mlr Tutorial

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Contents

1 Machine Learning in R: mlr Tutorial

This document provides an in-depth introduction to Machine Learning in R: mlr, a framework for machine learning experiments in **R**.

In this tutorial, we focus on basic functions and applications. More detailed technical information can be found in the manual pages which are regularly updated and reflect the documentation of the current package development version.

Offline versions of this tutorial are also available for download:

- current mlr release on CRAN
- the mlr devel version on GitHub

The tutorial aims to walkthrough basic data analysis tasks step by step. We will use simple examples from classification, regression, cluster and survival analysis to illustrate the main features of the package.

Enjoy reading!

1.1 Quick start

Here we show the `mlr` workflow to train, make predictions, and evaluate a learner on a classification problem. We walk through 5 basic steps that work on any learning problem or method supported by `mlr`.

```
library(mlr)
data(iris)

## 1) Define the task
## Specify the type of analysis (e.g. classification) and provide data and response variable
task = makeClassifTask(data = iris, target = "Species")

## 2) Define the learner
## Choose a specific algorithm (e.g. linear discriminant analysis)
lrn = makeLearner("classif.lda")

n = nrow(iris)
train.set = sample(n, size = 2/3*n)
test.set = setdiff(1:n, train.set)

## 3) Fit the model
## Train the learner on the task using a random subset of the data as training set
model = train(lrn, task, subset = train.set)

## 4) Make predictions
## Predict values of the response variable for new observations by the trained model
## using the other part of the data as test set
pred = predict(model, task = task, subset = test.set)

## 5) Evaluate the learner
## Calculate the mean misclassification error and accuracy
performance(pred, measures = list(mmce, acc))
## mmce  acc
## 0.02 0.98
```

2 Basics

2.1 Learning Tasks

Learning tasks encapsulate the data set and further relevant information about a machine learning problem, for example the name of the target variable for supervised problems.

2.1.1 Task types and creation

The tasks are organized in a hierarchy, with the generic `Task()` at the top. The following tasks can be instantiated and all inherit from the virtual superclass `Task()`:

- `RegrTask()` for regression problems,
- `ClassifTask()` for binary and multi-class classification problems with class-dependent costs can be handled as well),
- `SurvTask()` for survival analysis,
- `ClusterTask()` for cluster analysis,
- `MultilabelTask()` for multilabel classification problems,
- `CostSensTask()` for general cost sensitive classification (with example-specific costs).

To create a task, just call `make<TaskType>`, e.g., `makeClassifTask()`. All tasks require an identifier (argument `id`) and a `base::data.frame()` (argument `data`). If no ID is provided it is automatically generated using the variable name of the data. The ID will be later used to name results, for example of benchmark experiments, and to annotate plots. Depending on the nature of the learning problem, additional arguments may be required and are discussed in the following sections.

2.1.1.1 Regression

For supervised learning like regression (as well as classification and survival analysis) we, in addition to `data`, have to specify the name of the `target` variable.

```
data(BostonHousing, package = "mlbench")
regr.task = makeRegrTask(id = "bh", data = BostonHousing, target = "medv")
regr.task
## Supervised task: bh
## Type: regr
## Target: medv
## Observations: 506
## Features:
##    numerics     factors     ordered functionals
##          12           1           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
```

As you can see, the `Task()` records the type of the learning problem and basic information about the data set, e.g., the types of the features (`base::numeric()` vectors, `base::factors()` or ordered factors), the number of observations, or whether missing values are present.

Creating tasks for classification and survival analysis follows the same scheme, the data type of the target variables included in `data` is simply different. For each of these learning problems some specifics are described below.

2.1.1.2 Classification

For classification the target column has to be a `factor`.

In the following example we define a classification task for the `mlbench::BreastCancer()` data set and exclude the variable `Id` from all furthercmodel fitting and evaluation.

```
data(BreastCancer, package = "mlbench")
df = BreastCancer
df$Id = NULL
classif.task = makeClassifTask(id = "BreastCancer", data = df, target = "Class")
classif.task
## Supervised task: BreastCancer
## Type: classif
## Target: Class
## Observations: 699
## Features:
##    numerics     factors     ordered functionals
##           0           4           5           0
## Missings: TRUE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
## Classes: 2
##    benign malignant
##       458       241
## Positive class: benign
```

In binary classification the two classes are usually referred to as *positive* andc*negative* class with the positive class being the category of greater interest. This is relevant for many performance measures like the *true positive rate* or ROC analysis. Moreover, `mlr`, where possible, permits to set options (like the `setThreshold()` or `makeWeightedClassesWrapper()`) and returns and plots results (like class posterior probabilities) for the positive class only.

`makeClassifTask()` by default selects the first factor level of the target variable as the positive class, in the above example `benign`. Class `malignant` can be manually selected as follows:

```
classif.task = makeClassifTask(id = "BreastCancer", data = df, target = "Class", positive = "malignant")
```

2.1.1.3 Survival analysis

Survival tasks use two target columns. For left and right censored problems these consist of the survival time and a binary event indicator. For interval censored data the two target columns must be specified in the `"interval2"` format (see `survival::Surv()`).

```
data(lung, package = "survival")
lung$status = (lung$status == 2) ## convert to logical
surv.task = makeSurvTask(data = lung, target = c("time", "status"))
surv.task
## Supervised task: lung
## Type: surv
## Target: time,status
## Events: 165
## Observations: 228
## Features:
##    numerics     factors     ordered functionals
##           8           0           0           0
```

```
## Missings: TRUE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
```

The type of censoring can be specified via the argument `censoring`, which defaults to `"rcens"` for right censored data.

2.1.1.4 Multilabel classification

In multilabel classification each object can belong to more than one category at the same time.

The `data` are expected to contain as many target columns as there are class labels. The target columns should be logical vectors that indicate which class labels are present. The names of the target columns are taken as class labels and need to be passed to the `target` argument of `makeMultilabelTask`Task()‘.

In the following example we get the data of the yeast data set, extract the label names, and pass them to the `target` argument in `makeMultilabelTask`Task()‘.

```
yeast = getTaskData(yeast.task)

labels = colnames(yeast)[1:14]
yeast.task = makeMultilabelTask(id = "multi", data = yeast, target = labels)
yeast.task
## Supervised task: multi
## Type: multilabel
## Target: label1,label2,label3,label4,label5,label6,label7,label8,label9,label10,label11,label12,label
## Observations: 2417
## Features:
##    numerics     factors     ordered functionals
##         103           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
## Classes: 14
##  label1  label2  label3  label4  label5  label6  label7  label8  label9
##     762    1038     983     862     722     597     428     480     178
## label10 label11 label12 label13 label14
##     253     289    1816    1799      34
```

See also the tutorial page multilabel.

2.1.1.5 Cluster analysis

As cluster analysis is unsupervised, the only mandatory argument to construct a cluster analysis task is the `data`. Below we create a learning task from the data set `datasets::mtcars()`.

```
data(mtcars, package = "datasets")
cluster.task = makeClusterTask(data = mtcars)
cluster.task
## Unsupervised task: mtcars
## Type: cluster
## Observations: 32
## Features:
##    numerics     factors     ordered functionals
```

```
##          11           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
```

2.1.1.6 Cost-sensitive classification

The standard objective in classification is to obtain a high prediction accuracy, i.e., to minimize the number of errors. All types of misclassification errors are thereby deemed equally severe. However, in many applications different kinds of errors cause different costs.

In case of *class-dependent costs*, that solely depend on the actual and predicted class labels, it is sufficient to create an ordinary `ClassifTask()`.

In order to handle *example-specific costs* it is necessary to generate a `CostSensTask()`. In this scenario, each example (x, y) is associated with an individual cost vector of length K with K denoting the number of classes. The k-th component indicates the cost of assigning x to class k. Naturally, it is assumed that the cost of the intended class label y is minimal.

As the cost vector contains all relevant information about the intended class y, only the feature values x and a `cost` matrix, which contains the cost vectors for all examples in the data set, are required to create the `CostSensTask()`.

In the following example we use the `datasets::iris()` data and an artificial cost matrix (which is generated as proposed by Beygelzimer et al., 2005):

```
df = iris
cost = matrix(runif(150 * 3, 0, 2000), 150) * (1 - diag(3))[df$Species,]
df$Species = NULL

costsens.task = makeCostSensTask(data = df, cost = cost)
costsens.task
## Supervised task: df
## Type: costsens
## Observations: 150
## Features:
##    numerics     factors     ordered functionals
##           4           0           0           0
## Missings: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
## Classes: 3
## y1, y2, y3
```

For more details see the page on cost sensitive classification.

2.1.2 Further settings

The `Task()` help page also lists several other arguments to describe further details of the learning problem.

For example, we could include a `blocking` factor in the task. This would indicate that some observations "belong together" and should not be separated when splitting the data into training and test sets for resampling.

Another option is to assign `weights` to observations. These can simply indicate observation frequencies or result from the sampling scheme used to collect the data. Note that you should use this option only if the

weights really belong to the task. If you plan to train some learning algorithms with different weights on the same `Task()`, `mlr` offers several other ways to set observation or class weights (for supervised classification). See for example the tutorial page about training or function `makeWeightedClassesWrapper()`.

2.1.3 Accessing a learning task

We provide many operators to access the elements stored in a `Task()`. The most important ones are listed in the documentation of `Task()` and `getTaskData()`.

To access the `TaskDesc()` that contains basic information about the task you can use:

```
getTaskDesc(classif.task)
## $id
## [1] "BreastCancer"
##
## $type
## [1] "classif"
##
## $target
## [1] "Class"
##
## $size
## [1] 699
##
## $n.feat
##    numerics     factors     ordered functionals
##           0           4           5           0
##
## $has.missings
## [1] TRUE
##
## $has.weights
## [1] FALSE
##
## $has.blocking
## [1] FALSE
##
## $has.coordinates
## [1] FALSE
##
## $class.levels
## [1] "benign"    "malignant"
##
## $positive
## [1] "malignant"
##
## $negative
## [1] "benign"
##
## $class.distribution
##
##    benign malignant
##       458       241
##
```

```
## attr(,"class")
## [1] "ClassifTaskDesc"    "SupervisedTaskDesc" "TaskDesc"
```

Note that `TaskDesc()` have slightly different elements for different types of `Task()`s. Frequently required elements can also be accessed directly.

```
### Get the ID
getTaskId(classif.task)
## [1] "BreastCancer"
### Get the type of task
getTaskType(classif.task)
## [1] "classif"
### Get the names of the target columns
getTaskTargetNames(classif.task)
## [1] "Class"
### Get the number of observations
getTaskSize(classif.task)
## [1] 699
### Get the number of input variables
getTaskNFeats(classif.task)
## [1] 9
### Get the class levels in classif.task
getTaskClassLevels(classif.task)
## [1] "benign"    "malignant"
```

Moreover, `mlr` provides several functions to extract data from a `Task()`.

```
### Accessing the data set in classif.task
str(getTaskData(classif.task))
## 'data.frame':    699 obs. of  10 variables:
##  $ Cl.thickness   : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 5 5 3 6 4 8 1 2 2 4 ...
##  $ Cell.size      : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 1 4 1 8 1 10 1 1 1 2 ...
##  $ Cell.shape     : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 1 4 1 8 1 10 1 2 1 1 ...
##  $ Marg.adhesion  : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 1 5 1 1 3 8 1 1 1 1 ...
##  $ Epith.c.size   : Ord.factor w/ 10 levels "1"<"2"<"3"<"4"<..: 2 7 2 3 2 7 2 2 2 2 ...
##  $ Bare.nuclei    : Factor w/ 10 levels "1","2","3","4",..: 1 10 2 4 1 10 10 1 1 1 ...
##  $ Bl.cromatin    : Factor w/ 10 levels "1","2","3","4",..: 3 3 3 3 3 9 3 3 1 2 ...
##  $ Normal.nucleoli: Factor w/ 10 levels "1","2","3","4",..: 1 2 1 7 1 7 1 1 1 1 ...
##  $ Mitoses        : Factor w/ 9 levels "1","2","3","4",..: 1 1 1 1 1 1 1 1 5 1 ...
##  $ Class          : Factor w/ 2 levels "benign","malignant": 1 1 1 1 1 2 1 1 1 1 ...
### Get the names of the input variables in cluster.task
getTaskFeatureNames(cluster.task)
##  [1] "mpg"  "cyl"  "disp" "hp"   "drat" "wt"   "qsec" "vs"   "am"   "gear"
## [11] "carb"
### Get the values of the target variables in surv.task
head(getTaskTargets(surv.task))
##   time status
## 1  306   TRUE
## 2  455   TRUE
## 3 1010  FALSE
## 4  210   TRUE
## 5  883   TRUE
## 6 1022  FALSE
### Get the cost matrix in costsens.task
head(getTaskCosts(costsens.task))
```

```
##      y1         y2        y3
## [1,]  0  669.29445  590.6579
## [2,]  0 1683.51667  808.3662
## [3,]  0 1605.76846  218.4530
## [4,]  0  881.55286 1835.8541
## [5,]  0   51.96546  885.0618
## [6,]  0  903.19228 1268.3677
```

Note that `getTaskData()` offers many options for converting the data set into a convenient format. This especially comes in handy when you integrate a new learner from another **R** package into `mlr`. In this regard function `getTaskFormula()` is also useful.

2.1.4 Modifying a learning task

`mlr` provides several functions to alter an existing `Task()`, which is often more convenient than creating a new `Task()` from scratch. Here are some examples.

```
### Select observations and/or features
cluster.task = subsetTask(cluster.task, subset = 4:17)

### It may happen, especially after selecting observations, that features are constant.
### These should be removed.
removeConstantFeatures(cluster.task)
## Removing 1 columns: am
## Unsupervised task: mtcars
## Type: cluster
## Observations: 14
## Features:
##    numerics     factors     ordered functionals
##          10           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
### Remove selected features
dropFeatures(surv.task, c("meal.cal", "wt.loss"))
## Supervised task: lung
## Type: surv
## Target: time,status
## Events: 165
## Observations: 228
## Features:
##    numerics     factors     ordered functionals
##           6           0           0           0
## Missings: TRUE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
### Standardize numerical features
task = normalizeFeatures(cluster.task, method = "range")
summary(getTaskData(task))
##       mpg              cyl              disp              hp
##  Min.   :0.0000   Min.   :0.0000   Min.   :0.0000   Min.   :0.0000
##  1st Qu.:0.3161   1st Qu.:0.5000   1st Qu.:0.1242   1st Qu.:0.2801
```

```
##  Median :0.5107   Median :1.0000   Median :0.4076   Median :0.6311
##  Mean   :0.4872   Mean   :0.7143   Mean   :0.4430   Mean   :0.5308
##  3rd Qu.:0.6196   3rd Qu.:1.0000   3rd Qu.:0.6618   3rd Qu.:0.7473
##  Max.   :1.0000   Max.   :1.0000   Max.   :1.0000   Max.   :1.0000
##       drat             wt             qsec             vs
##  Min.   :0.0000   Min.   :0.0000   Min.   :0.0000   Min.   :0.0000
##  1st Qu.:0.2672   1st Qu.:0.1275   1st Qu.:0.2302   1st Qu.:0.0000
##  Median :0.3060   Median :0.1605   Median :0.3045   Median :0.0000
##  Mean   :0.4544   Mean   :0.3268   Mean   :0.3752   Mean   :0.4286
##  3rd Qu.:0.7026   3rd Qu.:0.3727   3rd Qu.:0.4908   3rd Qu.:1.0000
##  Max.   :1.0000   Max.   :1.0000   Max.   :1.0000   Max.   :1.0000
##        am           gear             carb
##  Min.   :0.5   Min.   :0.0000   Min.   :0.0000
##  1st Qu.:0.5   1st Qu.:0.0000   1st Qu.:0.3333
##  Median :0.5   Median :0.0000   Median :0.6667
##  Mean   :0.5   Mean   :0.2857   Mean   :0.6429
##  3rd Qu.:0.5   3rd Qu.:0.7500   3rd Qu.:1.0000
##  Max.   :0.5   Max.   :1.0000   Max.   :1.0000
```

For more functions and more detailed explanations have a look at the data preprocessing page.

2.1.5 Example tasks and convenience functions

For your convenience `mlr` provides pre-defined `Task()`s for each type of learning problem. These are also used throughout this tutorial in order to get shorter and more readable code. A list of all `Task()`s can be found in the Appendix.

Moreover, `mlr`'s function `convertMLBenchObjToTask()` can generate `Task()`s from the data sets and data generating functions in package `mlbench::mlbench()`.

2.2 Learners

The following classes provide a unified interface to all popular machine learning methods in **R**: (cost-sensitive) classification, regression, survival analysis, and clustering. Many are already integrated in `mlr`, others are not, but the package is specifically designed to make extensions simple.

Section integrated learners shows the already implemented machine learning methods and their properties. If your favorite method is missing, either open an issue or take a look at how to integrate a learning method yourself. This basic introduction demonstrates how to use already implemented learners.

2.2.1 Constructing a learner

A learner in `mlr` is generated by calling `makeLearner()`. In the constructor you need to specify which learning method you want to use. Moreover, you can:

- Set hyperparameters.
- Control the output for later prediction, e.g., for classification whether you want a factor of predicted class labels or probabilities.
- Set an ID to name the object (some methods will later use this ID to name results or annotate plots).

```
### Classification tree, set it up for predicting probabilities
classif.lrn = makeLearner("classif.randomForest", predict.type = "prob", fix.factors.prediction = TRUE)

### Regression gradient boosting machine, specify hyperparameters via a list
```

```
regr.lrn = makeLearner("regr.gbm", par.vals = list(n.trees = 500, interaction.depth = 3))

### Cox proportional hazards model with custom name
surv.lrn = makeLearner("surv.coxph", id = "cph")

### K-means with 5 clusters
cluster.lrn = makeLearner("cluster.kmeans", centers = 5)

### Multilabel Random Ferns classification algorithm
multilabel.lrn = makeLearner("multilabel.rFerns")
```

The first argument specifies which algorithm to use. The naming convention is `classif.<R_method_name>` for classification methods, `regr.<R_method_name>` for regression methods, `surv.<R_method_name>` for survival analysis, `cluster.<R_method_name>` for clustering methods, and `multilabel.<R_method_name>` for multilabel classification.

Hyperparameter values can be specified either via the `...` argument or as a `list` via `par.vals`.

Occasionally, `factor` features may cause problems when fewer levels are present in the test data set than in the training data. By setting `fix.factors.prediction = TRUE` these are avoided by adding a factor level for missing data in the test data set.

Let's have a look at two of the learners created above.

```
classif.lrn
## Learner classif.randomForest from package randomForest
## Type: classif
## Name: Random Forest; Short name: rf
## Class: classif.randomForest
## Properties: twoclass,multiclass,numerics,factors,ordered,prob,class.weights,oobpreds,featimp
## Predict-Type: prob
## Hyperparameters:
surv.lrn
## Learner cph from package survival
## Type: surv
## Name: Cox Proportional Hazard Model; Short name: coxph
## Class: surv.coxph
## Properties: numerics,factors,weights
## Predict-Type: response
## Hyperparameters:
```

All generated learners are objects of class Learner (`makeLearner()`). This class contains the properties of the method, e.g., which types of features it can handle, what kind of output is possible during prediction, and whether multi-class problems, observations weights or missing values are supported.

As you might have noticed, there is currently no special learner class for cost-sensitive classification. For ordinary misclassification costs you can use standard classification methods. For example-dependent costs there are several ways to generate cost-sensitive learners from ordinary regression and classification learners. This is explained in greater detail in the section about cost-sensitive classification.

2.2.2 Accessing a learner

The Learner (`makeLearner()`) object is a `list` and the following elements contain information regarding the hyperparameters and the type of prediction.

```
### Get the configured hyperparameter settings that deviate from the defaults
cluster.lrn$par.vals
## $centers
## [1] 5
### Get the set of hyperparameters
classif.lrn$par.set
##                      Type  len   Def   Constr Req Tunable Trafo
## ntree             integer    -   500 1 to Inf   -    TRUE     -
## mtry              integer    -     - 1 to Inf   -    TRUE     -
## replace           logical    -  TRUE        -   -    TRUE     -
## classwt     numericvector <NA>     - 0 to Inf   -    TRUE     -
## cutoff      numericvector <NA>     -   0 to 1   -    TRUE     -
## strata            untyped    -     -        -   -   FALSE     -
## sampsize    integervector <NA>     - 1 to Inf   -    TRUE     -
## nodesize          integer    -     1 1 to Inf   -    TRUE     -
## maxnodes          integer    -     - 1 to Inf   -    TRUE     -
## importance        logical    - FALSE        -   -    TRUE     -
## localImp          logical    - FALSE        -   -    TRUE     -
## proximity         logical    - FALSE        -   -   FALSE     -
## oob.prox          logical    -     -        -   Y   FALSE     -
## norm.votes        logical    -  TRUE        -   -   FALSE     -
## do.trace          logical    - FALSE        -   -   FALSE     -
## keep.forest       logical    -  TRUE        -   -   FALSE     -
## keep.inbag        logical    - FALSE        -   -   FALSE     -
### Get the type of prediction
regr.lrn$predict.type
## [1] "response"
```

Slot `$par.set` is an object of class `ParamSet` (`ParamHelpers::makeParamSet()`). It contains, among others, the type of hyperparameters (e.g., numeric, logical), potential default values and the range of allowed values.

Moreover, `mlr` provides function `getHyperPars()` or its alternative `getLearnerParVals()` to access the current hyperparameter setting of a Learner (`makeLearner()`) and `getParamSet()` to get a description of all possible settings. These are particularly useful in case of wrapped Learner (`makeLearner()`)s, for example if a learner is fused with a feature selection strategy, and both, the learner as well the feature selection method, have hyperparameters. For details see the section on wrapped learners.

```
### Get current hyperparameter settings
getHyperPars(cluster.lrn)
## $centers
## [1] 5
### Get a description of all possible hyperparameter settings
getParamSet(classif.lrn)
##                      Type  len   Def   Constr Req Tunable Trafo
## ntree             integer    -   500 1 to Inf   -    TRUE     -
## mtry              integer    -     - 1 to Inf   -    TRUE     -
## replace           logical    -  TRUE        -   -    TRUE     -
## classwt     numericvector <NA>     - 0 to Inf   -    TRUE     -
## cutoff      numericvector <NA>     -   0 to 1   -    TRUE     -
## strata            untyped    -     -        -   -   FALSE     -
## sampsize    integervector <NA>     - 1 to Inf   -    TRUE     -
## nodesize          integer    -     1 1 to Inf   -    TRUE     -
## maxnodes          integer    -     - 1 to Inf   -    TRUE     -
## importance        logical    - FALSE        -   -    TRUE     -
## localImp          logical    - FALSE        -   -    TRUE     -
```

```
## proximity         logical    - FALSE        -   -   FALSE     -
## oob.prox          logical    -     -        -   Y   FALSE     -
## norm.votes        logical    -  TRUE        -   -   FALSE     -
## do.trace          logical    - FALSE        -   -   FALSE     -
## keep.forest       logical    -  TRUE        -   -   FALSE     -
## keep.inbag        logical    - FALSE        -   -   FALSE     -
```

We can also use `getParamSet()` or its alias `getLearnerParamSet()` to get a quick overview about the available hyperparameters and defaults of a learning method without explicitly constructing it (by calling `makeLearner()`).

```
getParamSet("classif.randomForest")
##                      Type  len   Def   Constr Req Tunable Trafo
## ntree             integer    -   500 1 to Inf   -    TRUE     -
## mtry              integer    -     - 1 to Inf   -    TRUE     -
## replace           logical    -  TRUE        -   -    TRUE     -
## classwt     numericvector <NA>     - 0 to Inf   -    TRUE     -
## cutoff      numericvector <NA>     -   0 to 1   -    TRUE     -
## strata            untyped    -     -        -   -   FALSE     -
## sampsize    integervector <NA>     - 1 to Inf   -    TRUE     -
## nodesize          integer    -     1 1 to Inf   -    TRUE     -
## maxnodes          integer    -     - 1 to Inf   -    TRUE     -
## importance        logical    - FALSE        -   -    TRUE     -
## localImp          logical    - FALSE        -   -    TRUE     -
## proximity         logical    - FALSE        -   -   FALSE     -
## oob.prox          logical    -     -        -   Y   FALSE     -
## norm.votes        logical    -  TRUE        -   -   FALSE     -
## do.trace          logical    - FALSE        -   -   FALSE     -
## keep.forest       logical    -  TRUE        -   -   FALSE     -
## keep.inbag        logical    - FALSE        -   -   FALSE     -
```

Functions for accessing a Learner's meta information are available in `mlr`. We can use `getLearnerId()`, `getLearnerShortName()` and `getLearnerType()` to get Learner's ID, short name and type, respectively. Moreover, in order to show the required packages for the Learner, one can call `getLearnerPackages()`.

```
### Get object's id
getLearnerId(surv.lrn)
## [1] "cph"
### Get the short name
getLearnerShortName(classif.lrn)
## [1] "rf"
### Get the type of the learner
getLearnerType(multilabel.lrn)
## [1] "multilabel"
### Get required packages
getLearnerPackages(cluster.lrn)
## [1] "stats" "clue"
```

2.2.3 Modifying a learner

There are also some functions that enable you to change certain aspects of a Learner (`makeLearner()`) without needing to create a new Learner (`makeLearner()`) from scratch. Here are some examples.

```
### Change the ID
surv.lrn = setLearnerId(surv.lrn, "CoxModel")
surv.lrn
## Learner CoxModel from package survival
## Type: surv
## Name: Cox Proportional Hazard Model; Short name: coxph
## Class: surv.coxph
## Properties: numerics,factors,weights
## Predict-Type: response
## Hyperparameters:
### Change the prediction type, predict a factor with class labels instead of probabilities
classif.lrn = setPredictType(classif.lrn, "response")

### Change hyperparameter values
cluster.lrn = setHyperPars(cluster.lrn, centers = 4)

### Go back to default hyperparameter values
regr.lrn = removeHyperPars(regr.lrn, c("n.trees", "interaction.depth"))
```

2.2.4 Listing learners

A list of all learners integrated in `mlr` and their respective properties is shown in the Appendix.

