesize = integer(),
  nodedepth = integer(),
  splitrule = character(),
  nsplit = 10,
  block.size = integer(),
  samptype = c("swor", "swr"),
  membership = FALSE,
```
RFSRCModel

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 minimum size of terminal nodes.
nodedepth maximum depth to which a tree should be grown.
splitrule splitting rule (see rfsr).
snsplit 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.
membrane logical indicating whether to return terminal node membership.
sampsize function specifying the bootstrap size.
nimpute number of iterations of the missing data imputation algorithm.
ntime integer number of time points to constrain ensemble calculations for survival outcomes.
proximity whether and how to return proximity of cases as measured by the frequency of sharing the same terminal nodes.
distance whether and how to return distance between cases as measured by the ratio of the sum of edges from each case to the root node.
forest.wt whether and how to return the forest weight matrix.
xvar.wt vector of non-negative weights representing the probability of selecting a 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 completion.
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

```r
## 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)
```
RPartModel

Recursive Partitioning and Regression Tree Models

Description

Fit an \texttt{rpart} model.

Usage

\begin{verbatim}
RPartModel(
  minsplit = 20,
  minbucket = round(minsplit/3),
  cp = 0.01,
  maxcompete = 4,
  maxsurrogate = 5,
  usesurrogate = 2,
  xval = 10,
  surrogatestyle = 0,
  maxdepth = 30
)
\end{verbatim}

Arguments

- \texttt{minsplit}: minimum number of observations that must exist in a node in order for a split to be attempted.
- \texttt{minbucket}: minimum number of observations in any terminal node.
- \texttt{cp}: complexity parameter.
- \texttt{maxcompete}: number of competitor splits retained in the output.
- \texttt{maxsurrogate}: number of surrogate splits retained in the output.
- \texttt{usesurrogate}: how to use surrogates in the splitting process.
- \texttt{xval}: number of cross-validations.
- \texttt{surrogatestyle}: controls the selection of a best surrogate.
- \texttt{maxdepth}: maximum depth of any node of the final tree, with the root node counted as depth 0.

Details

- \textbf{Response types}: \texttt{factor}, \texttt{numeric}, \texttt{Surv}
- \textbf{Automatic tuning of grid parameter}: \texttt{cp}

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

Value

\texttt{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(
  ...,
  y,
  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"),
  ...)
SelectedInput

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 performance. If not specified, default metrics defined in the performance functions are used. Recipe selection is based on the first calculated metric.

cutoff argument passed to the metrics functions.

stat function or character string naming a function to compute a summary statistic on resampled metric values for recipe selection.

y 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

```r
## 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)
```

Description

Model selection from a candidate set.

Usage

```r
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 performance. If not specified, default metrics defined in the performance functions are used. Model selection is based on the first calculated metric.

cutoff argument passed to the metrics functions.

stat function or character string naming a function to compute a summary statistic on resampled metric values for model selection.

x list of models followed by arguments passed to their method function.

### Details

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

### Value

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

### See Also

fit, resample

### Examples

```r
## 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)
```
settings

MachineShop Settings

Description

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

Usage

settings(...)

Arguments

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

Value

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

Settings

ccontrol 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: \{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: \{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: \{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-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: \{Mean = "base::mean"\}].

stats.Resample function, function name, or vector of these with which to compute summary statistics on resampled performance metrics [default: \{Mean = "base::mean", Median = "stats::median", SD = "stats::sd", Min = "base::min", Max = "base::max"\}].

Examples

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

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

## View one setting
settings("control")

## View multiple settings
settings("control", "grid")
```
## Restore the previous settings

```r
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**

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

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

## S3 method for class 'ModelSpecification'
set_monitor(object, which = c("all", "control", "optim"), ...)
```

**Arguments**

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

**Value**

Argument object updated with the supplied parameters.

**See Also**

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

CVControl() %>% set_monitor(verbos = 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 = 2.576,
  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, ...)
set_optim

## 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(),
  ...
set_optim

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

kappa
upper confidence bound parameter ("ucb") to balance exploitation against exploration. It multiplies the predictive standard deviation added to the predictive mean in the acquisition function. The default value of 2.576 corresponds to the 99th percentile of a normal distribution. 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 package "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 function with the same number of rows as model evaluations will be included in a TrainingStep summary of optimization results; other types of return values will be ignored.

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

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

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

params list of optimization parameters as supplied to set_optim_method.

monitor list of the progress and verbose values.

label character descriptor for the optimization method.

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

Details

The optimization functions implement the following methods.

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

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

set_optim_grid exhaustive or random grid search.


set_optim_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


See Also

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

Examples

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