If you would like a list of available learners, maybe only with certain properties or suitable for a certain learning `Task()` use function `listLearners()`.

```
### List everything in mlr
lrns = listLearners()
## Warning in listLearners.character(obj = NA_character_, properties, quiet, : The following learners c
## classif.mxff,regr.mxff
## Check ?learners to see which packages you need or install mlr with all suggestions.
head(lrns[c("class", "package")])
##                 class      package
## 1         classif.ada    ada,rpart
## 2  classif.adaboostm1        RWeka
## 3 classif.bartMachine  bartMachine
## 4    classif.binomial        stats
## 5  classif.blackboost mboost,party
## 6    classif.boosting adabag,rpart
### List classifiers that can output probabilities
lrns = listLearners("classif", properties = "prob")
## Warning in listLearners.character("classif", properties = "prob"): The following learners could not
## classif.mxff,regr.mxff
## Check ?learners to see which packages you need or install mlr with all suggestions.
head(lrns[c("class", "package")])
##                 class      package
## 1         classif.ada    ada,rpart
## 2  classif.adaboostm1        RWeka
## 3 classif.bartMachine  bartMachine
## 4    classif.binomial        stats
## 5  classif.blackboost mboost,party
## 6    classif.boosting adabag,rpart
### List classifiers that can be applied to iris (i.e., multiclass) and output probabilities
lrns = listLearners(iris.task, properties = "prob")
```

```
## Warning in listLearners.character(td$type, union(props, properties), quiet, : The following learners
## classif.mxff,regr.mxff
## Check ?learners to see which packages you need or install mlr with all suggestions.
head(lrns[c("class", "package")])
##                class      package
## 1 classif.adaboostm1        RWeka
## 2   classif.boosting adabag,rpart
## 3        classif.C50          C50
## 4    classif.cforest        party
## 5      classif.ctree        party
## 6   classif.cvglmnet       glmnet
### The calls above return character vectors, but you can also create learner objects
head(listLearners("cluster", create = TRUE), 2)
## Warning in listLearners.character("cluster", create = TRUE): The following learners could not be cons
## classif.mxff,regr.mxff
## Check ?learners to see which packages you need or install mlr with all suggestions.
## [[1]]
## Learner cluster.cmeans from package e1071,clue
## Type: cluster
## Name: Fuzzy C-Means Clustering; Short name: cmeans
## Class: cluster.cmeans
## Properties: numerics,prob
## Predict-Type: response
## Hyperparameters: centers=2
##
##
## [[2]]
## Learner cluster.Cobweb from package RWeka
## Type: cluster
## Name: Cobweb Clustering Algorithm; Short name: cobweb
## Class: cluster.Cobweb
## Properties: numerics
## Predict-Type: response
## Hyperparameters:
```

2.3 Predicting Outcomes for New Data

Predicting the target values for new observations is implemented the same way as most of the other predict methods in **R**. In general, all you need to do is call `predict` (`predict.WrappedModel()`) on the object returned by `train()` and pass the data you want predictions for.

There are two ways to pass the data:

- Either pass the `Task()` via the `task` argument or
- pass a `data.frame` via the `newdata` argument.

The first way is preferable if you want predictions for data already included in a `Task()`.

Just as `train()`, the `predict` (`predict.WrappedModel()`) function has a `subset` argument, so you can set aside different portions of the data in `Task()` for training and prediction (more advanced methods for splitting the data in train and test set are described in the section on resampling).

In the following example we fit a gradient boosting machine (`gbm::gbm()`) to every second observation of the `BostonHousing` (`mlbench::BostonHousing()`) data set and make predictions on the remaining data in `bh.task()`.

```
n = getTaskSize(bh.task)
train.set = seq(1, n, by = 2)
test.set = seq(2, n, by = 2)
lrn = makeLearner("regr.gbm", n.trees = 100)
mod = train(lrn, bh.task, subset = train.set)

task.pred = predict(mod, task = bh.task, subset = test.set)
task.pred
## Prediction: 253 observations
## predict.type: response
## threshold:
## time: 0.00
##    id truth response
## 2   2  21.6 22.23910
## 4   4  33.4 23.20101
## 6   6  28.7 22.32445
## 8   8  27.1 22.12672
## 10 10  18.9 22.12672
## 12 12  18.9 22.12672
## ... (#rows: 253, #cols: 3)
```

The second way is useful if you want to predict data not included in the `Task()`.

Here we cluster the `iris` data set without the target variable. All observations with an odd index are included in the `Task()` and used for training. Predictions are made for the remaining observations.

```
n = nrow(iris)
iris.train = iris[seq(1, n, by = 2), -5]
iris.test = iris[seq(2, n, by = 2), -5]
task = makeClusterTask(data = iris.train)
mod = train("cluster.kmeans", task)

newdata.pred = predict(mod, newdata = iris.test)
newdata.pred
## Prediction: 75 observations
## predict.type: response
## threshold:
## time: 0.00
##    response
## 2         2
## 4         2
## 6         2
## 8         2
## 10        2
## 12        2
## ... (#rows: 75, #cols: 1)
```

Note that for supervised learning you do not have to remove the target columns from the data. These columns are automatically removed prior to calling the underlying `predict` method of the learner.

2.3.1 Accessing the prediction

Function `predict()` returns a named `list` of class `Prediction()`. Its most important element is `$data` which is a `data.frame` that contains columns with the true values of the target variable (in case of supervised

learning problems) and the predictions. Use `as.data.frame` (`Prediction()`) for direct access.

In the following the predictions on the `BostonHousing` (`mlbench::BostonHousing()`) and the `iris` (`datasets::iris()`) data sets are shown. As you may recall, the predictions in the first case were made from a `Task()` and in the second case from a `data.frame`.

```
### Result of predict with data passed via task argument
head(as.data.frame(task.pred))
##    id truth response
## 2   2  21.6 22.23910
## 4   4  33.4 23.20101
## 6   6  28.7 22.32445
## 8   8  27.1 22.12672
## 10 10  18.9 22.12672
## 12 12  18.9 22.12672
### Result of predict with data passed via newdata argument
head(as.data.frame(newdata.pred))
##    response
## 2         2
## 4         2
## 6         2
## 8         2
## 10        2
## 12        2
```

As you can see when predicting from a `Task()`, the resulting `data.frame` contains an additional column, called `id`, which tells us which element in the original data set the prediction corresponds to.

A direct way to access the true and predicted values of the target variable(s) is provided by functions `getPredictionTruth` (`getPredictionResponse()`) and [`getPredictionResponse()`].

```
head(getPredictionTruth(task.pred))
## [1] 21.6 33.4 28.7 27.1 18.9 18.9
head(getPredictionResponse(task.pred))
## [1] 22.23910 23.20101 22.32445 22.12672 22.12672 22.12672
```

2.3.1.1 Regression: Extracting standard errors

Some learners provide standard errors for predictions, which can be accessed in `mlr`. An overview is given by calling the function `listLearners()` and setting `properties = "se"`. By assigning `FALSE` to `check.packages` learners from packages which are not installed will be included in the overview.

```
listLearners("regr", check.packages = FALSE, properties = "se")[c("class", "name")]
## Warning in listLearners.character("regr", check.packages = FALSE, properties = "se"): The following l
## classif.mxff,regr.mxff
## Check ?learners to see which packages you need or install mlr with all suggestions.
##          class
## 1   regr.bcart
## 2     regr.bgp
## 3  regr.bgpllm
## 4     regr.blm
## 5    regr.btgp
## 6 regr.btgpllm
##                                                                  name
## 1                                                       Bayesian CART
## 2                                          Bayesian Gaussian Process
## 3       Bayesian Gaussian Process with jumps to the Limiting Linear Model
```

```
## 4                                                    Bayesian Linear Model
## 5                                          Bayesian Treed Gaussian Process
## 6 Bayesian Treed Gaussian Process with jumps to the Limiting Linear Model
## ... (#rows: 17, #cols: 2)
```

In this example we train a linear regression model (`stats::lm()`) on the `BostonHousing` (`bh.task()`) dataset. In order to calculate standard errors set the `predict.type` to `"se"`:

```
### Create learner and specify predict.type
lrn.lm = makeLearner("regr.lm", predict.type = 'se')
mod.lm = train(lrn.lm, bh.task, subset = train.set)
task.pred.lm = predict(mod.lm, task = bh.task, subset = test.set)
task.pred.lm
## Prediction: 253 observations
## predict.type: se
## threshold:
## time: 0.01
##    id truth response        se
## 2   2  21.6 24.83734 0.7501615
## 4   4  33.4 28.38206 0.8742590
## 6   6  28.7 25.16725 0.8652139
## 8   8  27.1 19.38145 1.1963265
## 10 10  18.9 18.66449 1.1793944
## 12 12  18.9 21.25802 1.0727918
## ... (#rows: 253, #cols: 4)
```

The standard errors can then be extracted using `getPredictionSE()`.

```
head(getPredictionSE(task.pred.lm))
## [1] 0.7501615 0.8742590 0.8652139 1.1963265 1.1793944 1.0727918
```

2.3.1.2 Classification and clustering: Extracting probabilities

The predicted probabilities can be extracted from the `Prediction()` using function `getPredictionProbabilities()`. Here is another cluster analysis example. We use fuzzy c-means clustering (`e1071::cmeans()`) on the `mtcars` (`datasets::mtcars()`) data set.

```
lrn = makeLearner("cluster.cmeans", predict.type = "prob")
mod = train(lrn, mtcars.task)

pred = predict(mod, task = mtcars.task)
head(getPredictionProbabilities(pred))
##                             1          2
## Mazda RX4         0.020406481 0.97959352
## Mazda RX4 Wag     0.020366262 0.97963374
## Datsun 710        0.007339505 0.99266050
## Hornet 4 Drive    0.457088530 0.54291147
## Hornet Sportabout 0.981294666 0.01870533
## Valiant           0.242541933 0.75745807
```

For *classification problems* there are some more things worth mentioning. By default, class labels are predicted.

```
### Linear discriminant analysis on the iris data set
mod = train("classif.lda", task = iris.task)

pred = predict(mod, task = iris.task)
```

```
pred
## Prediction: 150 observations
## predict.type: response
## threshold:
## time: 0.00
##   id  truth response
## 1  1 setosa   setosa
## 2  2 setosa   setosa
## 3  3 setosa   setosa
## 4  4 setosa   setosa
## 5  5 setosa   setosa
## 6  6 setosa   setosa
## ... (#rows: 150, #cols: 3)
```

In order to get predicted posterior probabilities we have to create a Learner (`makeLearner()`) with the appropriate `predict.type`.

```
lrn = makeLearner("classif.rpart", predict.type = "prob")
mod = train(lrn, iris.task)

pred = predict(mod, newdata = iris)
head(as.data.frame(pred))
##    truth prob.setosa prob.versicolor prob.virginica response
## 1 setosa           1               0              0   setosa
## 2 setosa           1               0              0   setosa
## 3 setosa           1               0              0   setosa
## 4 setosa           1               0              0   setosa
## 5 setosa           1               0              0   setosa
## 6 setosa           1               0              0   setosa
```

In addition to the probabilities, class labels are predicted by choosing the class with the maximum probability and breaking ties at random.

As mentioned above, the predicted posterior probabilities can be accessed via the `getPredictionProbabilities()` function.

```
head(getPredictionProbabilities(pred))
##   setosa versicolor virginica
## 1      1          0         0
## 2      1          0         0
## 3      1          0         0
## 4      1          0         0
## 5      1          0         0
## 6      1          0         0
```

2.3.1.3 Classification: Confusion matrix

A confusion matrix can be obtained by calling `calculateConfusionMatrix()`. The columns represent predicted and the rows true class labels.

```
calculateConfusionMatrix(pred)
##             predicted
## true         setosa versicolor virginica -err.-
##   setosa         50          0         0      0
##   versicolor      0         49         1      1
```

```
##   virginica       0          5        45      5
##   -err.-          0          5         1      6
```

You can see the number of correctly classified observations on the diagonal of the matrix. Misclassified observations are on the off-diagonal. The total number of errors for single (true and predicted) classes is shown in the `-err.-` row and column, respectively.

To get relative frequencies additional to the absolute numbers we can set `relative = TRUE`.

```
conf.matrix = calculateConfusionMatrix(pred, relative = TRUE)
conf.matrix
## Relative confusion matrix (normalized by row/column):
##             predicted
## true         setosa    versicolor virginica -err.-
##   setosa     1.00/1.00 0.00/0.00  0.00/0.00 0.00
##   versicolor 0.00/0.00 0.98/0.91  0.02/0.02 0.02
##   virginica  0.00/0.00 0.10/0.09  0.90/0.98 0.10
##   -err.-          0.00      0.09       0.02 0.04
##
##
## Absolute confusion matrix:
##             predicted
## true         setosa versicolor virginica -err.-
##   setosa         50          0         0      0
##   versicolor      0         49         1      1
##   virginica       0          5        45      5
##   -err.-          0          5         1      6
```

It is possible to normalize by either row or column, therefore every element of the above relative confusion matrix contains two values. The first is the relative frequency grouped by row (the true label) and the second value grouped by column (the predicted label).

If you want to access the relative values directly you can do this through the `$relative.row` and `$relative.col` members of the returned object `conf.matrix`. For more details see the `ConfusionMatrix()` documentation page.

```
conf.matrix$relative.row
##            setosa versicolor virginica -err-
## setosa          1       0.00      0.00  0.00
## versicolor      0       0.98      0.02  0.02
## virginica       0       0.10      0.90  0.10
```

Finally, we can also add the absolute number of observations for each predicted and true class label to the matrix (both absolute and relative) by setting `sums = TRUE`.

```
calculateConfusionMatrix(pred, relative = TRUE, sums = TRUE)
## Relative confusion matrix (normalized by row/column):
##             predicted
## true         setosa    versicolor virginica -err.-    -n-
##   setosa     1.00/1.00 0.00/0.00  0.00/0.00 0.00      50
##   versicolor 0.00/0.00 0.98/0.91  0.02/0.02 0.02      54
##   virginica  0.00/0.00 0.10/0.09  0.90/0.98 0.10      46
##   -err.-          0.00      0.09       0.02 0.04      <NA>
##   -n-           50        50         50        <NA>      150
##
##
## Absolute confusion matrix:
```

```
##            setosa versicolor virginica -err.- -n-
## setosa         50          0         0      0  50
## versicolor      0         49         1      1  50
## virginica       0          5        45      5  50
## -err.-          0          5         1      6  NA
## -n-            50         54        46     NA 150
```

2.3.2 Classification: Adjusting the decision threshold

We can set the threshold value that is used to map the predicted posterior probabilities to class labels. Note that for this purpose we need to create a Learner (`makeLearner()`) that predicts probabilities. For binary classification, the threshold determines when the *positive* class is predicted. The default is 0.5. Now, we set the threshold for the positive class to 0.9 (that is, an example is assigned to the positive class if its posterior probability exceeds 0.9). Which of the two classes is the positive one can be seen by accessing the `Task()`. To illustrate binary classification, we use the `Sonar` (`mlbench::Sonar()`) data set from the `mlbench` package.

```
lrn = makeLearner("classif.rpart", predict.type = "prob")
mod = train(lrn, task = sonar.task)

### Label of the positive class
getTaskDesc(sonar.task)$positive
## [1] "M"
### Default threshold
pred1 = predict(mod, sonar.task)
pred1$threshold
##   M   R
## 0.5 0.5
### Set the threshold value for the positive class
pred2 = setThreshold(pred1, 0.9)
pred2$threshold
##   M   R
## 0.9 0.1
pred2
## Prediction: 208 observations
## predict.type: prob
## threshold: M=0.90,R=0.10
## time: 0.01
##   id truth    prob.M    prob.R response
## 1  1     R 0.1060606 0.8939394        R
## 2  2     R 0.7333333 0.2666667        R
## 3  3     R 0.0000000 1.0000000        R
## 4  4     R 0.1060606 0.8939394        R
## 5  5     R 0.9250000 0.0750000        M
## 6  6     R 0.0000000 1.0000000        R
## ... (#rows: 208, #cols: 5)
### We can also set the effect in the confusion matrix
calculateConfusionMatrix(pred1)
##         predicted
## true      M  R -err.-
##   M      95 16     16
##   R      10 87     10
##   -err.- 10 16     26
calculateConfusionMatrix(pred2)
```

```
##         predicted
## true      M  R -err.-
##   M      84 27     27
##   R       6 91      6
##   -err.-  6 27     33
```

Note that in the binary case `getPredictionProbabilities()` by default extracts the posterior probabilities of the positive class only.

```
head(getPredictionProbabilities(pred1))
## [1] 0.1060606 0.7333333 0.0000000 0.1060606 0.9250000 0.0000000
### But we can change that, too
head(getPredictionProbabilities(pred1, cl = c("M", "R")))
##           M         R
## 1 0.1060606 0.8939394
## 2 0.7333333 0.2666667
## 3 0.0000000 1.0000000
## 4 0.1060606 0.8939394
## 5 0.9250000 0.0750000
## 6 0.0000000 1.0000000
```

It works similarly for multiclass classification. The threshold has to be given by a named vector specifying the values by which each probability will be divided. The class with the maximum resulting value is then selected.

```
lrn = makeLearner("classif.rpart", predict.type = "prob")
mod = train(lrn, iris.task)
pred = predict(mod, newdata = iris)
pred$threshold
##     setosa versicolor  virginica
##  0.3333333  0.3333333  0.3333333
table(as.data.frame(pred)$response)
##
##     setosa versicolor  virginica
##         50         54         46
pred = setThreshold(pred, c(setosa = 0.01, versicolor = 50, virginica = 1))
pred$threshold
##     setosa versicolor  virginica
##       0.01      50.00       1.00
table(as.data.frame(pred)$response)
##
##     setosa versicolor  virginica
##         50          0        100
```

If you are interested in tuning the threshold (vector) have a look at the section about performance curves and threshold tuning.

2.3.3 Visualizing the prediction

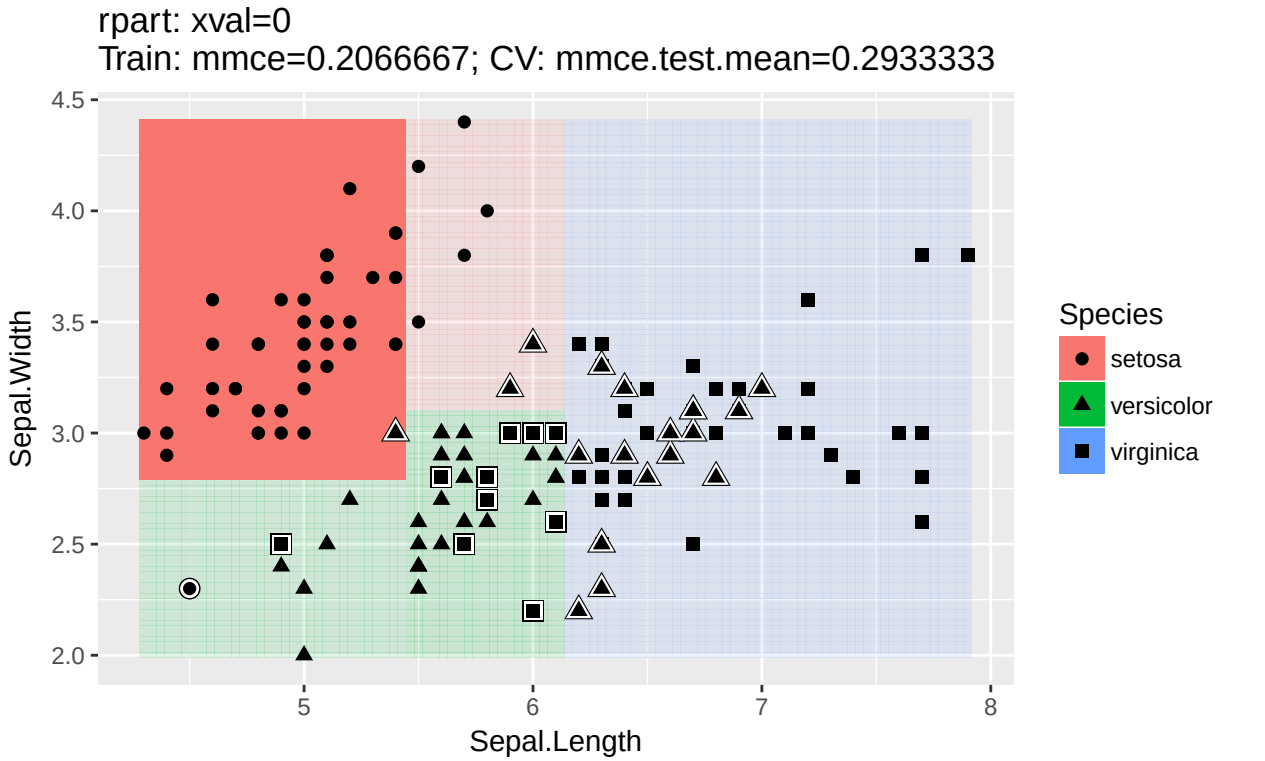
The function `plotLearnerPrediction()` allows to visualize predictions, e.g., for teaching purposes or exploring models. It trains the chosen learning method for 1 or 2 selected features and then displays the predictions with `ggplot2::ggplot()`.

For *classification*, we get a scatter plot of 2 features (by default the first 2 in the data set). The type of symbol shows the true class labels of the data points. Symbols with white border indicate misclassified

observations. The posterior probabilities (if the learner under consideration supports this) are represented by the background color where higher saturation means larger probabilities.

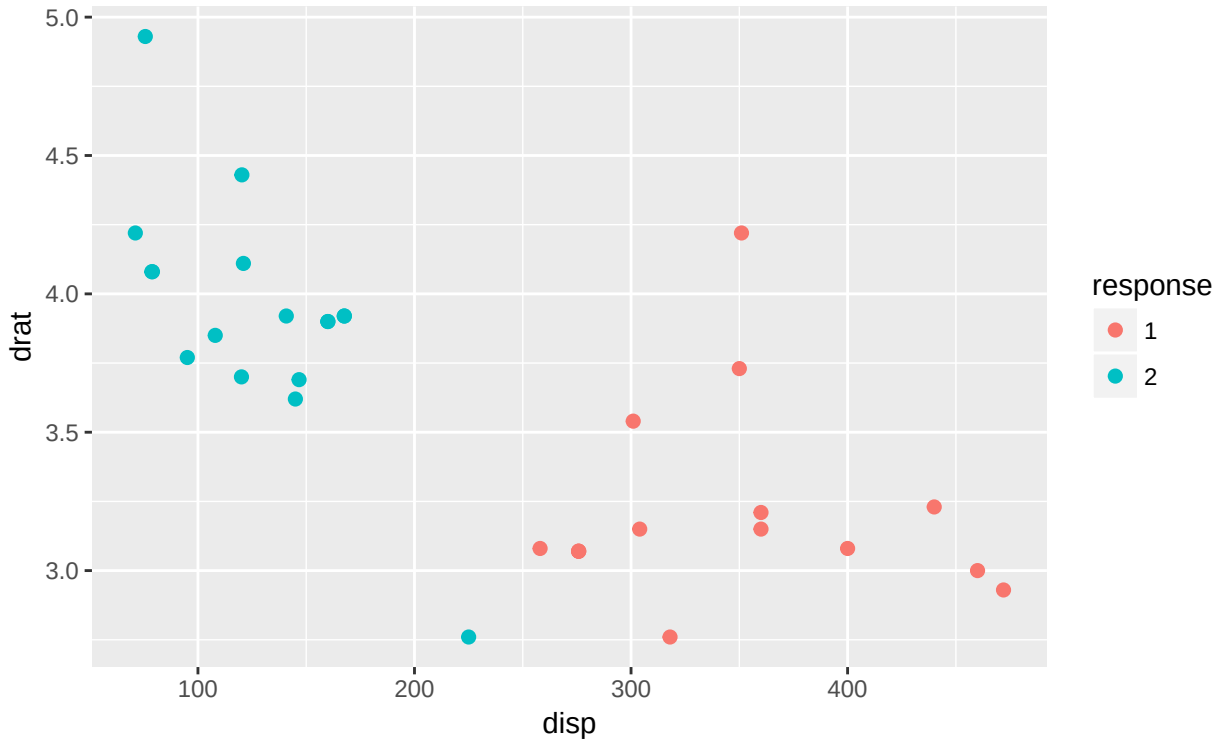
The plot title displays the ID of the Learner (`makeLearner()`) (in the following example CART), its parameters, its training performance and its cross-validation performance. mmce stands for *mean misclassification error*, i.e., the error rate. See the sections on performance and resampling for further explanations.

```
lrn = makeLearner("classif.rpart", id = "CART")
plotLearnerPrediction(lrn, task = iris.task)
```



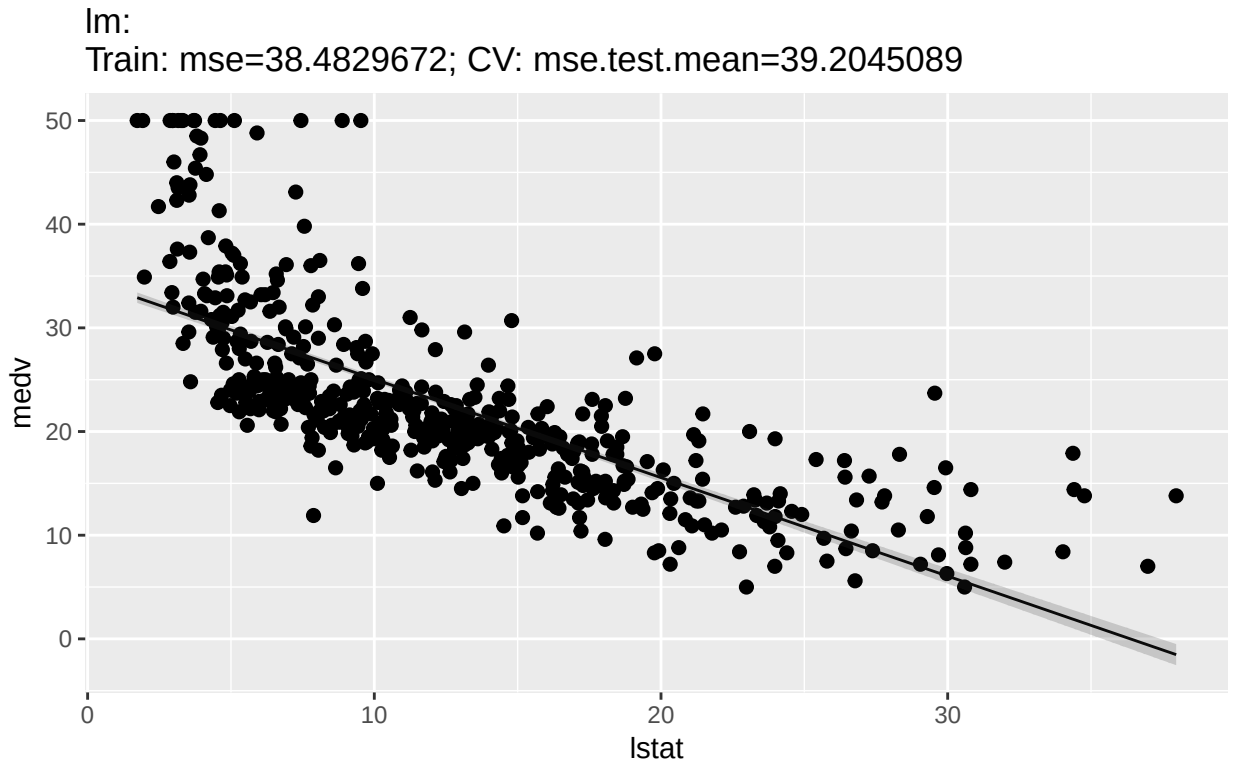
For *clustering* we also get a scatter plot of two selected features. The color of the points indicates the predicted cluster.

```
lrn = makeLearner("cluster.kmeans")
plotLearnerPrediction(lrn, task = mtcars.task, features = c("disp", "drat"), cv = 0)
## Warning in rgl.init(initValue, onlyNULL): RGL: unable to open X11 display
## Warning: 'rgl_init' failed, running with rgl.useNULL = TRUE
##
## This is package 'modeest' written by P. PONCET.
## For a complete list of functions, use 'library(help = "modeest")' or 'help.start()'.
```



For *regression*, there are two types of plots. The 1D plot shows the target values in relation to a single feature, the regression curve and, if the chosen learner supports this, the estimated standard error.

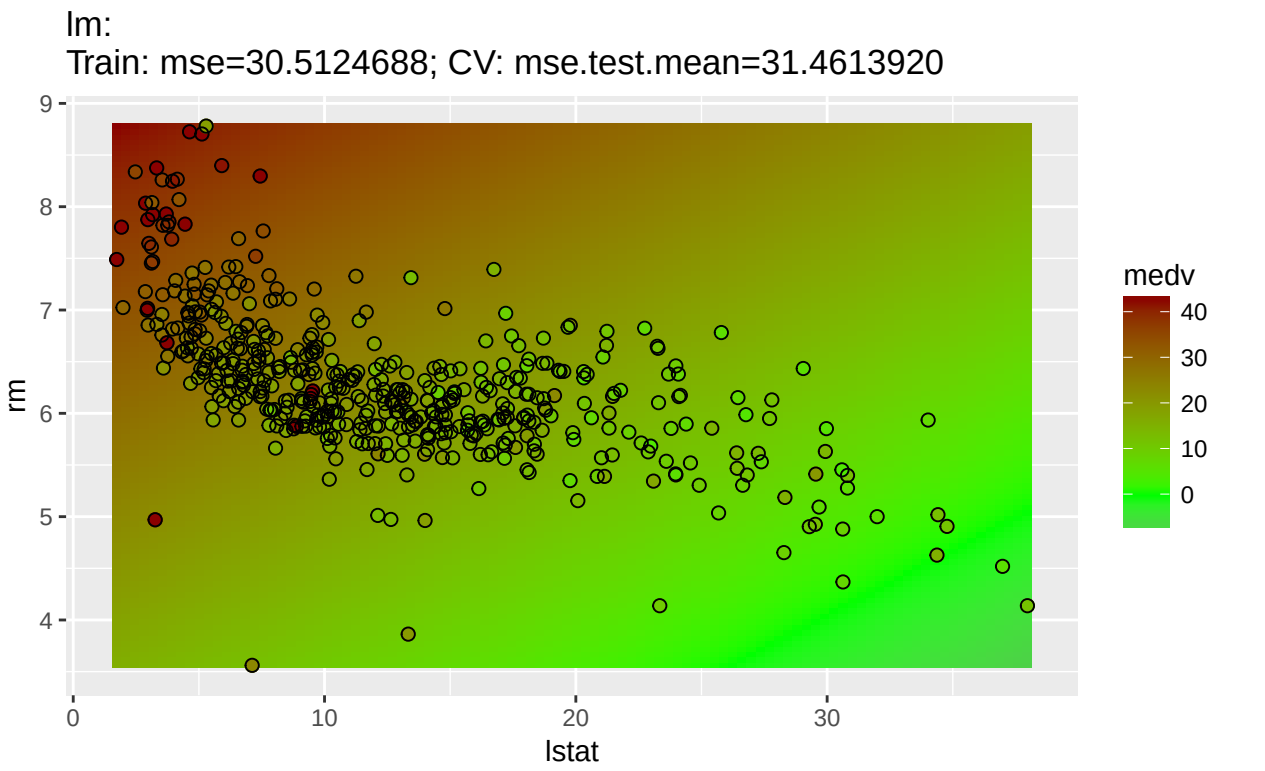
```
plotLearnerPrediction("regr.lm", features = "lstat", task = bh.task)
```



The 2D variant, as in the classification case, generates a scatter plot of 2 features. The fill color of the dots illustrates the value of the target variable `"medv"`, the background colors show the estimated mean. The plot

does not represent the estimated standard error.

```
plotLearnerPrediction("regr.lm", features = c("lstat", "rm"), task = bh.task)
```



2.4 Evaluating Learner Performance

The quality of the predictions of a model in `mlr` can be assessed with respect to a number of different performance measures. In order to calculate the performance measures, call `performance()` on the object returned by `predict` (`predict.WrappedModel()`) and specify the desired performance measures.

2.4.1 Available performance measures

`mlr` provides a large number of performance measures for all types of learning problems. Typical performance measures for *classification* are the mean misclassification error (mmce), accuracy (acc) or measures based on ROC analysis. For *regression* the mean of squared errors (mse) or mean of absolute errors (mae) are usually considered. For *clustering* tasks, measures such as the Dunn index (dunn) are provided, while for *survival* predictions, the Concordance Index (cindex) is supported, and for *cost-sensitive* predictions the misclassification penalty (mcp) and others. It is also possible to access the time to train the learner (timetrain), the time to compute the prediction (timepredict) and their sum (timeboth) as performance measures.

To see which performance measures are implemented, have a look at the table of performance measures and the `measures()` documentation page.

If you want to implement an additional measure or include a measure with non-standard misclassification costs, see the section on creating custom measures.

2.4.2 Listing measures

The properties and requirements of the individual measures are shown in the table of performance measures.

If you would like a list of available measures with certain properties or suitable for a certain learning `Task()` use the function `listMeasures()`.

```
### Performance measures for classification with multiple classes
listMeasures("classif", properties = "classif.multi")
##  [1] "featperc"         "mmce"             "lsr"
##  [4] "qsr"              "timeboth"         "multiclass.aunp"
##  [7] "timetrain"        "multiclass.aunu"  "ber"
## [10] "timepredict"      "multiclass.brier" "ssr"
## [13] "acc"              "logloss"          "wkappa"
## [16] "multiclass.au1p"  "multiclass.au1u"  "kappa"
### Performance measure suitable for the iris classification task
listMeasures(iris.task)
##  [1] "featperc"         "mmce"             "lsr"
##  [4] "qsr"              "timeboth"         "multiclass.aunp"
##  [7] "timetrain"        "multiclass.aunu"  "ber"
## [10] "timepredict"      "multiclass.brier" "ssr"
## [13] "acc"              "logloss"          "wkappa"
## [16] "multiclass.au1p"  "multiclass.au1u"  "kappa"
```

For convenience there exists a default measure for each type of learning problem, which is calculated if nothing else is specified. As defaults we chose the most commonly used measures for the respective types, e.g., the mean squared error (mse) for regression and the misclassification rate (mmce) for classification. The help page of function `getDefaultMeasure()` lists all defaults for all types of learning problems. The function itself returns the default measure for a given task type, `Task()` or `Learner()`.

```
### Get default measure for iris.task
getDefaultMeasure(iris.task)
## Name: Mean misclassification error
## Performance measure: mmce
## Properties: classif,classif.multi,req.pred,req.truth
## Minimize: TRUE
## Best: 0; Worst: 1
## Aggregated by: test.mean
## Arguments: list()
## Note: Defined as: mean(response != truth)
### Get the default measure for linear regression
getDefaultMeasure(makeLearner("regr.lm"))
## Name: Mean of squared errors
## Performance measure: mse
## Properties: regr,req.pred,req.truth
## Minimize: TRUE
## Best: 0; Worst: Inf
## Aggregated by: test.mean
## Arguments: list()
## Note: Defined as: mean((response - truth)^2)
```

2.4.3 Calculate performance measures

In the following example we fit a gradient boosting machine (`gbm::gbm()`) on a subset of the `BostonHousing` (`mlbench::BostonHousing()`) data set and calculate the default measure mean squared error (mse) on the remaining observations.

```
n = getTaskSize(bh.task)
lrn = makeLearner("regr.gbm", n.trees = 1000)
```

```
mod = train(lrn, task = bh.task, subset = seq(1, n, 2))
pred = predict(mod, task = bh.task, subset = seq(2, n, 2))

performance(pred)
##      mse
## 42.91952
```

The following code computes the median of squared errors (medse) instead.

```
performance(pred, measures = medse)
##    medse
## 9.063252
```

Of course, we can also calculate multiple performance measures at once by simply passing a list of measures which can also include your own measure.

Calculate the mean squared error, median squared error and mean absolute error (mae).

```
performance(pred, measures = list(mse, medse, mae))
##       mse     medse       mae
## 42.919524  9.063252  4.558664
```

For the other types of learning problems and measures, calculating the performance basically works in the same way.

2.4.3.1 Requirements of performance measures

Note that in order to calculate some performance measures it is required that you pass the `Task()` or the fitted model (`makeWrappedModel()`) in addition to the `Prediction()`.

For example in order to assess the time needed for training (timetrain), the fitted model has to be passed.

```
performance(pred, measures = timetrain, model = mod)
## timetrain
##     0.693
```

For many performance measures in cluster analysis the `Task()` is required.

```
lrn = makeLearner("cluster.kmeans", centers = 3)
mod = train(lrn, mtcars.task)
pred = predict(mod, task = mtcars.task)

### Calculate the Dunn index
performance(pred, measures = dunn, task = mtcars.task)
##      dunn
## 0.2278991
```

Moreover, some measures require a certain type of prediction. For example in binary classification in order to calculate the AUC (auc) – the area under the ROC (receiver operating characteristic) curve – we have to make sure that posterior probabilities are predicted. For more information on ROC analysis, see the section on ROC analysis.

```
lrn = makeLearner("classif.rpart", predict.type = "prob")
mod = train(lrn, task = sonar.task)
pred = predict(mod, task = sonar.task)

performance(pred, measures = auc)
##       auc
## 0.9224018
```

Also bear in mind that many of the performance measures that are available for classification, e.g., the false positive rate (fpr), are only suitable for binary problems.

2.4.4 Access a performance measure

Performance measures in `mlr` are objects of class `Measure` (`makeMeasure()`). If you are interested in the properties or requirements of a single measure you can access it directly. See the help page of `Measure` (`makeMeasure()`) for information on the individual slots.

```
### Mean misclassification error
str(mmce)
## List of 10
##  $ id        : chr "mmce"
##  $ minimize  : logi TRUE
##  $ properties: chr [1:4] "classif" "classif.multi" "req.pred" "req.truth"
##  $ fun       :function (task, model, pred, feats, extra.args)
##  $ extra.args: list()
##  $ best      : num 0
##  $ worst     : num 1
##  $ name      : chr "Mean misclassification error"
##  $ note      : chr "Defined as: mean(response != truth)"
##  $ aggr      :List of 4
##   ..$ id        : chr "test.mean"
##   ..$ name      : chr "Test mean"
##   ..$ fun       :function (task, perf.test, perf.train, measure, group, pred)
##   ..$ properties: chr "req.test"
##   ..- attr(*, "class")= chr "Aggregation"
##  - attr(*, "class")= chr "Measure"
```

2.4.5 Binary classification

For binary classification specialized techniques exist to analyze the performance.

2.4.5.1 Plot performance versus threshold

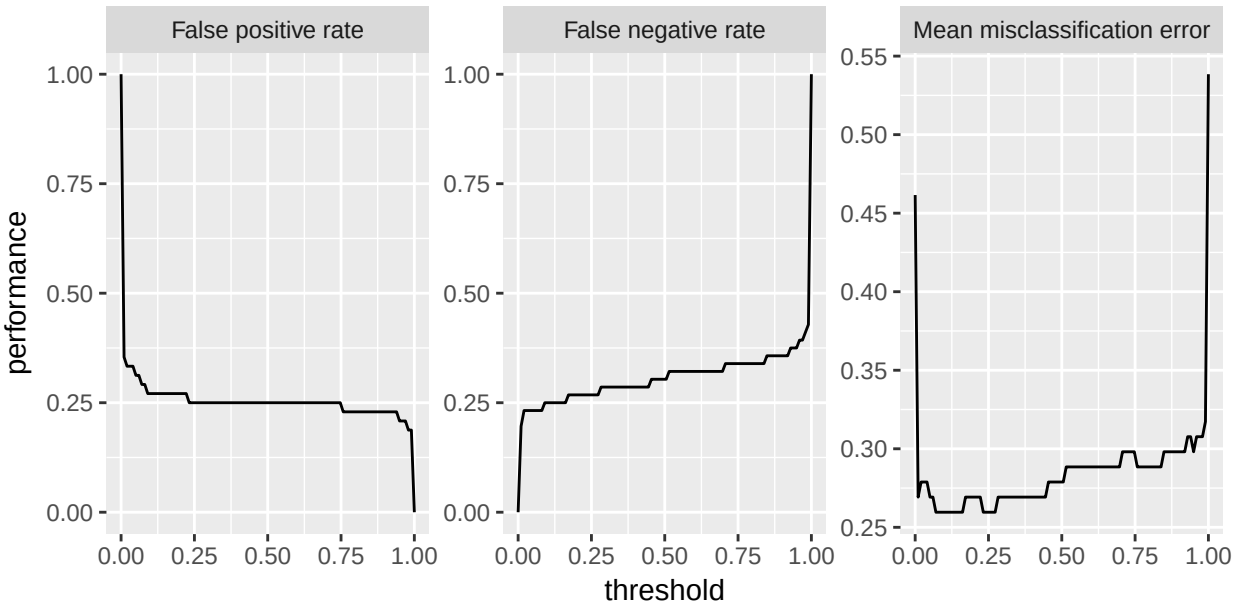
As you may recall (see the previous section on making predictions) in binary classification we can adjust the threshold used to map probabilities to class labels. Helpful in this regard is are the functions `generateThreshVsPerfData()` and `plotThreshVsPerf()`, which generate and plot, respectively, the learner performance versus the threshold.

For more performance plots and automatic threshold tuning see the section on ROC analysis.

In the following example we consider the `mlbench::Sonar()` data set and plot the false positive rate (fpr), the false negative rate (fnr) as well as the misclassification rate (mmce) for all possible threshold values.

```
lrn = makeLearner("classif.lda", predict.type = "prob")
n = getTaskSize(sonar.task)
mod = train(lrn, task = sonar.task, subset = seq(1, n, by = 2))
pred = predict(mod, task = sonar.task, subset = seq(2, n, by = 2))

### Performance for the default threshold 0.5
performance(pred, measures = list(fpr, fnr, mmce))
##       fpr       fnr      mmce
## 0.2500000 0.3035714 0.2788462
```

```
### Plot false negative and positive rates as well as the error rate versus the threshold
d = generateThreshVsPerfData(pred, measures = list(fpr, fnr, mmce))
plotThreshVsPerf(d)
```



There is an experimental `ggvis` plotting function `plotThreshVsPerfGGVIS()` which performs similarly to `plotThreshVsPerf()` but instead of creating facetted subplots to visualize multiple learners and/or multiple measures, one of them is mapped to an interactive sidebar which selects what to display.

```
plotThreshVsPerfGGVIS(d)
```

2.4.5.2 ROC measures

For binary classification a large number of specialized measures exist, which can be nicely formatted into one matrix, see for example the receiver operating characteristic page on wikipedia.

We can generate a similiar table with the `calculateROCMeasures()` function.

```
r = calculateROCMeasures(pred)
r
##     predicted
## true M         R
##    M 39        17        tpr: 0.7  fnr: 0.3
##    R 12        36        fpr: 0.25 tnr: 0.75
##      ppv: 0.76 for: 0.32 lrp: 2.79 acc: 0.72
##      fdr: 0.24 npv: 0.68 lrm: 0.4  dor: 6.88
##
##
## Abbreviations:
## tpr - True positive rate (Sensitivity, Recall)
## fpr - False positive rate (Fall-out)
## fnr - False negative rate (Miss rate)
## tnr - True negative rate (Specificity)
## ppv - Positive predictive value (Precision)
## for - False omission rate
## lrp - Positive likelihood ratio (LR+)
```

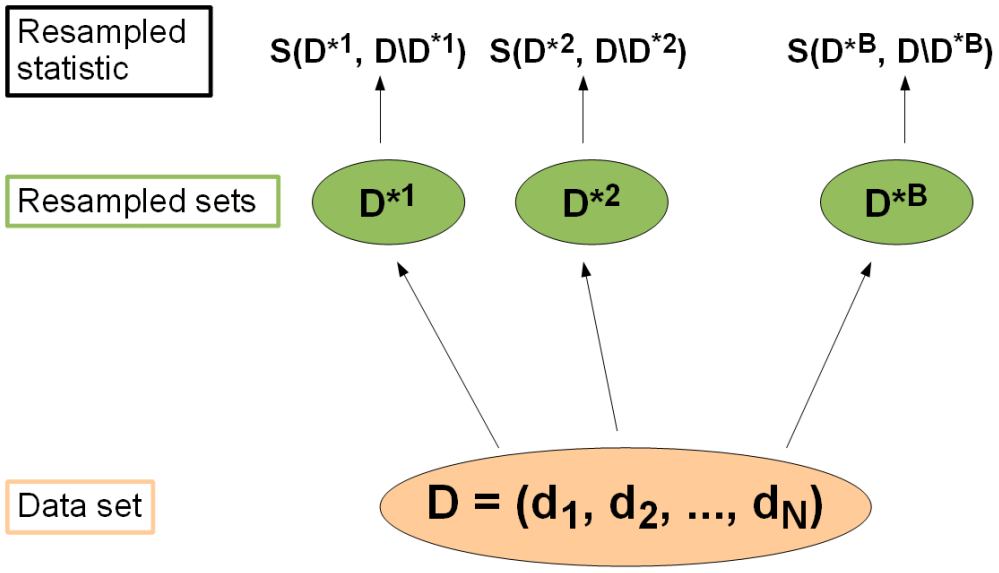


Figure 1: Resampling Figure

```
## fdr - False discovery rate
## npv - Negative predictive value
## acc - Accuracy
## lrm - Negative likelihood ratio (LR-)
## dor - Diagnostic odds ratio
```

The top left 2×2 matrix is the confusion matrix, which shows the relative frequency of correctly and incorrectly classified observations. Below and to the right a large number of performance measures that can be inferred from the confusion matrix are added. By default some additional info about the measures is printed. You can turn this off using the `abbreviations` argument of the `print` (`calculateROCMeasures()`) method: `print(r, abbreviations = FALSE)`.

2.5 Resampling

Resampling strategies are usually used to assess the performance of a learning algorithm: The entire data set is (repeatedly) split into training sets D^{*b} and test sets $D \setminus D^{*b}$, $b = 1, \ldots, B$. The learner is trained on each training set, predictions are made on the corresponding test set (sometimes on the training set as well) and the performance measure $S(D^{*b}, D \setminus D^{*b})$ is calculated. Then the B individual performance values are aggregated, most often by calculating the mean. There exist various different resampling strategies, for example cross-validation and bootstrap, to mention just two popular approaches.

If you want to read up on further details, the paper Resampling Strategies for Model Assessment and Selection by Simon is probably not a bad choice. Bernd has also published a paper Resampling methods for meta-model validation with recommendations for evolutionary computation which contains detailed descriptions and lots of statistical background information on resampling methods.

2.5.1 Defining the resampling strategy

In `mlr` the resampling strategy can be defined via function `makeResampleDesc()`. It requires a string that specifies the resampling method and, depending on the selected strategy, further information like the number of iterations. The supported resampling strategies are:

- Cross-validation (`"CV"`),
- Leave-one-out cross-validation (`"LOO"`),
- Repeated cross-validation (`"RepCV"`),
- Out-of-bag bootstrap and other variants like *b632* (`"Bootstrap"`),
- Subsampling, also called Monte-Carlo cross-validation (`"Subsample"`),
- Holdout (training/test) (`"Holdout"`).