```r
set_predict

Resampling Prediction Control

Description

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

Usage

```r
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 resampling.
- **nunique**: number of unique values at or below which numeric data are stratified as categorical.
- **prop**: minimum proportion of data in each strata.
- **size**: minimum number of values in each strata.
- **...**: arguments passed to other methods.

Details

The arguments control resampling strata which are constructed from numeric proportions for `BinomialVariate`; original values for character, factor, logical, numeric, and ordered; first columns of values for `matrix`; and numeric times within event statuses for `Surv`. Stratification of survival data by event status only can be achieved by setting `breaks = 1`. Numeric values are stratified into quantile bins and categorical values into factor levels. The number of bins will be the largest integer less than or equal to `breaks` satisfying the `prop` and `size` control argument thresholds. Categorical levels below the thresholds will be pooled iteratively by reassigned 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.
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
**See Also**

*fit, resample*

**Examples**

```r
## 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)
```

**Description**

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

**Usage**

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

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

**step_kmedoids**


**See Also**

`kmeans`, `recipe`, `prep`, `bake`

**Examples**

```r
library(recipes)

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

pairs(kmeans_data, lower.panel = NULL)
tidy(kmeans_rec, number = 1)
tidy(kmeans_prep, number = 1)
```

---

**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**

```r
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 functions for the centering and scaling; not applied to selected variables.
- **method**: character string specifying one of the clustering methods provided by the `cluster` package. The `clara` (clustering large applications) method is an extension of `pam` (partitioning around medoids) designed to handle large datasets.
- **metric**: character string specifying the distance metric for calculating dissimilarities between observations as "euclidean", "manhattan", or "jaccard" (clara only).
- **optimize**: logical indicator or 0:5 integer level specifying optimization for the `pam` clustering method.
- **num_samp**: number of sub-datasets to sample for the `clara` clustering method.
- **samp_size**: number of cases to include in each sub-dataset.
- **replace**: logical indicating whether to replace the original variables.
- **prefix**: if the original variables are not replaced, the selected variables are added to the dataset with the character string prefix added to their names; otherwise, the original variable names are retained.
- **role**: analysis role that added step variables should be assigned. By default, they are designated as model predictors.
- **skip**: logical indicating whether to skip the step when the recipe is baked. While all operations are baked when `prep` is run, some operations may not be applicable to new data (e.g. processing outcome variables). Care should be taken when using `skip = TRUE` as it may affect the computations for subsequent operations.
- **id**: unique character string to identify the step.
- **x**: `step_kmedoids` object.
**Details**

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

**Value**

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

**References**


**See Also**

pam, clara, recipe, prep, bake

**Examples**

```r
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)
```

---

**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

```r
step_lincomp(
  recipe,
  ..., 
  transform,
  num_comp = 5,
  options = list(),
  center = TRUE,
  scale = TRUE,
  replace = TRUE,
  prefix = "LinComp",
  role = "predictor",
  skip = FALSE,
  id = recipes::rand_id("lincomp")
)
```

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

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

Arguments

- `recipe` recipe object to which the step will be added.
- `...` one or more selector functions to choose which variables will be used to compute the components. See `selections` for more details. These are not currently used by the tidy method.
- `transform` function whose first argument `x` is a matrix of variables with which to compute linear combinations and second argument `step` is the current step. The function should return a transformation matrix or `Matrix` of variable weights in its columns, or return a list with element `weights` containing the transformation matrix and possibly with other elements to be included as attributes in output from the tidy method.
- `num_comp` number of components to derive. The value of `num_comp` will be constrained to a minimum of 1 and maximum of the number of original variables when `prep` is run.
- `options` list of elements to be added to the step object for use in the `transform` function.
- `center, scale` logicals indicating whether to mean center and standard deviation scale the original variables prior to deriving components, or functions or names of functions for the centering and scaling.
- `replace` logical indicating whether to replace the original variables.
- `prefix` character string prefix added to a sequence of zero-padded integers to generate names for the resulting new variables.
- `role` analysis role that added step variables should be assigned. By default, they are designated as model predictors.
### step_sbf