For example if you want to use 3-fold cross-validation type:

```
### 3-fold cross-validation
rdesc = makeResampleDesc("CV", iters = 3)
rdesc
## Resample description: cross-validation with 3 iterations.
## Predict: test
## Stratification: FALSE
```

For holdout estimation use:

```
### Holdout estimation
rdesc = makeResampleDesc("Holdout")
rdesc
## Resample description: holdout with 0.67 split rate.
## Predict: test
## Stratification: FALSE
```

In order to save you some typing `mlr` contains some pre-defined resample descriptions for very common strategies like holdout (`hout` (`makeResampleDesc()`)) as well as cross-validation with different numbers of folds (e.g., `cv5` (`makeResampleDesc()`) or `cv10` (`makeResampleDesc()`)).

```
hout
## Resample description: holdout with 0.67 split rate.
## Predict: test
## Stratification: FALSE
cv3
## Resample description: cross-validation with 3 iterations.
## Predict: test
## Stratification: FALSE
```

2.5.2 Performing the resampling

Function `resample()` evaluates a Learner (`makeLearner()`) on a given machine learning `Task()` using the selected resampling strategy (`makeResampleDesc()`).

As a first example, the performance of linear regression (`stats::lm()`) on the `BostonHousing` (`mlbench::BostonHousing()`) data set is calculated using *3-fold cross-validation*.

Generally, for *K-fold cross-validation* the data set D is partitioned into K subsets of (approximately) equal size. In the b-th of the K iterations, the b-th subset is used for testing, while the union of the remaining parts forms the training set.

As usual, you can either pass a Learner (`makeLearner()`) object to `resample()` or, as done here, provide the class name `"regr.lm"` of the learner. Since no performance measure is specified the default for regression

learners (mean squared error, mse) is calculated.

```
### Specify the resampling strategy (3-fold cross-validation)
rdesc = makeResampleDesc("CV", iters = 3)

### Calculate the performance
r = resample("regr.lm", bh.task, rdesc)
## Resampling: cross-validation
## Measures:             mse
## [Resample] iter 1:    37.1457491
## [Resample] iter 2:    19.3752451
## [Resample] iter 3:    19.4389392
##
## Aggregated Result: mse.test.mean=25.3199778
##
r
## Resample Result
## Task: BostonHousing-example
## Learner: regr.lm
## Aggr perf: mse.test.mean=25.3199778
## Runtime: 0.0584648
```

The result `r` is an object of class `resample()` result. It contains performance results for the learner and some additional information like the runtime, predicted values, and optionally the models fitted in single resampling iterations.

```
### Peak into r
names(r)
##  [1] "learner.id"     "task.id"        "task.desc"      "measures.train"
##  [5] "measures.test"  "aggr"           "pred"           "models"
##  [9] "err.msgs"       "err.dumps"      "extract"        "runtime"
r$aggr
## mse.test.mean
##      25.31998
r$measures.test
##   iter      mse
## 1    1 37.14575
## 2    2 19.37525
## 3    3 19.43894
```

`r$measures.test` gives the performance on each of the 3 test data sets. `r$aggr` shows the aggregated performance value. Its name `"mse.test.mean"` indicates the performance measure, mse, and the method, `test.mean` (`aggregations()`), used to aggregate the 3 individual performances. `test.mean` (`aggregations()`) is the default aggregation scheme for most performance measures and, as the name implies, takes the mean over the performances on the test data sets.

Resampling in `mlr` works the same way for all types of learning problems and learners. Below is a classification example where a classification tree (rpart) (`rpart::rpart()`) is evaluated on the `Sonar` (`mlbench::sonar()`) data set by subsampling with 5 iterations.

In each subsampling iteration the data set D is randomly partitioned into a training and a test set according to a given percentage, e.g., 2/3 training and 1/3 test set. If there is just one iteration, the strategy is commonly called *holdout* or *test sample estimation*.

You can calculate several measures at once by passing a `list` of Measures (`makeMeasure()`)s to `resample()`. Below, the error rate (mmce), false positive and false negative rates (fpr, fnr), and the time it takes to train the learner (timetrain) are estimated by *subsampling* with 5 iterations.

```
### Subsampling with 5 iterations and default split ratio 2/3
rdesc = makeResampleDesc("Subsample", iters = 5)

### Subsampling with 5 iterations and 4/5 training data
rdesc = makeResampleDesc("Subsample", iters = 5, split = 4/5)

### Classification tree with information splitting criterion
lrn = makeLearner("classif.rpart", parms = list(split = "information"))

### Calculate the performance measures
r = resample(lrn, sonar.task, rdesc, measures = list(mmce, fpr, fnr, timetrain))
## Resampling: subsampling
## Measures:             mmce        fpr         fnr         timetrain
## [Resample] iter 1:    0.2142857   0.2380952   0.1904762   0.0170000
## [Resample] iter 2:    0.2857143   0.3157895   0.2608696   0.0250000
## [Resample] iter 3:    0.3333333   0.1764706   0.4400000   0.0210000
## [Resample] iter 4:    0.1904762   0.1666667   0.2083333   0.0210000
## [Resample] iter 5:    0.2619048   0.3809524   0.1428571   0.0210000
##
## Aggregated Result: mmce.test.mean=0.2571429,fpr.test.mean=0.2555949,fnr.test.mean=0.2485072,timetrai
##
r
## Resample Result
## Task: Sonar-example
## Learner: classif.rpart
## Aggr perf: mmce.test.mean=0.2571429,fpr.test.mean=0.2555949,fnr.test.mean=0.2485072,timetrain.test.m
## Runtime: 0.204438
```

If you want to add further measures afterwards, use `addRRMeasure()`.

```
### Add balanced error rate (ber) and time used to predict
addRRMeasure(r, list(ber, timepredict))
## Resample Result
## Task: Sonar-example
## Learner: classif.rpart
## Aggr perf: mmce.test.mean=0.2571429,fpr.test.mean=0.2555949,fnr.test.mean=0.2485072,timetrain.test.m
## Runtime: 0.204438
```

By default, `resample()` prints progress messages and intermediate results. You can turn this off by setting `show.info = FALSE`, as done in the code chunk below. (If you are interested in suppressing these messages permanently have a look at the tutorial page about configuring mlr.)

In the above example, the Learner (`makeLearner()`) was explicitly constructed. For convenience you can also specify the learner as a string and pass any learner parameters via the `...` argument of `resample()`.

```
r = resample("classif.rpart", parms = list(split = "information"), sonar.task, rdesc,
  measures = list(mmce, fpr, fnr, timetrain), show.info = FALSE)

r
## Resample Result
## Task: Sonar-example
## Learner: classif.rpart
## Aggr perf: mmce.test.mean=0.2047619,fpr.test.mean=0.2204025,fnr.test.mean=0.1992675,timetrain.test.m
## Runtime: 0.179133
```

2.5.3 Accessing resample results

Apart from the learner performance you can extract further information from the resample results, for example predicted values or the models fitted in individual resample iterations.

2.5.3.1 Predictions

Per default, the `resample()` result contains the predictions made during the resampling. If you do not want to keep them, e.g., in order to conserve memory, set `keep.pred = FALSE` when calling `resample()`.

The predictions are stored in slot `$pred` of the resampling result, which can also be accessed by function `getRRPredictions()`.

```
r$pred
## Resampled Prediction for:
## Resample description: subsampling with 5 iterations and 0.80 split rate.
## Predict: test
## Stratification: FALSE
## predict.type: response
## threshold:
## time (mean): 0.01
##    id truth response iter  set
## 1 195     M        M    1 test
## 2 108     M        M    1 test
## 3  59     R        R    1 test
## 4 158     M        M    1 test
## 5 208     M        M    1 test
## 6 155     M        M    1 test
## ... (#rows: 210, #cols: 5)
pred = getRRPredictions(r)
pred
## Resampled Prediction for:
## Resample description: subsampling with 5 iterations and 0.80 split rate.
## Predict: test
## Stratification: FALSE
## predict.type: response
## threshold:
## time (mean): 0.01
##    id truth response iter  set
## 1 195     M        M    1 test
## 2 108     M        M    1 test
## 3  59     R        R    1 test
## 4 158     M        M    1 test
## 5 208     M        M    1 test
## 6 155     M        M    1 test
## ... (#rows: 210, #cols: 5)
```

`pred` is an object of class `resample()` Prediction. Just as a `Prediction()` object (see the tutorial page on making predictions it has an element `$data` which is a `data.frame` that contains the predictions and in the case of a supervised learning problem the true values of the target variable(s). You can use `as.data.frame` (`Prediction()` to directly access the `$data` slot. Moreover, all getter functions for `Prediction()` objects like `getPredictionResponse()` or `getPredictionProbabilities()` are applicable.

```
head(as.data.frame(pred))
##    id truth response iter  set
```

```
## 1 195     M        M    1 test
## 2 108     M        M    1 test
## 3  59     R        R    1 test
## 4 158     M        M    1 test
## 5 208     M        M    1 test
## 6 155     M        M    1 test
head(getPredictionTruth(pred))
## [1] M M R M M M
## Levels: M R
head(getPredictionResponse(pred))
## [1] M M R M M M
## Levels: M R
```

The columns `iter` and `set` in the `data.frame` indicate the resampling iteration and the data set (`train` or `test`) for which the prediction was made.

By default, predictions are made for the test sets only. If predictions for the training set are required, set `predict = "train"` (for predictions on the train set only) or `predict = "both"` (for predictions on both train and test sets) in `makeResampleDesc()`. In any case, this is necessary for some bootstrap methods (*b632* and *b632+*) and some examples are shown later on.

Below, we use simple Holdout, i.e., split the data once into a training and test set, as resampling strategy and make predictions on both sets.

```
### Make predictions on both training and test sets
rdesc = makeResampleDesc("Holdout", predict = "both")

r = resample("classif.lda", iris.task, rdesc, show.info = FALSE)
r
## Resample Result
## Task: iris-example
## Learner: classif.lda
## Aggr perf: mmce.test.mean=0.0000000
## Runtime: 0.0175922
r$measures.train
##   iter mmce
## 1    1 0.03
```

(Please note that nonetheless the misclassification rate `r$aggr` is estimated on the test data only. How to calculate performance measures on the training sets is shown below.)

A second function to extract predictions from resample results is `getRRPredictionList()` which returns a `list` of predictions split by data set (train/test) and resampling iteration.

```
predList = getRRPredictionList(r)
predList
## $train
## $train$`1`
## Prediction: 100 observations
## predict.type: response
## threshold:
## time: 0.00
##      id      truth   response
## 73   73 versicolor versicolor
## 12   12     setosa     setosa
## 30   30     setosa     setosa
## 100 100 versicolor versicolor
```

```
## 14   14     setosa     setosa
## 13   13     setosa     setosa
## ... (#rows: 100, #cols: 3)
##
##
## $test
## $test$`1`
## Prediction: 50 observations
## predict.type: response
## threshold:
## time: 0.00
##      id     truth  response
## 4     4    setosa    setosa
## 120 120 virginica virginica
## 147 147 virginica virginica
## 150 150 virginica virginica
## 36   36    setosa    setosa
## 113 113 virginica virginica
## ... (#rows: 50, #cols: 3)
```

2.5.3.2 Learner models

In each resampling iteration a Learner (`makeLearner()`) is fitted on the respective training set. By default, the resulting `WrappedModel` (`makeWrappedModel()`)s are not included in the `resample()` result and slot `$models` is empty. In order to keep them, set `models = TRUE` when calling `resample()`, as in the following survival analysis example.

```
### 3-fold cross-validation
rdesc = makeResampleDesc("CV", iters = 3)

r = resample("surv.coxph", lung.task, rdesc, show.info = FALSE, models = TRUE)
r$models
## [[1]]
## Model for learner.id=surv.coxph; learner.class=surv.coxph
## Trained on: task.id = lung-example; obs = 111; features = 8
## Hyperparameters:
##
## [[2]]
## Model for learner.id=surv.coxph; learner.class=surv.coxph
## Trained on: task.id = lung-example; obs = 112; features = 8
## Hyperparameters:
##
## [[3]]
## Model for learner.id=surv.coxph; learner.class=surv.coxph
## Trained on: task.id = lung-example; obs = 111; features = 8
## Hyperparameters:
```

2.5.3.3 The extract option

Keeping complete fitted models can be memory-intensive if these objects are large or the number of resampling iterations is high. Alternatively, you can use the `extract` argument of `resample()` to retain only the information you need. To this end you need to pass a function to `extract` which is applied to each `WrappedModel` (`makeWrappedModel()`) object fitted in each resampling iteration.

Below, we cluster the `datasets::mtcars()` data using the k-means algorithm with $k = 3$ and keep only the cluster centers.

```
### 3-fold cross-validation
rdesc = makeResampleDesc("CV", iters = 3)

### Extract the compute cluster centers
r = resample("cluster.kmeans", mtcars.task, rdesc, show.info = FALSE,
  centers = 3, extract = function(x) getLearnerModel(x)$centers)
r$extract
## [[1]]
##        mpg      cyl     disp       hp     drat       wt     qsec        vs
## 1 14.25714 8.000000 397.7143 238.4286 3.315714 4.310571 16.45857 0.0000000
## 2 16.26667 7.333333 272.9333 145.0000 2.863333 3.586667 18.36333 0.3333333
## 3 24.04167 4.666667 124.8500 101.0833 4.005000 2.510667 18.20000 0.7500000
##          am     gear     carb
## 1 0.2857143 3.571429 4.285714
## 2 0.0000000 3.000000 2.000000
## 3 0.6666667 4.166667 2.583333
##
## [[2]]
##        mpg cyl     disp       hp     drat       wt     qsec    vs   am
## 1 26.96250   4 103.2625  87.7500 4.038750 2.252250 19.17250 0.875 0.75
## 2 20.01667   6 176.3667 125.1667 3.723333 3.060000 17.60333 0.500 0.50
## 3 14.52857   8 356.8000 192.8571 3.157143 4.169857 17.21857 0.000 0.00
##    gear     carb
## 1 4.125 1.500000
## 2 4.000 3.833333
## 3 3.000 3.142857
##
## [[3]]
##        mpg      cyl     disp        hp     drat       wt     qsec
## 1 17.01429 7.428571 276.0571 150.71429 2.994286 3.601429 18.11857
## 2 25.87143 4.285714 112.7000  77.71429 4.064286 2.469286 19.34571
## 3 15.85714 8.000000 366.0000 238.42857 3.451429 3.825714 15.97714
##          vs        am     gear     carb
## 1 0.2857143 0.0000000 3.000000 2.142857
## 2 0.8571429 0.7142857 4.000000 1.857143
## 3 0.0000000 0.2857143 3.571429 4.000000
```

As a second example, we extract the variable importances from fitted regression trees using function `getFeatureImportance()`. (For more detailed information on this topic see the feature selection page.)

```
### Extract the variable importance in a regression tree
r = resample("regr.rpart", bh.task, rdesc, show.info = FALSE, extract = getFeatureImportance)
r$extract
## [[1]]
## FeatureImportance:
## Task: BostonHousing-example
##
## Learner: regr.rpart
## Measure: NA
## Contrast: NA
## Aggregation: function (x)  x
## Replace: NA
```

```
## Number of Monte-Carlo iterations: NA
## Local: FALSE
##       crim       zn    indus chas     nox    rm      age      dis rad tax
## 1 4024.545 1391.391 3988.385    0 2777.08 18189 3153.081 3821.744   0   0
##   ptratio        b    lstat
## 1 3684.97 439.2913 12181.12
##
## [[2]]
## FeatureImportance:
## Task: BostonHousing-example
##
## Learner: regr.rpart
## Measure: NA
## Contrast: NA
## Aggregation: function (x)  x
## Replace: NA
## Number of Monte-Carlo iterations: NA
## Local: FALSE
##      crim       zn    indus     chas      nox       rm      age      dis
## 1 4196.57 4569.979 6572.307 194.1832 930.3136 11015.25 5620.492 2128.454
##   rad      tax ptratio b    lstat
## 1   0 2399.372 1880.27 0 17519.93
##
## [[3]]
## FeatureImportance:
## Task: BostonHousing-example
##
## Learner: regr.rpart
## Measure: NA
## Contrast: NA
## Aggregation: function (x)  x
## Replace: NA
## Number of Monte-Carlo iterations: NA
## Local: FALSE
##       crim       zn    indus chas     nox       rm      age      dis
## 1 8332.523 390.2531 8864.274    0 8859.31 13399.81 7916.243 3163.789
##        rad      tax  ptratio b    lstat
## 1 741.4216 1204.485 1816.896 0 16358.64
```

2.5.4 Stratification and blocking

- *Stratification* with respect to a categorical variable makes sure that all its values are present in each training and test set in approximately the same proportion as in the original data set. Stratification is possible with regard to categorical target variables (and thus for supervised classification and survival analysis) or categorical explanatory variables.
- *Blocking* refers to the situation that subsets of observations belong together and must not be separated during resampling. Hence, for one train/test set pair the entire block is either in the training set or in the test set.

2.5.4.1 Stratification with respect to the target variable(s)

For classification, it is usually desirable to have the same proportion of the classes in all of the partitions

of the original data set. This is particularly useful in the case of imbalanced classes and small data sets. Otherwise, it may happen that observations of less frequent classes are missing in some of the training sets which can decrease the performance of the learner, or lead to model crashes. In order to conduct stratified resampling, set `stratify = TRUE` in `makeResampleDesc()`.

```
### 3-fold cross-validation
rdesc = makeResampleDesc("CV", iters = 3, stratify = TRUE)

r = resample("classif.lda", iris.task, rdesc, show.info = FALSE)
r
## Resample Result
## Task: iris-example
## Learner: classif.lda
## Aggr perf: mmce.test.mean=0.0198693
## Runtime: 0.0366127
```

Stratification is also available for survival tasks. Here the stratification balances the censoring rate.

2.5.4.2 Stratification with respect to explanatory variables

Sometimes it is required to also stratify on the input data, e.g., to ensure that all subgroups are represented in all training and test sets. To stratify on the input columns, specify `factor` columns of your task data via `stratify.cols`.

```
rdesc = makeResampleDesc("CV", iters = 3, stratify.cols = "chas")

r = resample("regr.rpart", bh.task, rdesc, show.info = FALSE)
r
## Resample Result
## Task: BostonHousing-example
## Learner: regr.rpart
## Aggr perf: mse.test.mean=21.7548424
## Runtime: 0.0555286
```

2.5.4.3 Blocking

If some observations "belong together" and must not be separated when splitting the data into training and test sets for resampling, you can supply this information via a `blocking factor` when creating the task.

```
### 5 blocks containing 30 observations each
task = makeClassifTask(data = iris, target = "Species", blocking = factor(rep(1:5, each = 30)))
task
## Supervised task: iris
## Type: classif
## Target: Species
## Observations: 150
## Features:
##    numerics     factors     ordered functionals
##           4           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: TRUE
## Has coordinates: FALSE
## Classes: 3
##     setosa versicolor  virginica
```

```
##         50         50         50
## Positive class: NA
```

2.5.5 Resample descriptions and resample instances

As already mentioned, you can specify a resampling strategy using function `makeResampleDesc()`.

```
rdesc = makeResampleDesc("CV", iters = 3)
rdesc
## Resample description: cross-validation with 3 iterations.
## Predict: test
## Stratification: FALSE
str(rdesc)
## List of 4
##  $ id      : chr "cross-validation"
##  $ iters   : int 3
##  $ predict : chr "test"
##  $ stratify: logi FALSE
##  - attr(*, "class")= chr [1:2] "CVDesc" "ResampleDesc"
str(makeResampleDesc("Subsample", stratify.cols = "chas"))
## List of 6
##  $ split        : num 0.667
##  $ id           : chr "subsampling"
##  $ iters        : int 30
##  $ predict      : chr "test"
##  $ stratify     : logi FALSE
##  $ stratify.cols: chr "chas"
##  - attr(*, "class")= chr [1:2] "SubsampleDesc" "ResampleDesc"
```

The result `rdesc` inherits from class `ResampleDesc` (`makeResampleDesc()`) (short for resample description) and, in principle, contains all necessary information about the resampling strategy including the number of iterations, the proportion of training and test sets, stratification variables, etc.

Given either the size of the data set at hand or the `Task()`, function `makeResampleInstance()` draws the training and test sets according to the `ResampleDesc` (`makeResampleDesc()`).

```
### Create a resample instance based an a task
rin = makeResampleInstance(rdesc, iris.task)
rin
## Resample instance for 150 cases.
## Resample description: cross-validation with 3 iterations.
## Predict: test
## Stratification: FALSE
str(rin)
## List of 5
##  $ desc      :List of 4
##   ..$ id      : chr "cross-validation"
##   ..$ iters   : int 3
##   ..$ predict : chr "test"
##   ..$ stratify: logi FALSE
##   ..- attr(*, "class")= chr [1:2] "CVDesc" "ResampleDesc"
##  $ size      : int 150
##  $ train.inds:List of 3
##   ..$ : int [1:100] 41 2 90 39 62 48 78 23 143 102 ...
```

```
##   ..$ : int [1:100] 30 5 90 77 58 39 62 23 102 117 ...
##   ..$ : int [1:100] 30 41 2 5 77 58 48 78 143 71 ...
##  $ test.inds :List of 3
##   ..$ : int [1:50] 4 5 8 10 15 24 28 30 31 32 ...
##   ..$ : int [1:50] 2 6 7 11 12 14 18 21 22 25 ...
##   ..$ : int [1:50] 1 3 9 13 16 17 19 20 23 26 ...
##  $ group     : Factor w/ 0 levels:
##  - attr(*, "class")= chr "ResampleInstance"
### Create a resample instance given the size of the data set
rin = makeResampleInstance(rdesc, size = nrow(iris))
str(rin)
## List of 5
##  $ desc      :List of 4
##   ..$ id      : chr "cross-validation"
##   ..$ iters   : int 3
##   ..$ predict : chr "test"
##   ..$ stratify: logi FALSE
##   ..- attr(*, "class")= chr [1:2] "CVDesc" "ResampleDesc"
##  $ size      : int 150
##  $ train.inds:List of 3
##   ..$ : int [1:100] 23 4 1 55 84 11 20 75 52 17 ...
##   ..$ : int [1:100] 4 118 1 78 84 11 146 19 45 41 ...
##   ..$ : int [1:100] 23 118 55 78 146 19 20 75 45 41 ...
##  $ test.inds :List of 3
##   ..$ : int [1:50] 7 8 10 12 16 19 21 22 24 25 ...
##   ..$ : int [1:50] 2 6 9 13 14 17 18 20 23 29 ...
##   ..$ : int [1:50] 1 3 4 5 11 15 28 31 32 35 ...
##  $ group     : Factor w/ 0 levels:
##  - attr(*, "class")= chr "ResampleInstance"
### Access the indices of the training observations in iteration 3
rin$train.inds[[3]]
##   [1]  23 118  55  78 146  19  20  75  45  41  52  17  70  40  49  86  39
##  [18]  80  85  22 104  62 129  33  18 127 132  69 133  29  57  79  77 113
##  [35] 114  68  96  13  73  34   9  81 141   8   6  53  83 134  16  63  95
##  [52] 125  74   2  58  89  92  14 102  38 117 110  91  36  66  27  94  71
##  [69]  82  42 128 105  51  26 115 144  76  21 139   7 116 143  25  88  30
##  [86]  50  12  90 106 108 103  99  47 107 148  10  44  87  24 137
```

The result `rin` inherits from class `ResampleInstance` (`makeResampleInstance()`) and contains `lists` of index vectors for the train and test sets.

If a `ResampleDesc` (`makeResampleDesc()`) is passed to `resample()`, it is instantiated internally. Naturally, it is also possible to pass a `ResampleInstance` (`makeResampleInstance()`) directly.

While the separation between resample descriptions, resample instances, and the `resample()` function itself seems overly complicated, it has several advantages:

- Resample instances readily allow for paired experiments, that is comparing the performance of several learners on exactly the same training and test sets. This is particularly useful if you want to add another method to a comparison experiment you already did. Moreover, you can store the resample instance along with your data in order to be able to reproduce your results later on.

```
rdesc = makeResampleDesc("CV", iters = 3)
rin = makeResampleInstance(rdesc, task = iris.task)

### Calculate the performance of two learners based on the same resample instance
```

```
r.lda = resample("classif.lda", iris.task, rin, show.info = FALSE)
r.rpart = resample("classif.rpart", iris.task, rin, show.info = FALSE)
r.lda$aggr
## mmce.test.mean
##     0.02666667
r.rpart$aggr
## mmce.test.mean
##     0.06666667
```

- In order to add further resampling methods you can simply derive from the `ResampleDesc` (`makeResampleDesc()`) and `ResampleInstance` (`makeResampleInstance()`) classes, but you do neither have to touch `resample()` nor any further methods that use the resampling strategy.