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

**id**
unique character string to identify the step.

**x**
`step_lincomp` object.

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

### See Also
`recipe`, `prep`, `bake`

### Examples
```r
library(recipes)

pca_mat <- function(x, step) {
  prcomp(x)$rotation[, 1:step$num_comp, drop = FALSE]
}

rec <- recipe(rating ~ ., data = attitude)
lincomp_rec <- rec %>%
  step_lincomp(all_numeric(), -all_outcomes(),
              transform = pca_mat, num_comp = 3, prefix = "PCA")

lincomp_prep <- prep(lincomp_rec, training = attitude)
lincomp_data <- bake(lincomp_prep, attitude)

pairs(lincomp_data, lower.panel = NULL)

tidy(lincomp_rec, number = 1)
tidy(lincomp_prep, number = 1)
```

---

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

```r
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

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

```r
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(), -all_outcomes(),
            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)
```

Description

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

Usage

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

- **shrinkage**
  - numeric shrinkage (quadratic) penalty for the components to improve conditioning; larger values produce more shrinkage of component loadings toward zero.

- **center, scale**
  - logicals indicating whether to mean center and standard deviation scale the original variables prior to deriving components, or functions or names of functions for the centering and scaling.

- **max_iter**
  - maximum number of algorithm iterations allowed.

- **tol**
  - numeric tolerance for the convergence criterion.

- **replace**
  - logical indicating whether to replace the original variables.

- **prefix**
  - character string prefix added to a sequence of zero-padded integers to generate names for the resulting new variables.

- **role**
  - analysis role that added step variables should be assigned. By default, they are designated as model predictors.
step_spca

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

id unique character string to identify the step.

x step_spca object.

Details

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

Value

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

References


See Also

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

Examples

```r
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)
```
Model Performance Summaries

Description

Summary statistics for resampled model performance metrics.

Usage

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

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

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

```r
## S3 method for class 'MLModelFit'
summary(object, .type = c("default", "glance", "tidy"), ...)
```

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

```r
## S3 method for class 'PerformanceCurve'
summary(object, stat = MachineShop::settings("stat.Curve"), ...)
```

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

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

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

Value

An object of summary statistics.

Examples

```r
## 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)
```

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


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)
SurvMatrix  SurvMatrix Class Constructors

Description
Create a matrix of survival events or probabilities.

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

Arguments

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

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`
SVMModel

Examples

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

SVMModel

Support Vector Machine Models

Description

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

Usage

```r
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).  
- `C`: cost of constraints violation defined as the regularization term in the Lagrange formulation.  
- `nu`: parameter needed for nu-svc, one-svc, and nu-svr.  
- `epsilon`: parameter in the insensitive-loss function used for eps-svr, nu-svr and eps-bsvm.  
- `cache`: cache memory in MB.  
- `tol`: tolerance of termination criterion.  
- `shrinking`: whether to use the shrinking-heuristics.  
- `sigma`: inverse kernel width used by the ANOVA, Bessel, and Laplacian kernels.  
- `degree`: degree of the ANOVA, Bessel, and polynomial kernel functions.  
- `...`: arguments passed to `SVMModel` 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 convenient 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`
Paired t-tests for Model Comparisons

Examples

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

Description

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

Usage

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

Arguments

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

Details

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

\[
t = \frac{\bar{x}_R}{\sqrt{Fs^2_R/R}}
\]

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

Value

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


Examples

```r
## 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)
```

---

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

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

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

**Details**

**Response types:** factor, numeric

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

**Value**

MLModel class object.

**See Also**

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

**Examples**

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

---

**Description**

Recipe tuning over a grid of parameter values.
Usage

TunedInput(object, ...)

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

Arguments

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

Value

TunedModelRecipe class object that inherits from TunedInput and recipe.

See Also

- `fit`, `resample`, `set_optim`

Examples

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

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

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

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

---

TunedModel  Tuned Model

**Description**

Model tuning over a grid of parameter values.

**Usage**

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

**Arguments**

- `object`  
  model function, function name, or object defining the model to be tuned.

- `grid`  
  single integer or vector of integers whose positions or names match the parameters in the model’s pre-defined tuning grid if one exists and which specify the number of values used to construct the grid; TuningGrid function, function name, or object; ParameterGrid object; or data frame containing parameter values at which to evaluate the model, such as that returned by expand_params.

- `control`  
  control function, function name, or object defining the resampling method to be employed.

- `metrics`  
  metric function, function name, or vector of these with which to calculate performance. If not specified, default metrics defined in the performance functions are used. Model selection is based on the first calculated metric.

- `cutoff`  
  argument passed to the metrics functions.