Usually, when calling `makeResampleInstance()` the train and test index sets are drawn randomly. Mainly for *holdout* (*test sample*) *estimation* you might want full control about the training and tests set and specify them manually. This can be done using function `makeFixedHoldoutInstance()`.

```
rin = makeFixedHoldoutInstance(train.inds = 1:100, test.inds = 101:150, size = 150)
rin
## Resample instance for 150 cases.
## Resample description: holdout with 0.67 split rate.
## Predict: test
## Stratification: FALSE
```

2.5.6 Aggregating performance values

In each resampling iteration $b = 1, \ldots, B$ we get performance values $S(D^{*b}, D \setminus D^{*b})$ (for each measure we wish to calculate), which are then aggregated to an overall performance.

For the great majority of common resampling strategies (like holdout, cross-validation, subsampling) performance values are calculated on the test data sets only and for most measures aggregated by taking the mean (`test.mean(aggregations())`).

Each performance `Measure` (`makeMeasure()`) in `mlr` has a corresponding default aggregation method which is stored in slot `$aggr`. The default aggregation for most measures is `test.mean(aggregations())`. One exception is the root mean square error (rmse).

```
### Mean misclassification error
mmce$aggr
## Aggregation function: test.mean
mmce$aggr$fun
## function (task, perf.test, perf.train, measure, group, pred)
## mean(perf.test)
## <bytecode: 0x8f46628>
## <environment: namespace:mlr>
### Root mean square error
rmse$aggr
## Aggregation function: test.rmse
rmse$aggr$fun
## function (task, perf.test, perf.train, measure, group, pred)
## sqrt(mean(perf.test^2))
## <bytecode: 0xc743228>
## <environment: namespace:mlr>
```

You can change the aggregation method of a `Measure` (`makeMeasure()`) via function `setAggregation()`. All available aggregation schemes are listed on the `aggregations()` documentation page.

2.5.6.1 Example: One measure with different aggregations

The aggregation schemes `test.median` (`aggregations()`), `test.min` (`aggregations()`), and `text.max` (`aggregations()`) compute the median, minimum, and maximum of the performance values on the test sets.

```
mseTestMedian = setAggregation(mse, test.median)
mseTestMin = setAggregation(mse, test.min)
mseTestMax = setAggregation(mse, test.max)

mseTestMedian
## Name: Mean of squared errors
## Performance measure: mse
## Properties: regr,req.pred,req.truth
## Minimize: TRUE
## Best: 0; Worst: Inf
## Aggregated by: test.median
## Arguments: list()
## Note: Defined as: mean((response - truth)^2)
rdesc = makeResampleDesc("CV", iters = 3)
r = resample("regr.lm", bh.task, rdesc, measures = list(mse, mseTestMedian, mseTestMin, mseTestMax))
## Resampling: cross-validation
## Measures:             mse       mse       mse       mse
## [Resample] iter 1:    21.152892421.152892421.152892421.1528924
## [Resample] iter 2:    23.715531923.715531923.715531923.7155319
## [Resample] iter 3:    30.821725530.821725530.821725530.8217255
##
## Aggregated Result: mse.test.mean=25.2300499,mse.test.median=23.7155319,mse.test.min=21.1528924,mse.te
##
r
## Resample Result
## Task: BostonHousing-example
## Learner: regr.lm
## Aggr perf: mse.test.mean=25.2300499,mse.test.median=23.7155319,mse.test.min=21.1528924,mse.test.max=3
## Runtime: 0.0465388
r$aggr
##   mse.test.mean mse.test.median    mse.test.min    mse.test.max
##        25.23005        23.71553        21.15289        30.82173
```

2.5.6.2 Example: Calculating the training error

Below we calculate the mean misclassification error (mmce) on the training and the test data sets. Note that we have to set `predict = "both"` when calling `makeResampleDesc()` in order to get predictions on both training and test sets.

```
mmceTrainMean = setAggregation(mmce, train.mean)
rdesc = makeResampleDesc("CV", iters = 3, predict = "both")
r = resample("classif.rpart", iris.task, rdesc, measures = list(mmce, mmceTrainMean))
## Resampling: cross-validation
## Measures:             mmce.train   mmce.test
## [Resample] iter 1:    0.0200000    0.1200000
## [Resample] iter 2:    0.0400000    0.0400000
## [Resample] iter 3:    0.0400000    0.0400000
##
## Aggregated Result: mmce.test.mean=0.0666667,mmce.train.mean=0.0333333
##
```

```
r$measures.train
##   iter mmce mmce
## 1    1 0.02 0.02
## 2    2 0.04 0.04
## 3    3 0.04 0.04
r$aggr
##  mmce.test.mean mmce.train.mean
##      0.06666667      0.03333333
```

2.5.6.3 Example: Bootstrap

In *out-of-bag bootstrap estimation* B new data sets $D^{*1}, \ldots, D^{*B}$ are drawn from the data set D with replacement, each of the same size as D. In the b-th iteration, D^{*b} forms the training set, while the remaining elements from D, i.e., $D \setminus D^{*b}$, form the test set.

The *b632* and *b632+* variants calculate a convex combination of the training performance and the out-of-bag bootstrap performance and thus require predictions on the training sets and an appropriate aggregation strategy.

```
### Use bootstrap as resampling strategy and predict on both train and test sets
rdesc = makeResampleDesc("Bootstrap", predict = "both", iters = 10)

### Set aggregation schemes for b632 and b632+ bootstrap
mmceB632 = setAggregation(mmce, b632)
mmceB632plus = setAggregation(mmce, b632plus)

mmceB632
## Name: Mean misclassification error
## Performance measure: mmce
## Properties: classif,classif.multi,req.pred,req.truth
## Minimize: TRUE
## Best: 0; Worst: 1
## Aggregated by: b632
## Arguments: list()
## Note: Defined as: mean(response != truth)
r = resample("classif.rpart", iris.task, rdesc, measures = list(mmce, mmceB632, mmceB632plus),
  show.info = FALSE)
head(r$measures.train)
##   iter       mmce       mmce       mmce
## 1    1 0.04666667 0.04666667 0.04666667
## 2    2 0.01333333 0.01333333 0.01333333
## 3    3 0.01333333 0.01333333 0.01333333
## 4    4 0.03333333 0.03333333 0.03333333
## 5    5 0.04666667 0.04666667 0.04666667
## 6    6 0.03333333 0.03333333 0.03333333
### Compare misclassification rates for out-of-bag, b632, and b632+ bootstrap
r$aggr
## mmce.test.mean      mmce.b632  mmce.b632plus
##     0.04654660     0.03972145     0.04025534
```

2.5.7 Convenience functions

The functionality described on this page allows for much control and flexibility. However, when quickly trying out some learners, it can get tedious to type all the code for defining the resampling strategy, setting the

aggregation scheme and so on. As mentioned above, `mlr` includes some pre-defined resample description objects for frequently used strategies like, e.g., 5-fold cross-validation (`cv5` (`makeResampleDesc()`)). Moreover, `mlr` provides special functions for the most common resampling methods, for example `holdout` (`resample()`), `crossval` (`resample()`), or `bootstrapB632` (`resample()`).

```
crossval("classif.lda", iris.task, iters = 3, measures = list(mmce, ber))
## Resampling: cross-validation
## Measures:             mmce      ber
## [Resample] iter 1:    0.0000000 0.0000000
## [Resample] iter 2:    0.0000000 0.0000000
## [Resample] iter 3:    0.0600000 0.0703704
##
## Aggregated Result: mmce.test.mean=0.0200000,ber.test.mean=0.0234568
##
## Resample Result
## Task: iris-example
## Learner: classif.lda
## Aggr perf: mmce.test.mean=0.0200000,ber.test.mean=0.0234568
## Runtime: 0.0433581
bootstrapB632plus("regr.lm", bh.task, iters = 3, measures = list(mse, mae))
## Resampling: OOB bootstrapping
## Measures:             mse.train   mae.train   mse.test    mae.test
## [Resample] iter 1:    21.7610219  3.3407793   21.5016399  3.1758042
## [Resample] iter 2:    20.4289067  3.2175218   26.7737066  3.6056414
## [Resample] iter 3:    22.3656903  3.4060824   25.8328927  3.7107234
##
## Aggregated Result: mse.b632plus=23.5635240,mae.b632plus=3.4361348
##
## Resample Result
## Task: BostonHousing-example
## Learner: regr.lm
## Aggr perf: mse.b632plus=23.5635240,mae.b632plus=3.4361348
## Runtime: 0.0794981
```

2.6 Tuning Hyperparameters

Many machine learning algorithms have hyperparameters that need to be set. If selected by the user they can be specified as explained on the tutorial page on learners – simply pass them to `makeLearner()`. Often suitable parameter values are not obvious and it is preferable to tune the hyperparameters, that is automatically identify values that lead to the best performance.

In order to tune a machine learning algorithm, you have to specify:

- the search space
- the optimization algorithm (aka tuning method)
- an evaluation method, i.e., a resampling strategy and a performance measure

An example of the search space could be searching values of the `C` parameter for `kernlab::ksvm()`:

```
### ex: create a search space for the C hyperparameter from 0.01 to 0.1
ps = makeParamSet(
  makeNumericParam("C", lower = 0.01, upper = 0.1)
)
```

An example of the optimization algorithm could be performing random search on the space:

```
### ex: random search with 100 iterations
ctrl = makeTuneControlRandom(maxit = 100L)
```

An example of an evaluation method could be 3-fold CV using accuracy as the performance measure:

```
rdesc = makeResampleDesc("CV", iters = 3L)
measure = acc
```

The evaluation method is already covered in detail in evaluation of learning methods and resampling.

In this tutorial, we show how to specify the search space and optimization algorithm, how to do the tuning and how to access the tuning result, and how to visualize the hyperparameter tuning effects through several examples.

Throughout this section we consider classification examples. For the other types of learning problems, you can follow the same process analogously.

We use the iris classification task (`iris.task()`) for illustration and tune the hyperparameters of an SVM (function `kernlab::ksvm()`) from the `kernlab` package) with a radial basis kernel. The following examples tune the cost parameter `C` and the RBF kernel parameter `sigma` of the `kernlab::ksvm()`) function.

2.6.1 Specifying the search space

We first must define a space to search when tuning our learner. For example, maybe we want to tune several specific values of a hyperparameter or perhaps we want to define a space from 10^{-10} to 10^{10} and let the optimization algorithm decide which points to choose.

In order to define a search space, we create a `ParamSet` (`ParamHelpers::makeParamSet()`) object, which describes the parameter space we wish to search. This is done via the function `ParamHelpers::makeParamSet()`.

For example, we could define a search space with just the values 0.5, 1.0, 1.5, 2.0 for both `C` and `gamma`. Notice how we name each parameter as it's defined in the `kernlab` package:

```
discrete_ps = makeParamSet(
  makeDiscreteParam("C", values = c(0.5, 1.0, 1.5, 2.0)),
  makeDiscreteParam("sigma", values = c(0.5, 1.0, 1.5, 2.0))
)
print(discrete_ps)
##           Type len Def      Constr Req Tunable Trafo
## C     discrete   -   - 0.5,1,1.5,2   -    TRUE     -
## sigma discrete   -   - 0.5,1,1.5,2   -    TRUE     -
```

We could also define a continuous search space (using `makeNumericParam` (`ParamHelpers::makeNumericParam()`) instead of `makeDiscreteParam` (`ParamHelpers::makeDiscreteParam()`)) from 10^{-10} to 10^{10} for both parameters through the use of the `trafo` argument (trafo is short for transformation). Transformations work like this: All optimizers basically see the parameters on their original scale (from -10 to 10 in this case) and produce values on this scale during the search. Right before they are passed to the learning algorithm, the transformation function is applied.

Notice this time we use `makeNumericParam` (`ParamHelpers::makeNumericParam()`):

```
num_ps = makeParamSet(
  makeNumericParam("C", lower = -10, upper = 10, trafo = function(x) 10^x),
  makeNumericParam("sigma", lower = -10, upper = 10, trafo = function(x) 10^x)
)
```

Many other parameters can be created, check out the examples in `ParamHelpers::makeParamSet()`.

In order to standardize your workflow across several packages, whenever parameters in the underlying **R** functions should be passed in a `list` structure, `mlr` tries to give you direct access to each parameter and get rid of the list structure!

This is the case with the `kpar` argument of `kernlab::ksvm()`) which is a list of kernel parameters like `sigma`. This allows us to interface with learners from different packages in the same way when defining parameters to tune!

2.6.2 Specifying the optimization algorithm

Now that we have specified the search space, we need to choose an optimization algorithm for our parameters to pass to the `kernlab::ksvm()`) learner. Optimization algorithms are considered `TuneControl()` objects in `mlr`.

A grid search is one of the standard – albeit slow – ways to choose an appropriate set of parameters from a given search space.

In the case of `discrete_ps` above, since we have manually specified the values, grid search will simply be the cross product. We create the grid search object using the defaults, noting that we will have $4 \times 4 = 16$ combinations in the case of `discrete_ps`:

```
ctrl = makeTuneControlGrid()
```

In the case of `num_ps` above, since we have only specified the upper and lower bounds for the search space, grid search will create a grid using equally-sized steps. By default, grid search will span the space in 10 equal-sized steps. The number of steps can be changed with the `resolution` argument. Here we change to 15 equal-sized steps in the space defined within the `ParamSet` (`ParamHelpers::makeParamSet()`) object. For `num_ps`, this means 15 steps in the form of `10 ^ seq(-10, 10, length.out = 15)`:

```
ctrl = makeTuneControlGrid(resolution = 15L)
```

Many other types of optimization algorithms are available. Check out `TuneControl()` for some examples.

Since grid search is normally too slow in practice, we'll also examine random search. In the case of `discrete_ps`, random search will randomly choose from the specified values. The `maxit` argument controls the amount of iterations.

```
ctrl = makeTuneControlRandom(maxit = 10L)
```

In the case of `num_ps`, random search will randomly choose points within the space according to the specified bounds. Perhaps in this case we would want to increase the amount of iterations to ensure we adequately cover the space:

```
ctrl = makeTuneControlRandom(maxit = 200L)
```

2.6.3 Performing the tuning

Now that we have specified a search space and the optimization algorithm, it's time to perform the tuning. We will need to define a resampling strategy and make note of our performance measure.

We will use 3-fold cross-validation to assess the quality of a specific parameter setting. For this we need to create a resampling description just like in the resampling part of the tutorial.

```
rdesc = makeResampleDesc("CV", iters = 3L)
```

Finally, by combining all the previous pieces, we can tune the SVM parameters by calling `tuneParams()`. We will use `discrete_ps` with grid search:

```
discrete_ps = makeParamSet(
  makeDiscreteParam("C", values = c(0.5, 1.0, 1.5, 2.0)),
  makeDiscreteParam("sigma", values = c(0.5, 1.0, 1.5, 2.0))
)
ctrl = makeTuneControlGrid()
rdesc = makeResampleDesc("CV", iters = 3L)
res = tuneParams("classif.ksvm", task = iris.task, resampling = rdesc,
  par.set = discrete_ps, control = ctrl)
## [Tune] Started tuning learner classif.ksvm for parameter set:
##           Type len Def      Constr Req Tunable Trafo
## C     discrete   -   - 0.5,1,1.5,2   -    TRUE     -
## sigma discrete   -   - 0.5,1,1.5,2   -    TRUE     -
## With control class: TuneControlGrid
## Imputation value: 1
## [Tune-x] 1: C=0.5; sigma=0.5
## [Tune-y] 1: mmce.test.mean=0.0533333; time: 0.0 min
## [Tune-x] 2: C=1; sigma=0.5
## [Tune-y] 2: mmce.test.mean=0.0533333; time: 0.0 min
## [Tune-x] 3: C=1.5; sigma=0.5
## [Tune-y] 3: mmce.test.mean=0.0466667; time: 0.0 min
## [Tune-x] 4: C=2; sigma=0.5
## [Tune-y] 4: mmce.test.mean=0.0466667; time: 0.0 min
## [Tune-x] 5: C=0.5; sigma=1
## [Tune-y] 5: mmce.test.mean=0.0600000; time: 0.0 min
## [Tune-x] 6: C=1; sigma=1
## [Tune-y] 6: mmce.test.mean=0.0600000; time: 0.0 min
## [Tune-x] 7: C=1.5; sigma=1
## [Tune-y] 7: mmce.test.mean=0.0533333; time: 0.0 min
## [Tune-x] 8: C=2; sigma=1
## [Tune-y] 8: mmce.test.mean=0.0600000; time: 0.0 min
## [Tune-x] 9: C=0.5; sigma=1.5
## [Tune-y] 9: mmce.test.mean=0.0733333; time: 0.0 min
## [Tune-x] 10: C=1; sigma=1.5
## [Tune-y] 10: mmce.test.mean=0.0533333; time: 0.0 min
## [Tune-x] 11: C=1.5; sigma=1.5
## [Tune-y] 11: mmce.test.mean=0.0533333; time: 0.0 min
## [Tune-x] 12: C=2; sigma=1.5
## [Tune-y] 12: mmce.test.mean=0.0533333; time: 0.0 min
## [Tune-x] 13: C=0.5; sigma=2
## [Tune-y] 13: mmce.test.mean=0.0600000; time: 0.0 min
## [Tune-x] 14: C=1; sigma=2
## [Tune-y] 14: mmce.test.mean=0.0600000; time: 0.0 min
## [Tune-x] 15: C=1.5; sigma=2
## [Tune-y] 15: mmce.test.mean=0.0600000; time: 0.0 min
## [Tune-x] 16: C=2; sigma=2
## [Tune-y] 16: mmce.test.mean=0.0600000; time: 0.0 min
## [Tune] Result: C=1.5; sigma=0.5 : mmce.test.mean=0.0466667
res
## Tune result:
## Op. pars: C=1.5; sigma=0.5
## mmce.test.mean=0.0466667
```

`tuneParams()` simply performs the cross-validation for every element of the cross-product and selects the parameter setting with the best mean performance. As no performance measure was specified, by default the

error rate (mmce) is used.

Note that each measure (`makeMeasure()`) "knows" if it is minimized or maximized during tuning.

```
### error rate
mmce$minimize
## [1] TRUE
### accuracy
acc$minimize
## [1] FALSE
```

Of course, you can pass other measures and also a `list` of measures to `tuneParams()`. In the latter case the first measure is optimized during tuning, the others are simply evaluated. If you are interested in optimizing several measures simultaneously have a look at Advanced Tuning.

In the example below we calculate the accuracy (acc) instead of the error rate. We use function `setAggregation()`, as described on the resampling page, to additionally obtain the standard deviation of the accuracy. We also use random search with 100 iterations on the `num_set` we defined above and set `show.info` to `FALSE` to hide the output for all 100 iterations:

```
num_ps = makeParamSet(
  makeNumericParam("C", lower = -10, upper = 10, trafo = function(x) 10^x),
  makeNumericParam("sigma", lower = -10, upper = 10, trafo = function(x) 10^x)
)
ctrl = makeTuneControlRandom(maxit = 100L)
res = tuneParams("classif.ksvm", task = iris.task, resampling = rdesc, par.set = num_ps,
  control = ctrl, measures = list(acc, setAggregation(acc, test.sd)), show.info = FALSE)
res
## Tune result:
## Op. pars: C=2.77e+03; sigma=0.000686
## acc.test.mean=0.9733333,acc.test.sd=0.0115470
```

2.6.4 Accessing the tuning result

The result object `TuneResult()` allows you to access the best found settings `$x` and their estimated performance `$y`.

```
res$x
## $C
## [1] 2767.19
##
## $sigma
## [1] 0.0006856215
res$y
## acc.test.mean   acc.test.sd
##    0.97333333    0.01154701
```

We can generate a Learner (`makeLearner()`) with optimal hyperparameter settings as follows:

```
lrn = setHyperPars(makeLearner("classif.ksvm"), par.vals = res$x)
lrn
## Learner classif.ksvm from package kernlab
## Type: classif
## Name: Support Vector Machines; Short name: ksvm
## Class: classif.ksvm
## Properties: twoclass,multiclass,numerics,factors,prob,class.weights
```

```
## Predict-Type: response
## Hyperparameters: fit=FALSE,C=2.77e+03,sigma=0.000686
```

Then you can proceed as usual. Here we refit and predict the learner on the complete iris (`datasets::iris()`) data set:

```
m = train(lrn, iris.task)
predict(m, task = iris.task)
## Prediction: 150 observations
## predict.type: response
## threshold:
## time: 0.00
##   id  truth response
## 1  1 setosa   setosa
## 2  2 setosa   setosa
## 3  3 setosa   setosa
## 4  4 setosa   setosa
## 5  5 setosa   setosa
## 6  6 setosa   setosa
## ... (#rows: 150, #cols: 3)
```

But what if you wanted to inspect the other points on the search path, not just the optimal?

2.6.5 Investigating hyperparameter tuning effects

We can inspect all points evaluated during the search by using `generateHyperParsEffectData()`:

```
generateHyperParsEffectData(res)
## HyperParsEffectData:
## Hyperparameters: C,sigma
## Measures: acc.test.mean,acc.test.sd
## Optimizer: TuneControlRandom
## Nested CV Used: FALSE
## Snapshot of data:
##           C      sigma acc.test.mean acc.test.sd iteration exec.time
## 1  9.087234 -1.3383969     0.9200000  0.06000000         1     0.061
## 2  1.646101  7.8580028     0.2533333  0.04163332         2     0.062
## 3  6.657495  0.2534216     0.9266667  0.03055050         3     0.059
## 4 -7.178891 -5.5187732     0.2533333  0.04163332         4     0.077
## 5  9.663538 -3.8076717     0.9466667  0.03055050         5     0.073
## 6 -5.446035 -1.0537922     0.2533333  0.04163332         6     0.063
```

Note that the result of `generateHyperParsEffectData()` contains the parameter values *on the original scale*. In order to get the *transformed* parameter values instead, use the `trafo` argument:

```
generateHyperParsEffectData(res, trafo = TRUE)
## HyperParsEffectData:
## Hyperparameters: C,sigma
## Measures: acc.test.mean,acc.test.sd
## Optimizer: TuneControlRandom
## Nested CV Used: FALSE
## Snapshot of data:
##              C        sigma acc.test.mean acc.test.sd iteration exec.time
## 1 1.222457e+09 4.587785e-02     0.9200000  0.06000000         1     0.061
## 2 4.426909e+01 7.211121e+07     0.2533333  0.04163332         2     0.062
```

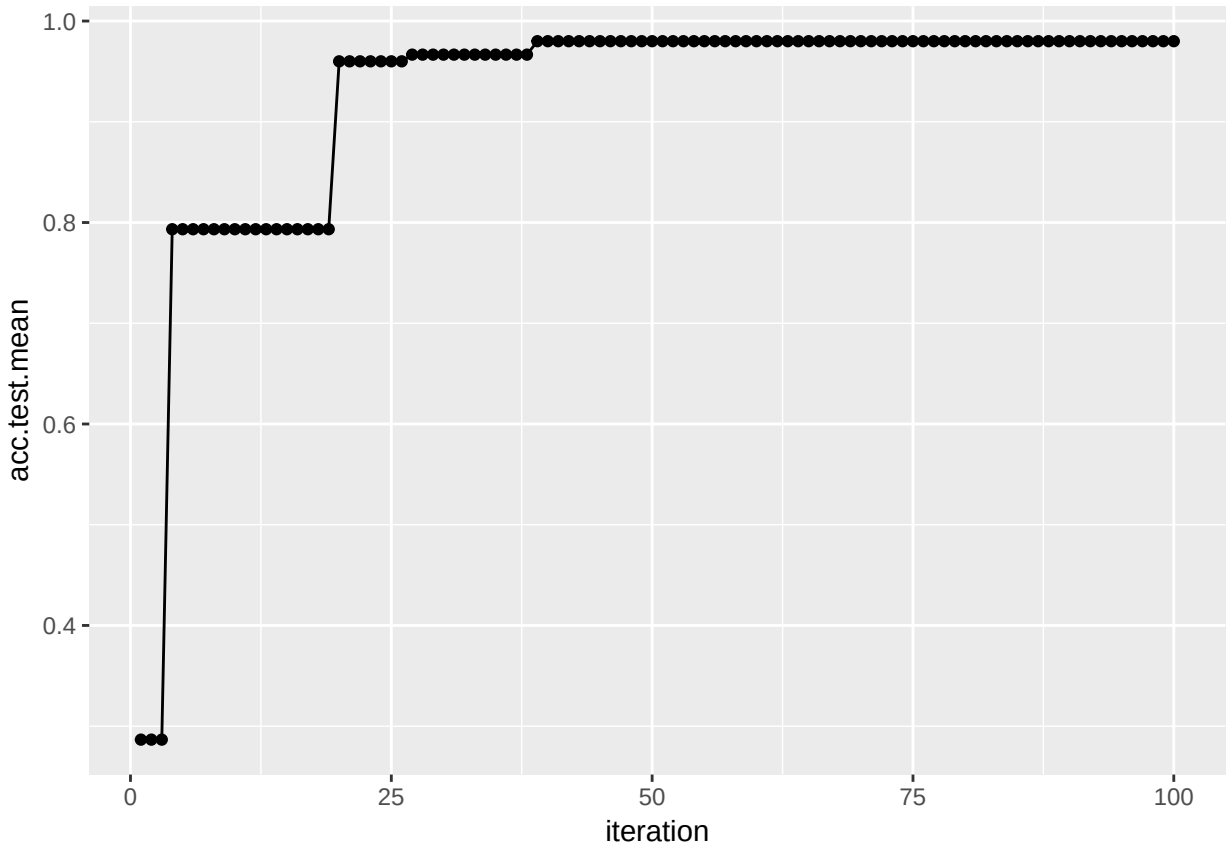
```
## 3 4.544596e+06 1.792345e+00     0.9266667  0.03055050         3     0.059
## 4 6.623823e-08 3.028494e-06     0.2533333  0.04163332         4     0.077
## 5 4.608273e+09 1.557142e-04     0.9466667  0.03055050         5     0.073
## 6 3.580674e-06 8.835025e-02     0.2533333  0.04163332         6     0.063
```

Note that we can also generate performance on the train data along with the validation/test data, as discussed on the resampling tutorial page:

```
rdesc2 = makeResampleDesc("Holdout", predict = "both")
res2 = tuneParams("classif.ksvm", task = iris.task, resampling = rdesc2, par.set = num_ps,
  control = ctrl, measures = list(acc, setAggregation(acc, train.mean)), show.info = FALSE)
generateHyperParsEffectData(res2)
## HyperParsEffectData:
## Hyperparameters: C,sigma
## Measures: acc.test.mean,acc.train.mean
## Optimizer: TuneControlRandom
## Nested CV Used: FALSE
## Snapshot of data:
##            C     sigma acc.test.mean acc.train.mean iteration exec.time
## 1 -2.5346578 -8.058910          0.30           0.35         1     0.032
## 2  6.0379349 -4.628623          0.96           0.99         2     0.050
## 3  1.4071660  9.574835          0.32           1.00         3     0.032
## 4  2.2464506 -8.229662          0.30           0.35         4     0.031
## 5  9.5797507 -4.879571          0.94           0.96         5     0.033
## 6 -0.5528879 -8.810588          0.30           0.35         6     0.038
```

We can also easily visualize the points evaluated by using `plotHyperParsEffect()`. In the example below, we plot the performance over iterations, using the `res` from the previous section but instead with 2 performance measures:

```
res = tuneParams("classif.ksvm", task = iris.task, resampling = rdesc, par.set = num_ps,
  control = ctrl, measures = list(acc, mmce), show.info = FALSE)
data = generateHyperParsEffectData(res)
plotHyperParsEffect(data, x = "iteration", y = "acc.test.mean",
  plot.type = "line")
```



Note that by default, we only plot the current global optima. This can be changed with the `global.only` argument.