- `stat`  
  function or character string naming a function to compute a summary statistic on resampled metric values for model tuning.

**Details**

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

**Response types:** factor, numeric, ordered, Surv
Value

TunedModel class object that inherits from MLModel.

See Also

fit, resample, set_optim

Examples

## Requires prior installation of suggested package gbm to run
## May require a long runtime

# Automatically generated grid
model_fit <- fit(sale_amount ~ ., data = ICHomes,
    model = TunedModel(GBMModel))
varimp(model_fit)
(tuned_model <- as.MLModel(model_fit))
summary(tuned_model)
plot(tuned_model, type = "l")

# 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.
Usage

TuningGrid(size = 3, random = FALSE)

Arguments

- **size**
  - single integer or vector of integers whose positions or names match the parameters in a model’s tuning grid and which specify the number of values used to construct the grid.

- **random**
  - number of unique points to sample at random from the grid defined by size. If size is a single unnamed integer, then random = Inf will include all values of all grid parameters in the constructed grid, whereas random = FALSE will include all values of default grid parameters.

Details

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

Value

TuningGrid class object.

See Also

TunedModel, expand_modelgrid

Examples

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

---

**unMLModelFit**

Revert an MLModelFit Object

Description

Function to revert an MLModelFit object to its original class.

Usage

unMLModelFit(object)

Arguments

- **object**
  - model fit result.
Value

The supplied object with its MLModelFit classes and fields removed.

---

### varimp

**Variable Importance**

**Description**

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

**Usage**

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

**Arguments**

- **object**: model fit result.
- **method**: character string specifying the calculation of variable importance as permutation-based ("permute") or model-specific ("model"). If model-specific importance is specified but not defined, the permutation-based method will be used instead with its default values (below). Permutation-based variable importance is defined as the relative change in model predictive performances between datasets with and without permuted values for the associated variable (Fisher et al. 2019).
- **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":
  - **select = NULL**: expression indicating predictor variables for which to compute variable importance (see `subset` for syntax) [default: all].
  - **samples = 1**: number of times to permute the values of each variable. Larger numbers of samples decrease variability in the estimates at the expense of increased computation time.
  - **prop = numeric()**: proportion of observations to sample without replacement at each round of variable permutations [default: all]. Subsampling of observations can decrease computation time.
  - **size = integer()**: number of observations to sample at each round of permutations [default: all].
  - **times = numeric()**: numeric vector of follow-up times at which to predict survival probabilities or NULL for predicted survival means.
  - **metric = NULL**: metric function or function name with which to calculate performance. If not specified, the first applicable default metric from the `performance` functions is used.
compare = c("-", "/") character specifying the relative change to compute in comparing model predictive performances between datasets with and without permuted values. The choices are difference ("-") and ratio ("/").

stats = MachineShop::settings("stat.TrainingParams") function, function name, or vector of these with which to compute summary statistics on the set of variable importance values from the permuted datasets.

na.rm = TRUE logical indicating whether to exclude missing variable importance values from the calculation of summary statistics.

progress = TRUE logical indicating whether to display iterative progress during computation.

Value

VariableImportance class object.

References


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)
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, 
    ...
)
XGBModel

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,
    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 automatically if not specified according to the following values available for supported response variable types.

factor: "multi:softprob", "binary:logistic" (2 levels only)
    "rank:pairwise", "rank:ndcg", "rank:map"
PoissonVariate: "count:poisson"
Surv: "survival:aft", "survival:cox"

The first values listed are the defaults for the corresponding response types.

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

aft_loss_distribution_scale numeric scaling parameter for the accelerated failure time distribution.

base_score initial prediction score of all observations, global bias.
XGBModel

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 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.

max_delta_step, tree_method, sketch_eps, scale_pos_weight, updater, refresh_leaf, process_type, grow_policy, max_leaves, max_bin, num_parallel_tree 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.

sample_type, normalize_type type of sampling and normalization algorithms.

rate_drop rate at which to drop trees during the dropout procedure.

one_drop integer indicating whether to drop at least one tree during the dropout procedure.

skip_drop probability of skipping the dropout procedure during a boosting iteration.

feature_selector, top_k character string specifying the feature selection and ordering method, and number of top variables to select in the "greedy" and "thrifty" feature selectors.

Details

Response types: factor, numeric, PoissonVariate, Surv

Automatic tuning of grid parameters:
- 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.
See Also

xgboost.fit.resample

Examples

```r
## 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)
```
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