For an in-depth exploration of generating hyperparameter tuning effects and plotting the data, check out Hyperparameter Tuning Effects.

2.6.6 Further comments

- Tuning works for all other tasks like regression, survival analysis and so on in a completely similar fashion.
- In longer running tuning experiments it is very annoying if the computation stops due to numerical or other errors. Have a look at `on.learner.error` in `configureMlr()` as well as the examples given in section configure mlr of this tutorial. You might also want to inform yourself about `impute.val` in `TuneControl()`.
- As we continually optimize over the same data during tuning, the estimated performance value might be optimistically biased. A clean approach to ensure unbiased performance estimation is nested resampling, where we embed the whole model selection process into an outer resampling loop.

2.7 Benchmark Experiments

In a benchmark experiment different learning methods are applied to one or several data sets with the aim to compare and rank the algorithms with respect to one or more performance measures.

In `mlr` a benchmark experiment can be conducted by calling function `benchmark()` on a `base::list()` of `makeLearner()`s and a `base::list()` of `Task()`s. `benchmark()` basically executes `resample()` for each

combination of `makeLearner()` and `Task()`. You can specify an individual resampling strategy for each `Task()` and select one or multiple performance measures to be calculated.

2.7.1 Conducting benchmark experiments

We start with a small example. Two learners, `MASS::lda()` and a `rpart::rpart()`, are applied to one classification problem (`sonar.task()`). As resampling strategy we choose `"Holdout"`. The performance is thus calculated on a single randomly sampled test data set.

In the example below we create a resample description (`makeResampleDesc()`), which is automatically instantiated by `benchmark()`. The instantiation is done only once per `Task()`, i.e., the same training and test sets are used for all learners. It is also possible to directly pass a `makeResampleInstance()`.

If you would like to use a *fixed test data set* instead of a randomly selected one, you can create a suitable `makeResampleInstance()` through function `makeFixedHoldoutInstance()`.

```
### Two learners to be compared
lrns = list(makeLearner("classif.lda"), makeLearner("classif.rpart"))

### Choose the resampling strategy
rdesc = makeResampleDesc("Holdout")

### Conduct the benchmark experiment
bmr = benchmark(lrns, sonar.task, rdesc)
## Task: Sonar-example, Learner: classif.lda
## Resampling: holdout
## Measures:             mmce
## [Resample] iter 1:    0.2571429
##
## Aggregated Result: mmce.test.mean=0.2571429
##
## Task: Sonar-example, Learner: classif.rpart
## Resampling: holdout
## Measures:             mmce
## [Resample] iter 1:    0.2714286
##
## Aggregated Result: mmce.test.mean=0.2714286
##
bmr
##         task.id    learner.id mmce.test.mean
## 1 Sonar-example   classif.lda      0.2571429
## 2 Sonar-example classif.rpart      0.2714286
```

For convenience, if you don't want to pass any additional arguments to `makeLearner()`, you don't need to generate the `makeLearner()`s explicitly, but it's sufficient to provide the learner name. In the above example we could also have written:

```
### Vector of strings
lrns = c("classif.lda", "classif.rpart")

### A mixed list of Learner objects and strings works, too
lrns = list(makeLearner("classif.lda", predict.type = "prob"), "classif.rpart")

bmr = benchmark(lrns, sonar.task, rdesc)
## Task: Sonar-example, Learner: classif.lda
## Resampling: holdout
```

```
## Measures:             mmce
## [Resample] iter 1:    0.3000000
##
## Aggregated Result: mmce.test.mean=0.3000000
##
## Task: Sonar-example, Learner: classif.rpart
## Resampling: holdout
## Measures:             mmce
## [Resample] iter 1:    0.3142857
##
## Aggregated Result: mmce.test.mean=0.3142857
##
bmr
##         task.id    learner.id mmce.test.mean
## 1 Sonar-example   classif.lda      0.3000000
## 2 Sonar-example classif.rpart      0.3142857
```

In the printed summary table every row corresponds to one pair of `Task()` and `makeLearner()`. The entries show the mean misclassification error, the default performance measure for classification, on the test data set.

The result `bmr` is an object of class `BenchmarkResult()`. Basically, it contains a `base::list()` of lists of `ResampleResult()` objects, first ordered by `Task()` and then by `makeLearner()`.

2.7.1.1 Making experiments reproducible

Typically, we would want our experiment results to be reproducible. `mlr` obeys the `set.seed` function, so make sure to use `set.seed` at the beginning of your script if you would like your results to be reproducible.

Note that if you are using parallel computing, you may need to adjust how you call `set.seed` depending on your usecase. One possibility is to use `set.seed(123, "L'Ecuyer")` in order to ensure the results are reproducible for each child process. See the examples in `parallel::mclapply()` for more information on reproducibility and parallel computing.

2.7.2 Accessing benchmark results

`mlr` provides several accessor functions, named `getBMR<WhatToExtract>`, that permit to retrieve information for further analyses. This includes for example the performances or predictions of the learning algorithms under consideration.

2.7.2.1 Learner performances

Let's have a look at the benchmark result above. `getBMRPerformances()` returns individual performances in resampling runs, while `getBMRAggrPerformances()` gives the aggregated values.

```
getBMRPerformances(bmr)
## $`Sonar-example`
## $`Sonar-example`$classif.lda
##   iter mmce
## 1    1  0.3
##
## $`Sonar-example`$classif.rpart
##   iter      mmce
## 1    1 0.3142857
getBMRAggrPerformances(bmr)
```

```
## $`Sonar-example`
## $`Sonar-example`$classif.lda
## mmce.test.mean
##            0.3
##
## $`Sonar-example`$classif.rpart
## mmce.test.mean
##      0.3142857
```

Since we used holdout as resampling strategy, individual and aggregated performance values coincide.

By default, nearly all "getter" functions return a nested `base::list()`, with the first level indicating the task and the second level indicating the learner. If only a single learner or, as in our case a single task is considered, setting `drop = TRUE` simplifies the result to a flat `base::list()`.

```
getBMRPerformances(bmr, drop = TRUE)
## $classif.lda
##   iter mmce
## 1    1  0.3
##
## $classif.rpart
##   iter      mmce
## 1    1 0.3142857
```

Often it is more convenient to work with `base::data.frame()`s. You can easily convert the result structure by setting `as.df = TRUE`.

```
getBMRPerformances(bmr, as.df = TRUE)
##         task.id    learner.id iter      mmce
## 1 Sonar-example   classif.lda    1 0.3000000
## 2 Sonar-example classif.rpart    1 0.3142857
getBMRAggrPerformances(bmr, as.df = TRUE)
##         task.id    learner.id mmce.test.mean
## 1 Sonar-example   classif.lda      0.3000000
## 2 Sonar-example classif.rpart      0.3142857
```

2.7.2.2 Predictions

Per default, the `BenchmarkResult()` contains the learner predictions. If you do not want to keep them, e.g., to conserve memory, set `keep.pred = FALSE` when calling `benchmark()`.

You can access the predictions using function `getBMRPredictions()`. Per default, you get a nested `base::list()` of `ResamplePrediction()`objects. As above, you can use the `drop` or `as.df` options to simplify the result.

```
getBMRPredictions(bmr)
## $`Sonar-example`
## $`Sonar-example`$classif.lda
## Resampled Prediction for:
## Resample description: holdout with 0.67 split rate.
## Predict: test
## Stratification: FALSE
## predict.type: prob
## threshold: M=0.50,R=0.50
## time (mean): 0.01
##    id truth       prob.M    prob.R response iter  set
```

```
## 1 110     M 1.030021e-02 0.9896998        R    1 test
## 2  87     R 7.021385e-01 0.2978615        M    1 test
## 3 128     M 1.830008e-03 0.9981700        R    1 test
## 4  38     R 1.741571e-04 0.9998258        R    1 test
## 5  65     R 8.870874e-06 0.9999911        R    1 test
## 6  12     R 2.029072e-01 0.7970928        R    1 test
## ... (#rows: 70, #cols: 7)
##
## $`Sonar-example`$classif.rpart
## Resampled Prediction for:
## Resample description: holdout with 0.67 split rate.
## Predict: test
## Stratification: FALSE
## predict.type: response
## threshold:
## time (mean): 0.01
##    id truth response iter  set
## 1 110     M        R    1 test
## 2  87     R        R    1 test
## 3 128     M        R    1 test
## 4  38     R        R    1 test
## 5  65     R        M    1 test
## 6  12     R        R    1 test
## ... (#rows: 70, #cols: 5)
head(getBMRPredictions(bmr, as.df = TRUE))
##         task.id  learner.id  id truth       prob.M    prob.R response iter
## 1 Sonar-example classif.lda 110     M 1.030021e-02 0.9896998        R    1
## 2 Sonar-example classif.lda  87     R 7.021385e-01 0.2978615        M    1
## 3 Sonar-example classif.lda 128     M 1.830008e-03 0.9981700        R    1
## 4 Sonar-example classif.lda  38     R 1.741571e-04 0.9998258        R    1
## 5 Sonar-example classif.lda  65     R 8.870874e-06 0.9999911        R    1
## 6 Sonar-example classif.lda  12     R 2.029072e-01 0.7970928        R    1
##    set
## 1 test
## 2 test
## 3 test
## 4 test
## 5 test
## 6 test
```

It is also easily possible to access results for certain learners or tasks via their IDs. For this purpose many "getter" functions have a `learner.ids` and a `task.ids` argument.

```
head(getBMRPredictions(bmr, learner.ids = "classif.rpart", as.df = TRUE))
##         task.id    learner.id  id truth response iter  set
## 1 Sonar-example classif.rpart 110     M        R    1 test
## 2 Sonar-example classif.rpart  87     R        R    1 test
## 3 Sonar-example classif.rpart 128     M        R    1 test
## 4 Sonar-example classif.rpart  38     R        R    1 test
## 5 Sonar-example classif.rpart  65     R        M    1 test
## 6 Sonar-example classif.rpart  12     R        R    1 test
```

If you don't like the default IDs, you can set the IDs of learners and tasks via the `id` option of `makeLearner()` and `makeTask()`. Moreover, you can conveniently change the ID of a `makeLearner()` via function `setLearnerid()`.

2.7.2.3 IDs

The IDs of all `makeLearner()`s, `Task()`s and Measure's (`makeMeasure()`) in a benchmark experiment can be retrieved as follows:

```
getBMRTaskIds(bmr)
## [1] "Sonar-example"
getBMRLearnerIds(bmr)
## [1] "classif.lda"   "classif.rpart"
getBMRMeasureIds(bmr)
## [1] "mmce"
```

2.7.2.4 Fitted models

Per default the `BenchmarkResult()` also contains the fitted models for all learners on all tasks. If you do not want to keep them set `models = FALSE` when calling `benchmark()`. The fitted models can be retrieved by function `getBMRModels()`. It returns a (possibly nested) `base::list()` of `WrappedModel` (`makeWrappedModel()`) objects.

```
getBMRModels(bmr)
## $`Sonar-example`
## $`Sonar-example`$classif.lda
## $`Sonar-example`$classif.lda[[1]]
## Model for learner.id=classif.lda; learner.class=classif.lda
## Trained on: task.id = Sonar-example; obs = 138; features = 60
## Hyperparameters:
##
##
## $`Sonar-example`$classif.rpart
## $`Sonar-example`$classif.rpart[[1]]
## Model for learner.id=classif.rpart; learner.class=classif.rpart
## Trained on: task.id = Sonar-example; obs = 138; features = 60
## Hyperparameters: xval=0
getBMRModels(bmr, drop = TRUE)
## $classif.lda
## $classif.lda[[1]]
## Model for learner.id=classif.lda; learner.class=classif.lda
## Trained on: task.id = Sonar-example; obs = 138; features = 60
## Hyperparameters:
##
##
## $classif.rpart
## $classif.rpart[[1]]
## Model for learner.id=classif.rpart; learner.class=classif.rpart
## Trained on: task.id = Sonar-example; obs = 138; features = 60
## Hyperparameters: xval=0
getBMRModels(bmr, learner.ids = "classif.lda")
## $`Sonar-example`
## $`Sonar-example`$classif.lda
## $`Sonar-example`$classif.lda[[1]]
## Model for learner.id=classif.lda; learner.class=classif.lda
## Trained on: task.id = Sonar-example; obs = 138; features = 60
## Hyperparameters:
```

2.7.2.5 Learners and measures

Moreover, you can extract the employed `makeLearner()`s and Measure's (`makeMeasure()`).

```
getBMRLearners(bmr)
## $classif.lda
## Learner classif.lda from package MASS
## Type: classif
## Name: Linear Discriminant Analysis; Short name: lda
## Class: classif.lda
## Properties: twoclass,multiclass,numerics,factors,prob
## Predict-Type: prob
## Hyperparameters:
##
##
## $classif.rpart
## Learner classif.rpart from package rpart
## Type: classif
## Name: Decision Tree; Short name: rpart
## Class: classif.rpart
## Properties: twoclass,multiclass,missings,numerics,factors,ordered,prob,weights,featimp
## Predict-Type: response
## Hyperparameters: xval=0
getBMRMeasures(bmr)
## [[1]]
## Name: Mean misclassification error
## Performance measure: mmce
## Properties: classif,classif.multi,req.pred,req.truth
## Minimize: TRUE
## Best: 0; Worst: 1
## Aggregated by: test.mean
## Arguments: list()
## Note: Defined as: mean(response != truth)
```

2.7.3 Merging benchmark results

Sometimes after completing a benchmark experiment it turns out that you want to extend it by another `makeLearner()` or another `Task()`. In this case you can perform an additional benchmark experiment and then use function `mergeBenchmarkResults()` to combine the results to a single `BenchmarkResult()` object that can be accessed and analyzed as usual.

For example in the benchmark experiment above we applied `MASS::lda()` and `rpart::rpart()` to the `sonar.task()`. We now perform a second experiment using a `randomForest::randomForest()` and quadratic discriminant analysis `MASS::qda()` and merge the results.

```
### First benchmark result
bmr
##         task.id    learner.id mmce.test.mean
## 1 Sonar-example   classif.lda      0.3000000
## 2 Sonar-example classif.rpart      0.3142857
### Benchmark experiment for the additional learners
lrns2 = list(makeLearner("classif.randomForest"), makeLearner("classif.qda"))
bmr2 = benchmark(lrns2, sonar.task, rdesc, show.info = FALSE)
bmr2
##         task.id           learner.id mmce.test.mean
```

```
## 1 Sonar-example classif.randomForest      0.1714286
## 2 Sonar-example          classif.qda      0.4000000
### Merge the results
mergeBenchmarkResults(list(bmr, bmr2))
##         task.id           learner.id mmce.test.mean
## 1 Sonar-example          classif.lda      0.3000000
## 2 Sonar-example        classif.rpart      0.3142857
## 3 Sonar-example classif.randomForest      0.1714286
## 4 Sonar-example          classif.qda      0.4000000
```

Note that in the above examples in each case a resample description (`makeResampleDesc()`) was passed to the `benchmark()` function. For this reason `MASS::lda()` and `rpart::rpart()` were most likely evaluated on a different training/test set pair than `randomForest::randomForest()` and `MASS::qda()`.

Differing training/test set pairs across learners pose an additional source of variation in the results, which can make it harder to detect actual performance differences between learners. Therefore, if you suspect that you will have to extend your benchmark experiment by another `makeLearner()` later on it's probably easiest to work with `makeResampleInstance()`s from the start. These can be stored and used for any additional experiments.

Alternatively, if you used a resample description in the first benchmark experiment you could also extract the `makeResampleInstance()`s from the `BenchmarkResult()` `bmr` and pass these to all further `benchmark()` calls.

```
rin = getBMRPredictions(bmr)[[1]][[1]]$instance
rin
## Resample instance for 208 cases.
## Resample description: holdout with 0.67 split rate.
## Predict: test
## Stratification: FALSE
### Benchmark experiment for the additional random forest
bmr3 = benchmark(lrns2, sonar.task, rin, show.info = FALSE)
bmr3
##         task.id           learner.id mmce.test.mean
## 1 Sonar-example classif.randomForest      0.1571429
## 2 Sonar-example          classif.qda      0.4857143
### Merge the results
mergeBenchmarkResults(list(bmr, bmr3))
##         task.id           learner.id mmce.test.mean
## 1 Sonar-example          classif.lda      0.3000000
## 2 Sonar-example        classif.rpart      0.3142857
## 3 Sonar-example classif.randomForest      0.1571429
## 4 Sonar-example          classif.qda      0.4857143
```

2.7.4 Benchmark analysis and visualization

`mlr` offers several ways to analyze the results of a benchmark experiment. This includes visualization, ranking of learning algorithms and hypothesis tests to assess performance differences between learners.

In order to demonstrate the functionality we conduct a slightly larger benchmark experiment with three learning algorithms that are applied to five classification tasks.

2.7.4.1 Example: Comparing lda, rpart and random Forest

We consider `MASS::lda()`, classification trees `rpart::rpart()`, and random forests `randomForest::randomForest()`. Since the default learner IDs are a little long, we choose shorter names in the **R** code below.

We use five classification tasks. Three are already provided by `mlr`, two more data sets are taken from package `mlbench::mlbench()` and converted to `Task()`s by function `convertMLBenchObjToTask()`.

For all tasks 10-fold cross-validation is chosen as resampling strategy. This is achieved by passing a single resample description (`makeResampleDesc()`) to `benchmark()`, which is then instantiated automatically once for each `Task()`. This way, the same instance is used for all learners applied to a single task.

It is also possible to choose a different resampling strategy for each `Task()` by passing a `base::list()` of the same length as the number of tasks that can contain both resample descriptions (`makeResampleDesc()`) and resample instances (`makeResampleInstance()`).

We use the mean misclassification error mmce as primary performance measure, but also calculate the balanced error rate ber and the training time `timetrain`.

```
### Create a list of learners
lrns = list(
  makeLearner("classif.lda", id = "lda"),
  makeLearner("classif.rpart", id = "rpart"),
  makeLearner("classif.randomForest", id = "randomForest")
)

### Get additional Tasks from package mlbench
ring.task = convertMLBenchObjToTask("mlbench.ringnorm", n = 600)
wave.task = convertMLBenchObjToTask("mlbench.waveform", n = 600)

tasks = list(iris.task, sonar.task, pid.task, ring.task, wave.task)
rdesc = makeResampleDesc("CV", iters = 10)
meas = list(mmce, ber, timetrain)
bmr = benchmark(lrns, tasks, rdesc, meas, show.info = FALSE)
bmr
##                         task.id   learner.id mmce.test.mean ber.test.mean
## 1                  iris-example          lda     0.02000000    0.02222222
## 2                  iris-example        rpart     0.08000000    0.07555556
## 3                  iris-example randomForest     0.05333333    0.05250000
## 4              mlbench.ringnorm          lda     0.35000000    0.34605671
## 5              mlbench.ringnorm        rpart     0.17333333    0.17313632
## 6              mlbench.ringnorm randomForest     0.05833333    0.05806121
## 7              mlbench.waveform          lda     0.19000000    0.18257244
## 8              mlbench.waveform        rpart     0.28833333    0.28765247
## 9              mlbench.waveform randomForest     0.16500000    0.16306057
## 10 PimaIndiansDiabetes-example          lda     0.22778537    0.27148893
## 11 PimaIndiansDiabetes-example        rpart     0.25133288    0.28967870
## 12 PimaIndiansDiabetes-example randomForest     0.23685919    0.27543146
## 13                Sonar-example          lda     0.24619048    0.23986694
## 14                Sonar-example        rpart     0.30785714    0.31153361
## 15                Sonar-example randomForest     0.17785714    0.17442696
##    timetrain.test.mean
## 1                0.0038
## 2                0.0046
## 3                0.0690
## 4                0.0117
## 5                0.0171
## 6                0.4085
```

```
## 7               0.0110
## 8               0.0127
## 9               0.4380
## 10              0.0050
## 11              0.0102
## 12              0.4447
## 13              0.0214
## 14              0.0208
## 15              0.2864
```

From the aggregated performance values we can see that for the iris- and PimaIndiansDiabetes-example linear discriminant analysis (`MASS::lda()`) performs well while for all other tasks the `randomForest::randomForest()` seems superior. Training takes longer for the `randomForest::randomForest()` than for the other learners.

In order to draw any conclusions from the average performances at least their variability has to be taken into account or, preferably, the distribution of performance values across resampling iterations.

The individual performances on the 10 folds for every task, learner, and measure are retrieved below.

```
perf = getBMRPerformances(bmr, as.df = TRUE)
head(perf)
##        task.id learner.id iter      mmce       ber timetrain
## 1 iris-example        lda    1 0.0000000 0.0000000     0.004
## 2 iris-example        lda    2 0.1333333 0.1666667     0.004
## 3 iris-example        lda    3 0.0000000 0.0000000     0.003
## 4 iris-example        lda    4 0.0000000 0.0000000     0.003
## 5 iris-example        lda    5 0.0000000 0.0000000     0.004
## 6 iris-example        lda    6 0.0000000 0.0000000     0.003
```

A closer look at the result reveals that the `randomForest::randomForest()` outperforms the classification tree (`rpart::rpart()`) in every instance, while linear discriminant analysis (`MASS::lda()`) performs better than `rpart::rpart()` most of the time. Additionally `MASS::lda()` sometimes even beats the `randomForest::randomForest()`. With increasing size of such `benchmark()` experiments, those tables become almost unreadable and hard to comprehend.

`mlr` features some plotting functions to visualize results of benchmark experiments that you might find useful. Moreover, `mlr` offers statistical hypothesis tests to assess performance differences between learners.

2.7.4.2 Integrated plots

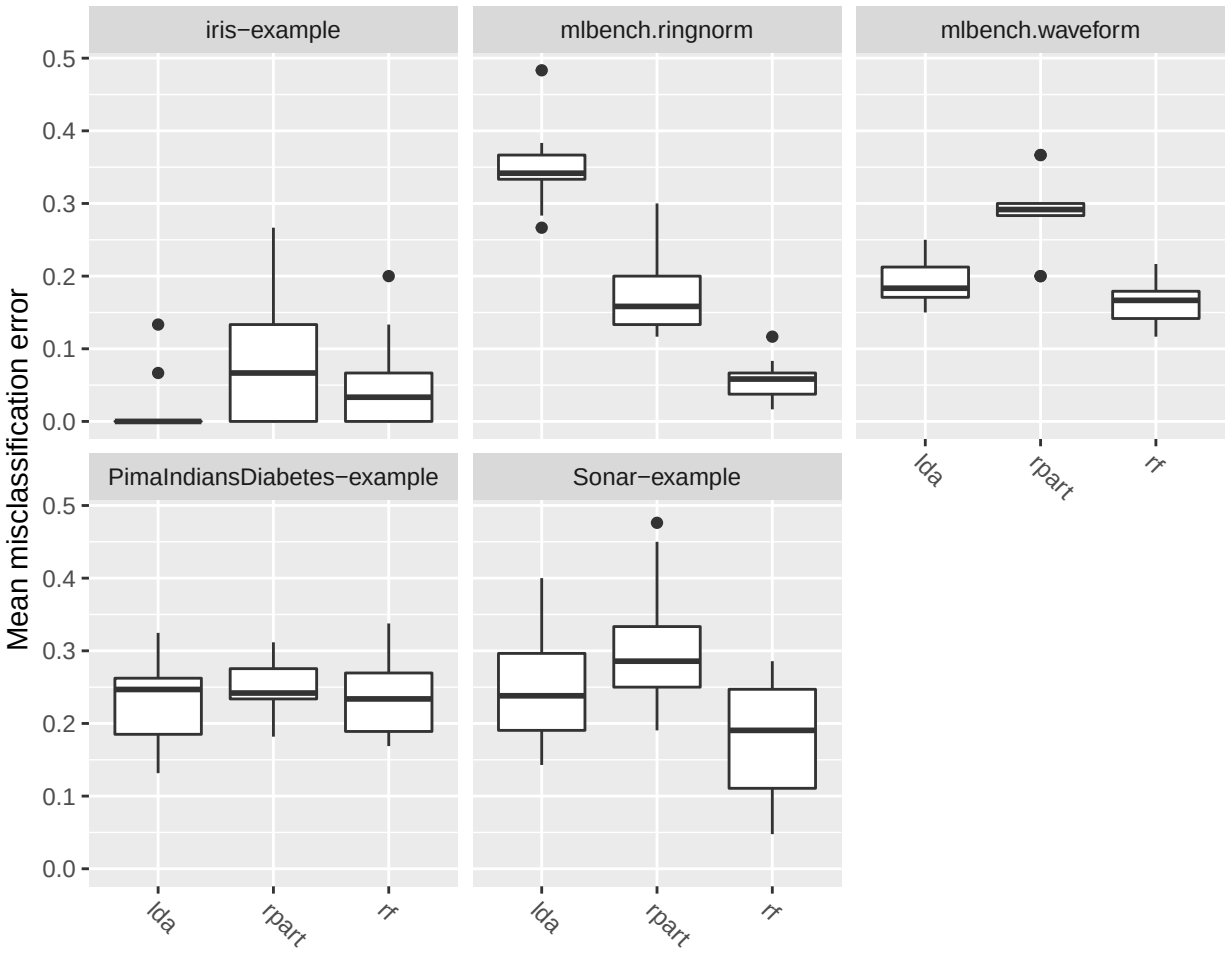
Plots are generated using `ggplot2::ggplot2()`. Further customization, such as renaming plot elements or changing colors, is easily possible.

2.7.4.2.1 Visualizing performances

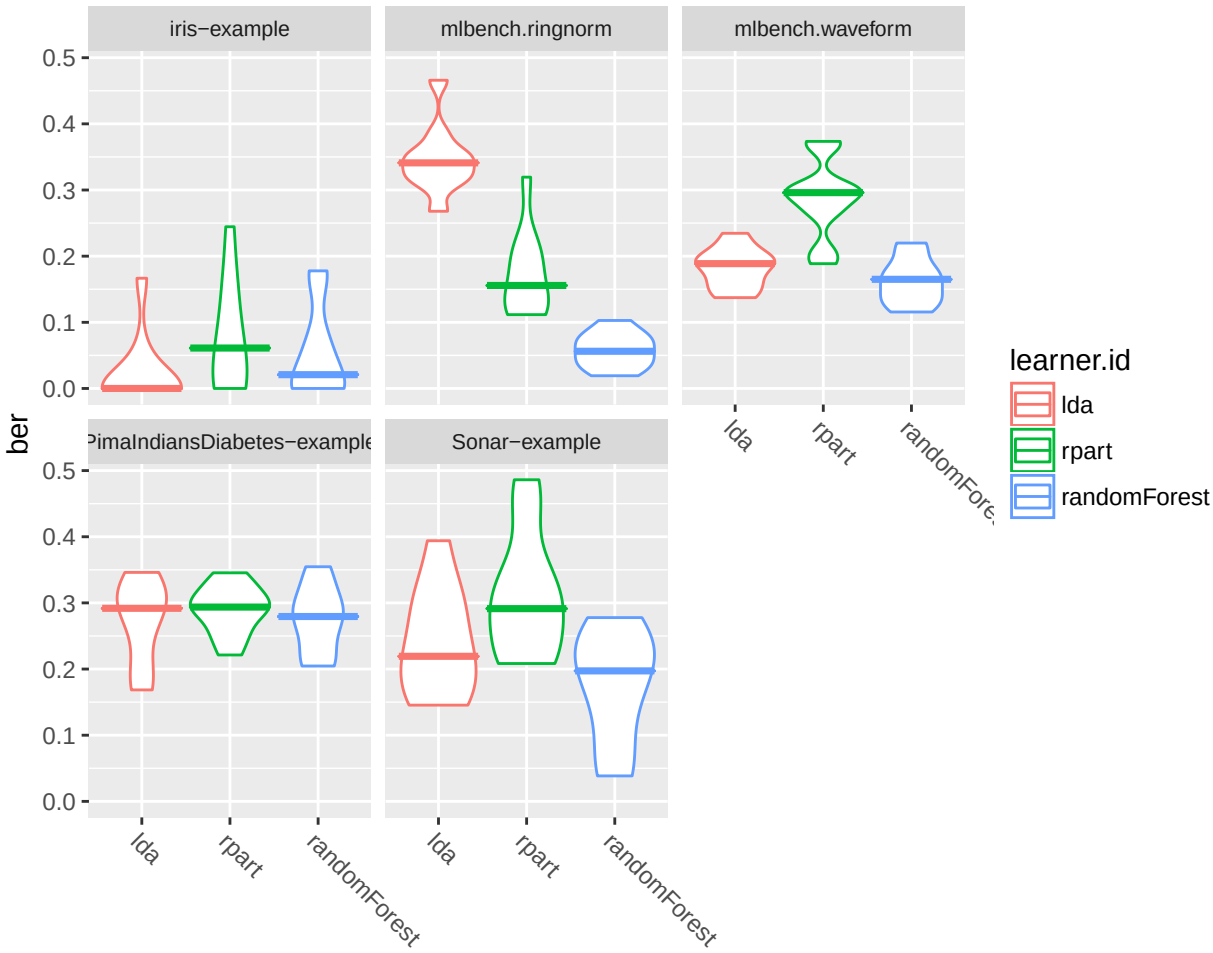
`plotBMRBoxplots()` creates box or violin plots which show the distribution of performance values across resampling iterations for one performance measure and for all learners and tasks (and thus visualize the output of `getBMRPerformances()`).

Below are both variants, box and violin plots. The first plot shows the mmce and the second plot the ber. Moreover, in the second plot we color the boxes according to the `learner.id`s.

```
plotBMRBoxplots(bmr, measure = mmce)
```




```
plotBMRBoxplots(bmr, measure = ber, style = "violin", pretty.names = FALSE) +
  aes(color = learner.id) +
  theme(strip.text.x = element_text(size = 8))
```



Note that by default the measure `names` and the learner `short.names` are used as axis labels.

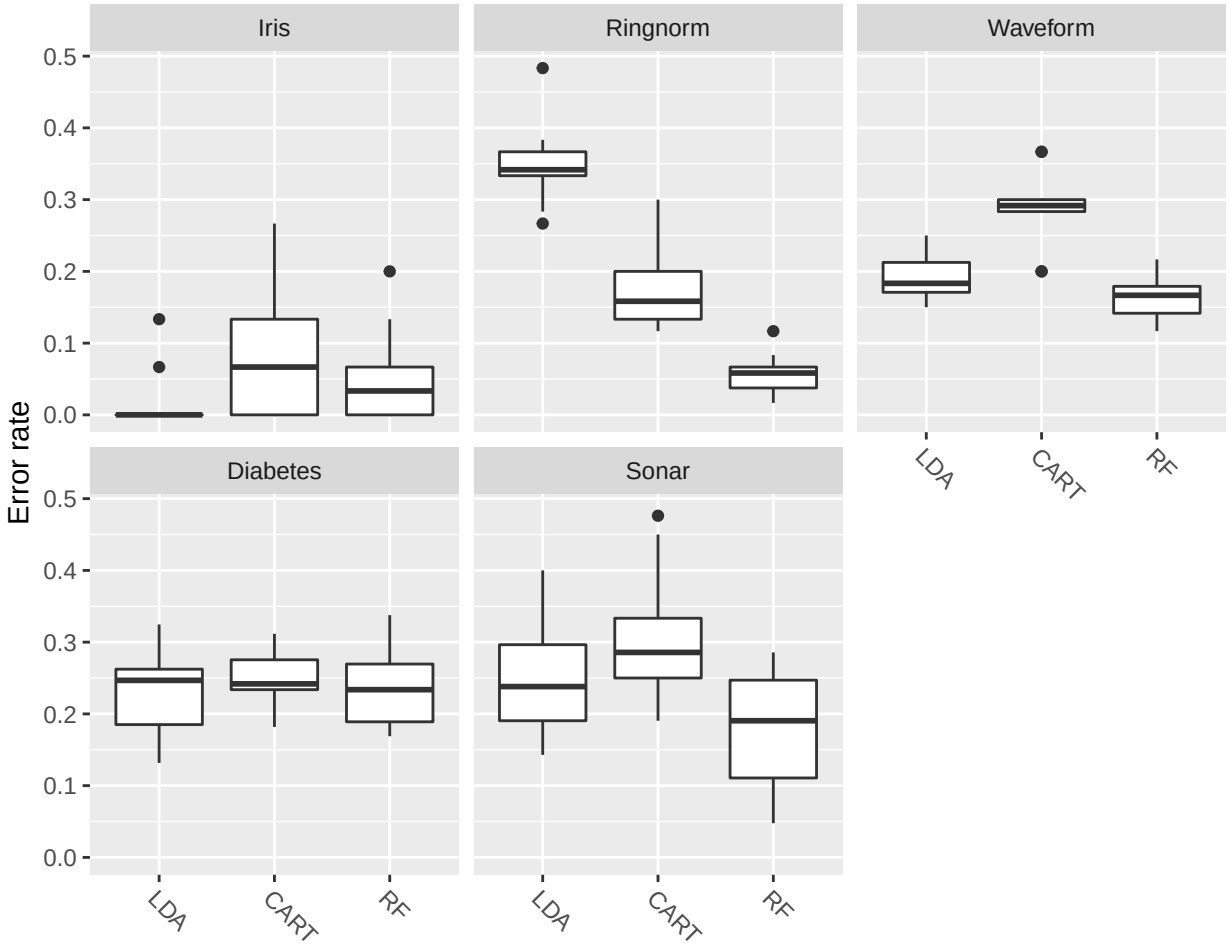
```
mmce$name
## [1] "Mean misclassification error"
mmce$id
## [1] "mmce"
getBMRLearnerIds(bmr)
## [1] "lda"          "rpart"        "randomForest"
getBMRLearnerShortNames(bmr)
## [1] "lda"   "rpart" "rf"
```

If you prefer the `ids` like, e.g., mmce and ber set `pretty.names = FALSE` (as done for the second plot). Of course you can also use the `ggplot2::ggplot2()` functionality like the `ggplot2::labs()` function to choose completely different labels.

One question which comes up quite often is how to change the panel headers (which default to the `Task()` IDs) and the learner names on the x-axis. For example looking at the above plots we would like to remove the "example" suffixes and the "mlbench" prefixes from the panel headers. Moreover, we want uppercase learner labels. Currently, the probably simplest solution is to change the factor levels of the plotted data as shown below.

```
plt = plotBMRBoxplots(bmr, measure = mmce)
head(plt$data)
##         task.id learner.id iter      mmce       ber timetrain
## 1 iris-example        lda    1 0.0000000 0.0000000     0.004
```

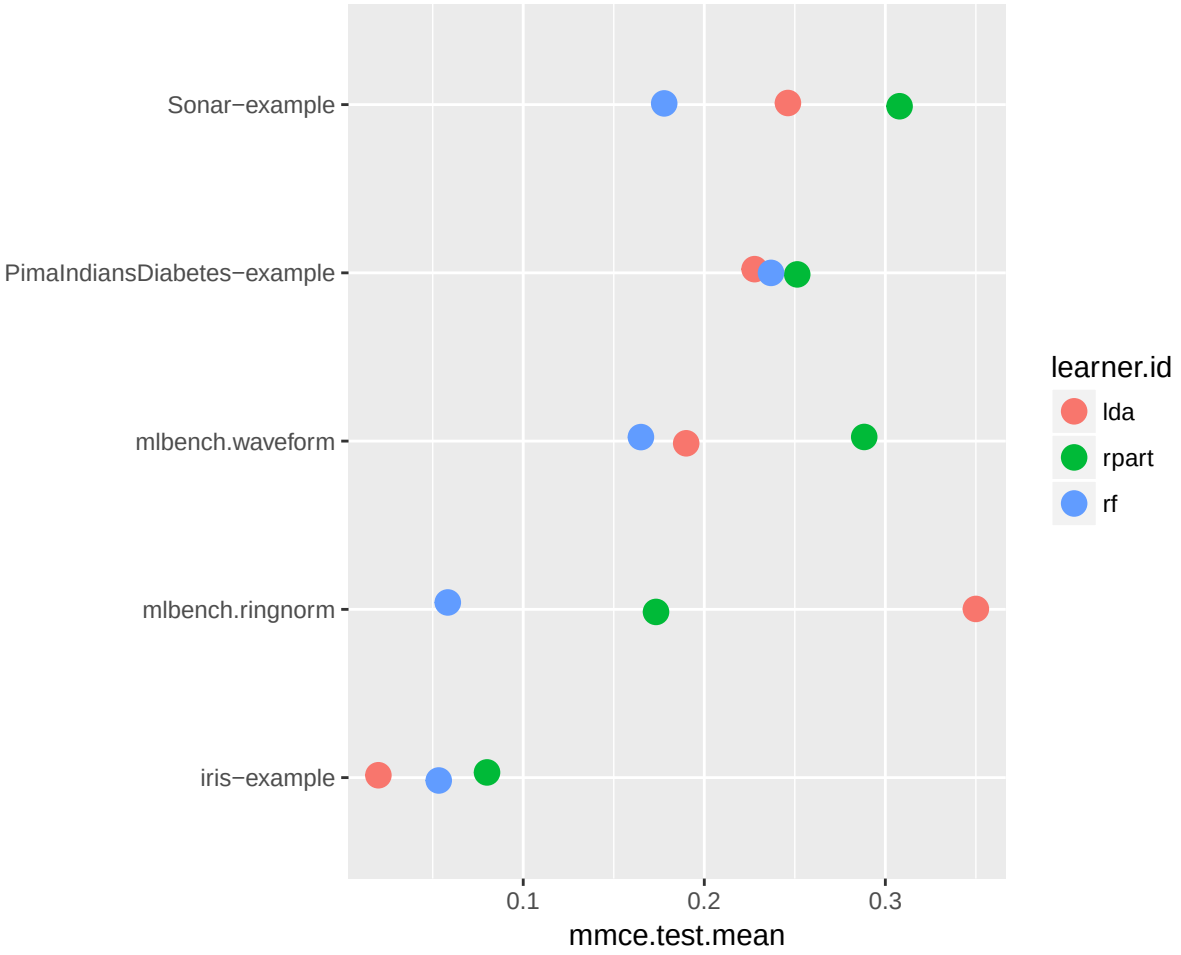
```
## 2 iris-example        lda    2 0.1333333 0.1666667     0.004
## 3 iris-example        lda    3 0.0000000 0.0000000     0.003
## 4 iris-example        lda    4 0.0000000 0.0000000     0.003
## 5 iris-example        lda    5 0.0000000 0.0000000     0.004
## 6 iris-example        lda    6 0.0000000 0.0000000     0.003
levels(plt$data$task.id) = c("Iris", "Ringnorm", "Waveform", "Diabetes", "Sonar")
levels(plt$data$learner.id) = c("LDA", "CART", "RF")

plt + ylab("Error rate")
```



2.7.4.2.2 Visualizing aggregated performances

The aggregated performance values (resulting from `getBMRAggrPerformances()`) can be visualized by function `plotBMRSummary()`. This plot draws one line for each task on which the aggregated values of one performance measure for all learners are displayed. By default, the first measure in the `base::list()` of Measure's (`makeMeasure()`) passed to `benchmark()` is used, in our example mmce. Moreover, a small vertical jitter is added to prevent overplotting.

```
plotBMRSummary(bmr)
```



2.7.4.2.3 Calculating and visualizing ranks

Additional to the absolute performance, relative performance, i.e., ranking the learners is usually of interest and might provide valuable additional insight.

Function `convertBMRToRankMatrix()` calculates ranks based on aggregated learner performances of one measure. We choose the mean misclassification error. The rank structure can be visualized by `plotBMRRanksAsBarChart()`.

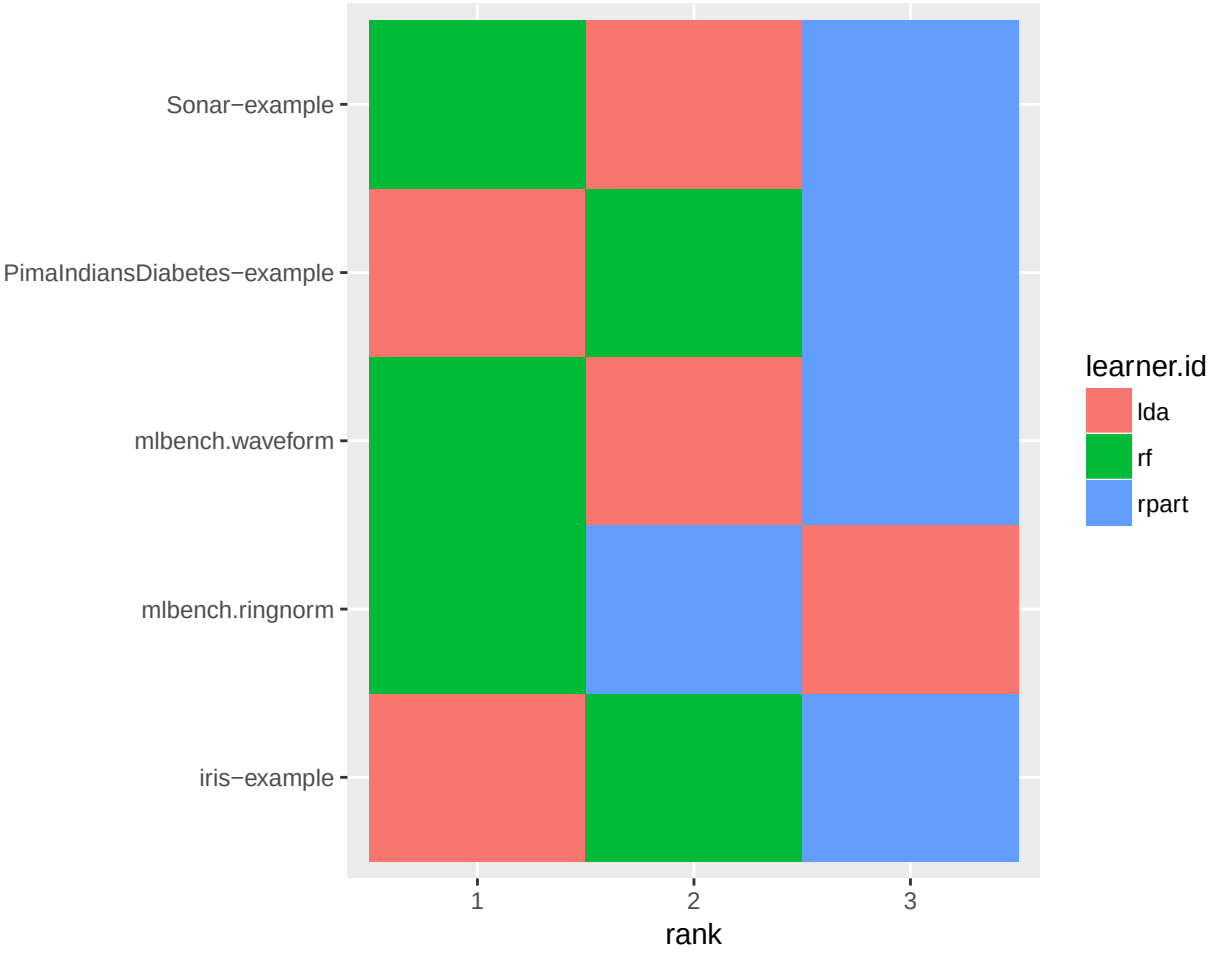
```
m = convertBMRToRankMatrix(bmr, mmce)
m
##              iris-example mlbench.ringnorm mlbench.waveform
## lda                     1                3                2
## rpart                   3                2                3
## randomForest            2                1                1
##              PimaIndiansDiabetes-example Sonar-example
## lda                                    1             2
## rpart                                  3             3
## randomForest                           2             1
```

Methods with best performance, i.e., with lowest mmce, are assigned the lowest rank. Linear discriminant analysis (`MASS::lda()`) is best for the iris and PimaIndiansDiabetes-examples while the

`randomForest::randomForest()` shows best results on the remaining tasks.

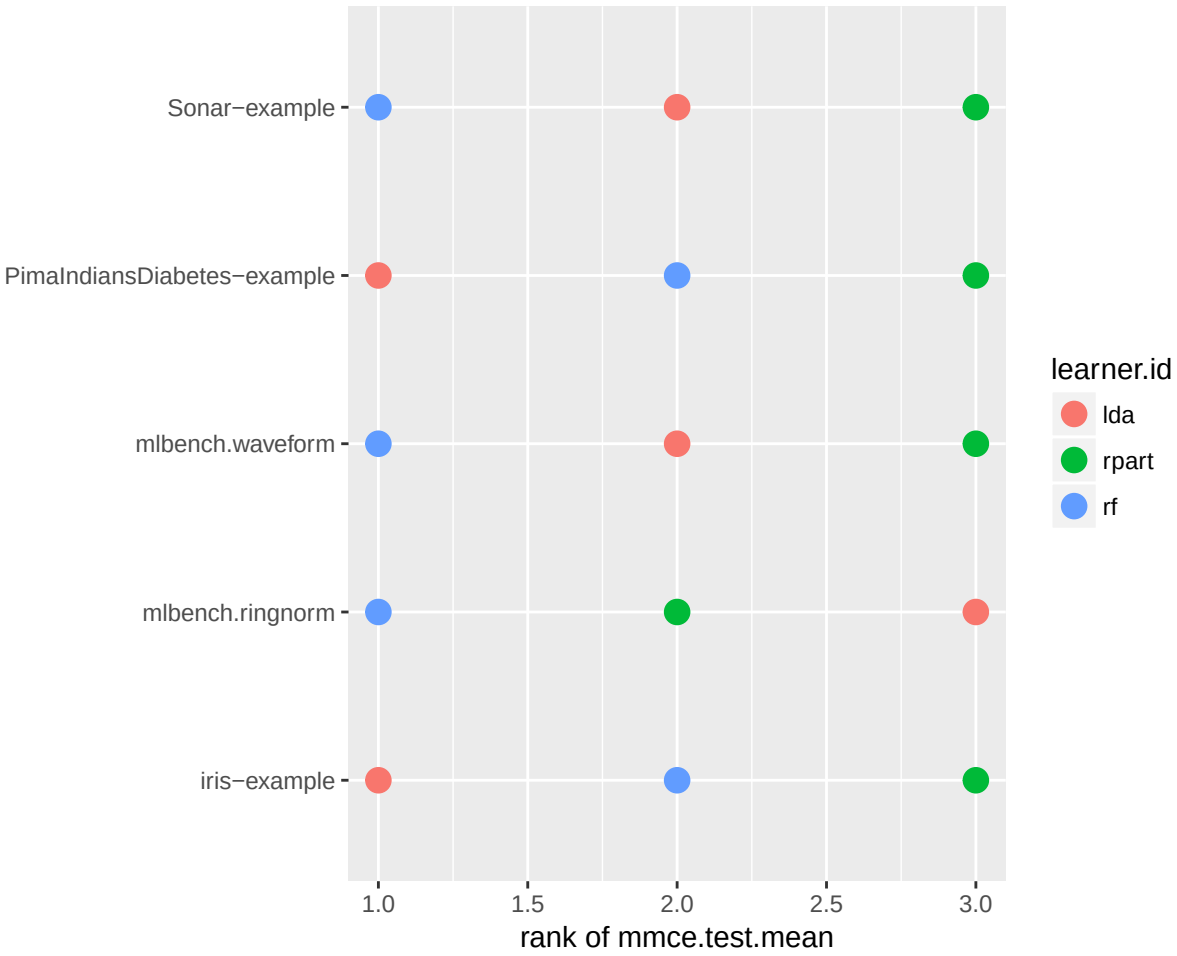
`plotBMRRanksAsBarChart()` with option `pos = "tile"` shows a corresponding heat map. The ranks are displayed on the x-axis and the learners are color-coded.

```
plotBMRRanksAsBarChart(bmr, pos = "tile")
```



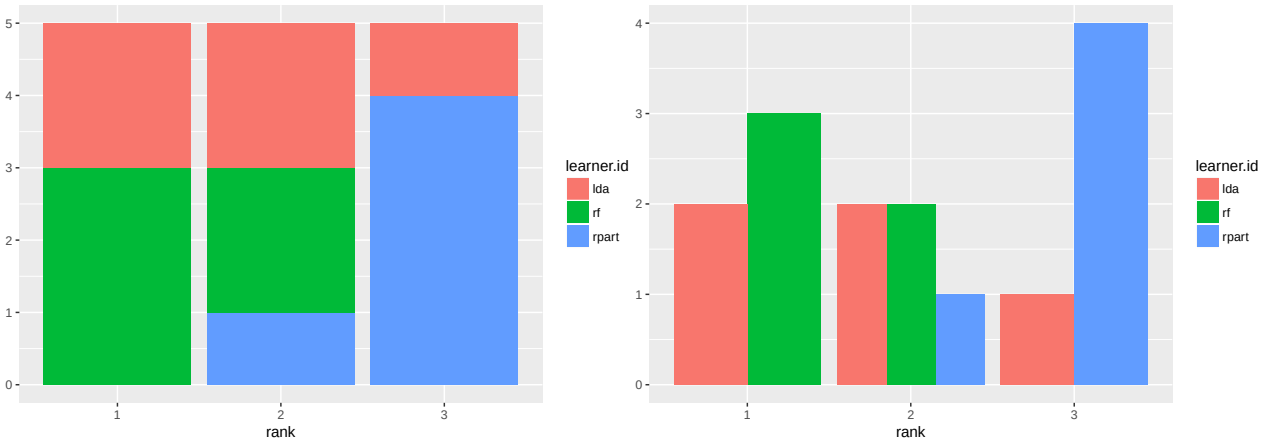
A similar plot can also be obtained via `plotBMRSummary()`. With option `trafo = "rank"` the ranks are displayed instead of the aggregated performances.

```
plotBMRSummary(bmr, trafo = "rank", jitter = 0)
```



Alternatively, you can draw stacked bar charts (the default) or bar charts with juxtaposed bars (`pos = "dodge"`) that are better suited to compare the frequencies of learners within and across ranks.

```
plotBMRRanksAsBarChart(bmr)
plotBMRRanksAsBarChart(bmr, pos = "dodge")
```



2.7.4.3 Comparing learners using hypothesis tests

Many researchers feel the need to display an algorithm's superiority by employing some sort of hypothesis

testing. As non-parametric tests seem better suited for such benchmark results the tests provided in `mlr` are the **Overall Friedman test** and the **Friedman-Nemenyi post hoc test**.

While the ad hoc `friedmanTestBMR()` based on `stats::friedman.test()` is testing the hypothesis whether there is a significant difference between the employed learners, the post hoc `friedmanPostHocTestBMR()` tests for significant differences between all pairs of learners. *Non parametric* tests often do have less power then their *parametric* counterparts but less assumptions about underlying distributions have to be made. This often means many **data sets** are needed in order to be able to show significant differences at reasonable significance levels.

In our example, we want to compare the three learners on the selected data sets. First we might we want to test the hypothesis whether there is a difference between the learners.

```
friedmanTestBMR(bmr)
##
##  Friedman rank sum test
##
## data:  mmce.test.mean and learner.id and task.id
## Friedman chi-squared = 5.2, df = 2, p-value = 0.07427
```

In order to keep the computation time for this tutorial small, the `makeLearner()`s are only evaluated on five tasks. This also means that we operate on a relatively low significance level $\alpha = 0.1$. As we can reject the null hypothesis of the Friedman test at a reasonable significance level we might now want to test where these differences lie exactly.

```
friedmanPostHocTestBMR(bmr, p.value = 0.1)
##
##  Pairwise comparisons using Nemenyi multiple comparison test
##              with q approximation for unreplicated blocked data
##
## data:  mmce.test.mean and learner.id and task.id
##
##              lda   rpart
## rpart        0.254 -
## randomForest 0.802 0.069
##
## P value adjustment method: none
```

At this level of significance, we can reject the null hypothesis that there exists no performance difference between the decision tree (`rpart::rpart()`) and the `randomForest::randomForest()`.

2.7.4.4 Critical differences diagram

In order to visualize differently performing learners, a critical differences diagramcan be plotted, using either the Nemenyi test (`test = "nemenyi"`) or the Bonferroni-Dunn test (`test = "bd"`).

The mean rank of learners is displayed on the x-axis.

- Choosing `test = "nemenyi"` compares all pairs of `makeLearner()`s to each other, thus the output are groups of not significantly different learners. The diagram connects all groups of learners where the mean ranks do not differ by more than the critical differences. Learners that are not connected by a bar are significantly different, and the learner(s) with the lower mean rank can be considered "better" at the chosen significance level.
- Choosing `test = "bd"` performs a *pairwise comparison with a baseline*. An interval which extends by the given *critical difference* in both directions is drawn around the `makeLearner()` chosen as baseline, though only comparisons with the baseline are possible. All learners within the interval are not

significantly different, while the baseline can be considered better or worse than a given learner which is outside of the interval.

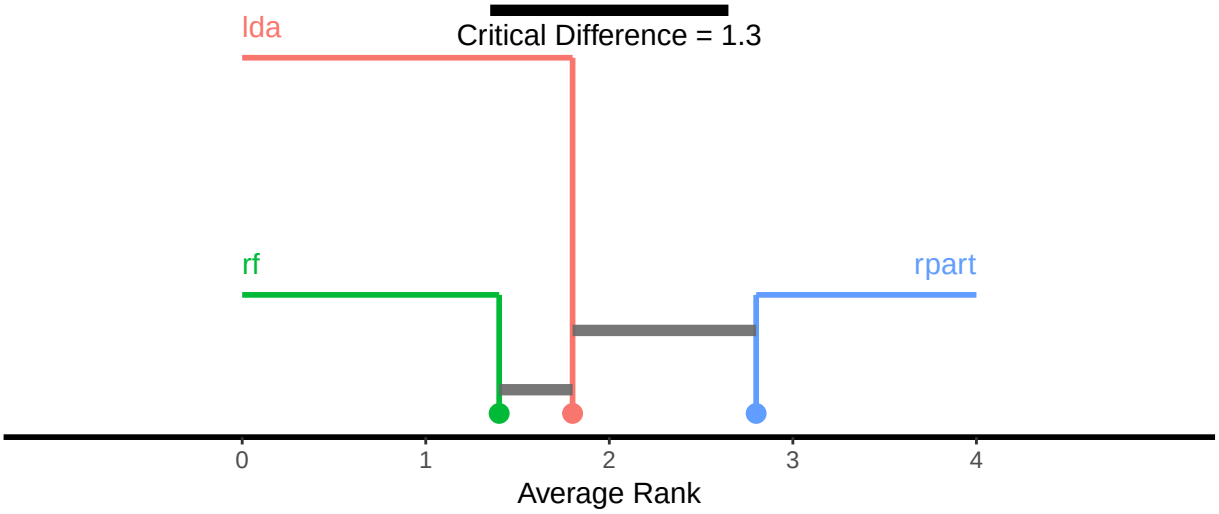
The critical difference CD is calculated by

$$CD = q_\alpha \cdot \sqrt{\frac{k(k+1)}{6N}},$$

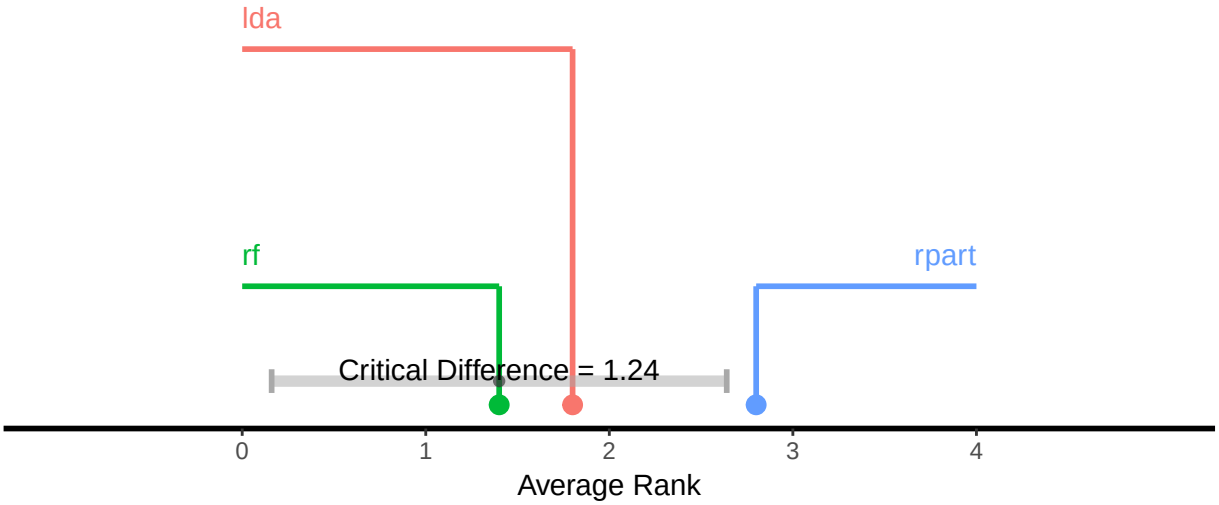
where N denotes the number of tasks, k is the number of learners, and q_α comes from the studentized range statistic divided by $\sqrt{2}$. For details see Demsar (2006).

Function `generateCritDifferencesData()` does all necessary calculations while function `plotCritDifferences()` draws the plot. See the tutorial page about visualization for details on data generation and plotting functions.

```
### Nemenyi test
g = generateCritDifferencesData(bmr, p.value = 0.1, test = "nemenyi")
plotCritDifferences(g) + coord_cartesian(xlim = c(-1,5), ylim = c(0,2))
```




```
### Bonferroni-Dunn test
g = generateCritDifferencesData(bmr, p.value = 0.1, test = "bd", baseline = "randomForest")
plotCritDifferences(g) + coord_cartesian(xlim = c(-1,5), ylim = c(0,2))
```

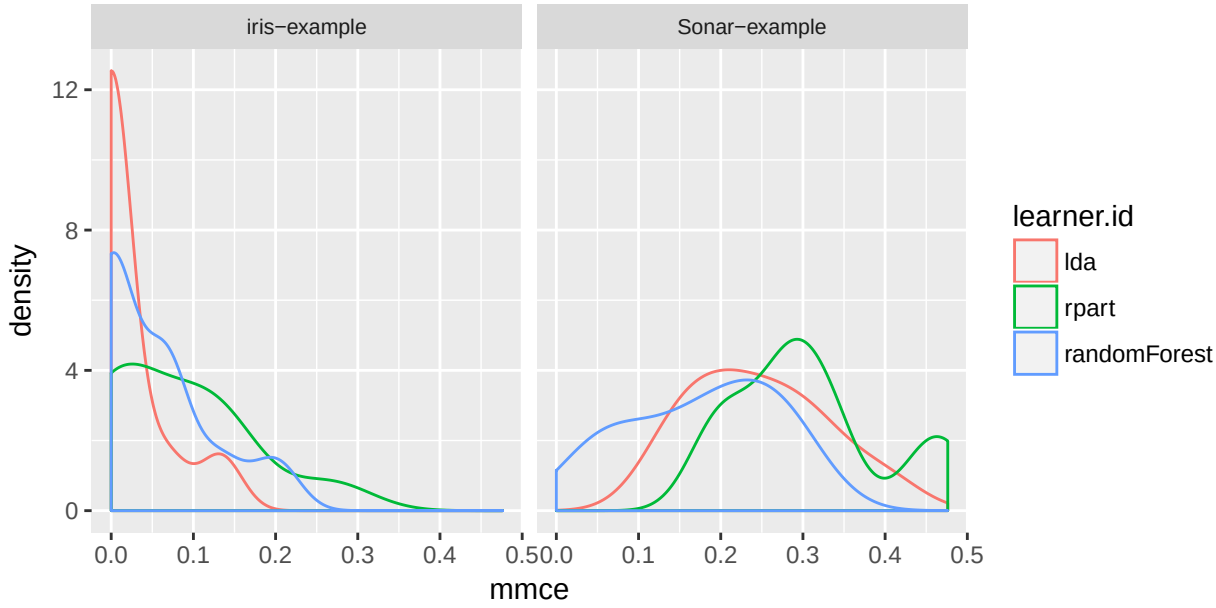


2.7.4.5 Custom plots

You can easily generate your own visualizations by customizing the `ggplot2::ggplot()` objects returned by the plots above, retrieve the data from the `ggplot2::ggplot()` objects and use them as basis for your own plots, or rely on the `base::data.frame()`s returned by `getBMRPerformances()` or `getBMRAggrPerformances()`. Here are some examples.

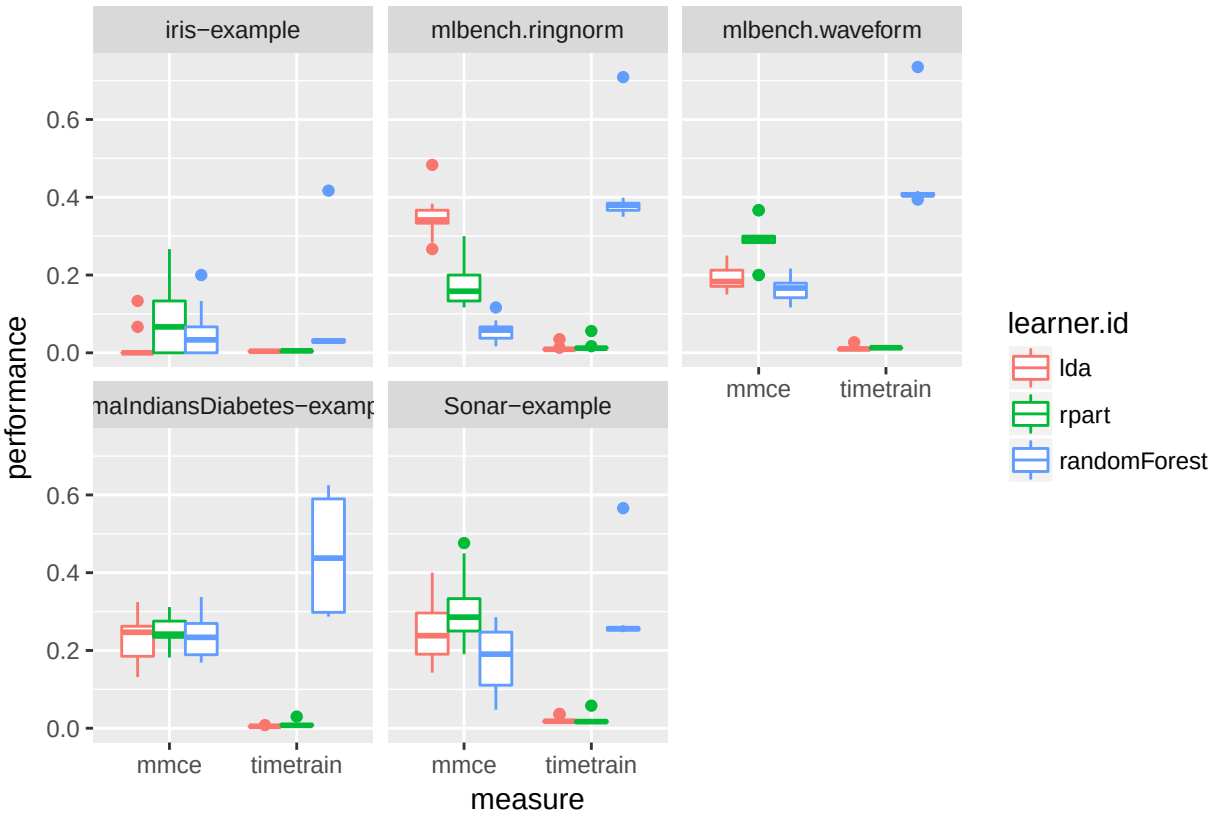
Instead of boxplots (as in `plotBMRBoxplots()`) we could create density plots to show the performance values resulting from individual resampling iterations.

```
perf = getBMRPerformances(bmr, as.df = TRUE)

### Density plots for two tasks
qplot(mmce, colour = learner.id, facets = . ~ task.id,
  data = perf[perf$task.id %in% c("iris-example", "Sonar-example"),], geom = "density") +
  theme(strip.text.x = element_text(size = 8))
```



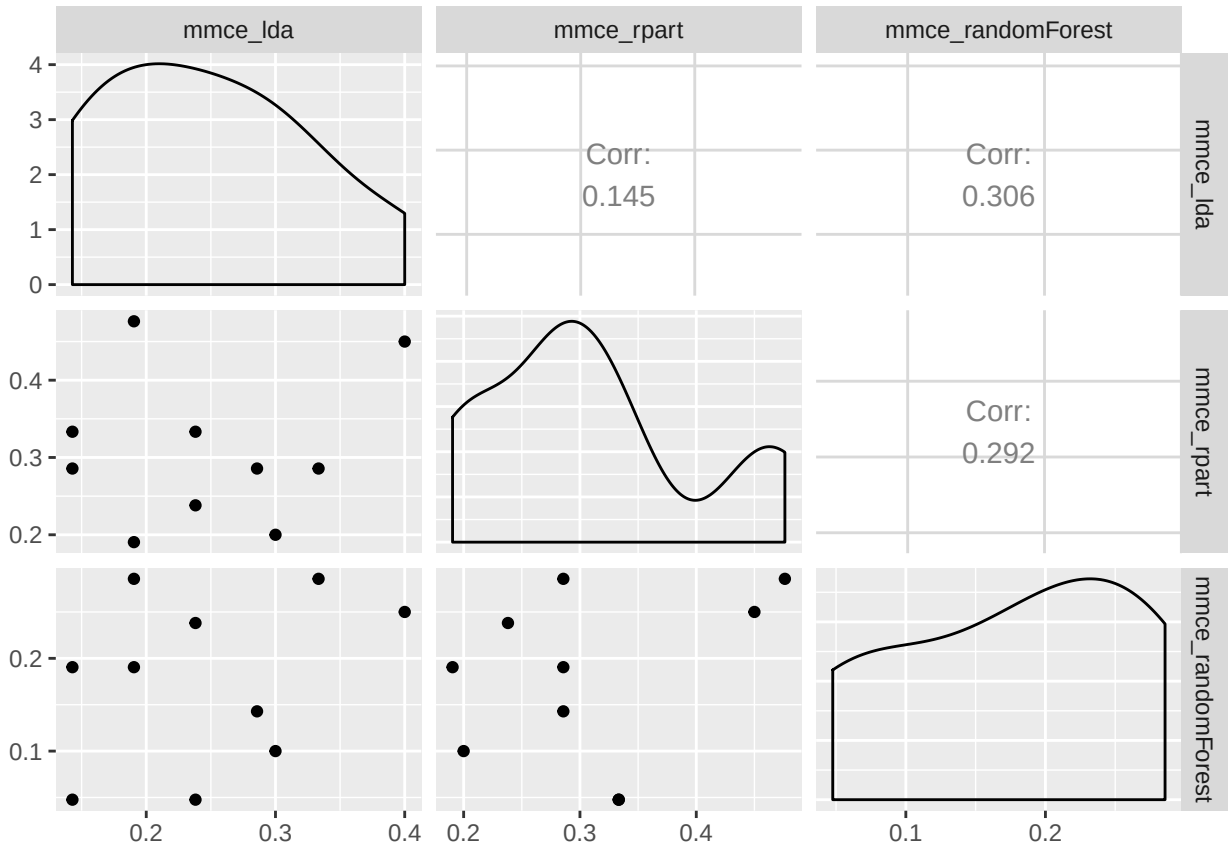
In order to plot multiple performance measures in parallel, `perf` is reshaped to long format. Below we generate grouped boxplots showing the error rate and the training time timetrain.

```
### Compare mmce and timetrain
df = reshape2::melt(perf, id.vars = c("task.id", "learner.id", "iter"))
df = df[df$variable != "ber",]
head(df)
##         task.id learner.id iter variable     value
## 1 iris-example        lda    1     mmce 0.0000000
## 2 iris-example        lda    2     mmce 0.1333333
## 3 iris-example        lda    3     mmce 0.0000000
## 4 iris-example        lda    4     mmce 0.0000000
## 5 iris-example        lda    5     mmce 0.0000000
## 6 iris-example        lda    6     mmce 0.0000000
qplot(variable, value, data = df, colour = learner.id, geom = "boxplot",
  xlab = "measure", ylab = "performance") +
  facet_wrap(~ task.id, nrow = 2)
```



It might also be useful to assess if learner performances in single resampling iterations, i.e., in one fold, are related. This might help to gain further insight, for example by having a closer look at train and test sets from iterations where one learner performs exceptionally well while another one is fairly bad. Moreover, this might be useful for the construction of ensembles of learning algorithms. Below, function `GGally::ggpairs()` from package `GGally::GGally()` is used to generate a scatterplot matrix of mean misclassification errors on the `mlbench::Sonar()` data set.

```
perf = getBMRPerformances(bmr, task.id = "Sonar-example", as.df = TRUE)
df = reshape2::melt(perf, id.vars = c("task.id", "learner.id", "iter"))
df = df[df$variable == "mmce",]
df = reshape2::dcast(df, task.id + iter ~ variable + learner.id)
head(df)
##         task.id iter  mmce_lda mmce_rpart mmce_randomForest
## 1 Sonar-example    1 0.2857143  0.2857143        0.14285714
## 2 Sonar-example    2 0.2380952  0.2380952        0.23809524
## 3 Sonar-example    3 0.3333333  0.2857143        0.28571429
## 4 Sonar-example    4 0.2380952  0.3333333        0.04761905
## 5 Sonar-example    5 0.1428571  0.2857143        0.19047619
## 6 Sonar-example    6 0.4000000  0.4500000        0.25000000
GGally::ggpairs(df, 3:5)
```



2.7.5 Further comments

- Note that for supervised classification `mlr` offers some more plots that operate on `BenchmarkResult()` objects and allow you to compare the performance of learning algorithms. See for example the tutorial page on ROC analysis and functions `generateThreshVsPerfData()`, `plotROCCurves()`, and `plotViperCharts()` as well as the page about classifier calibration and function `generateCalibrationData()`.
- In the examples shown in this section we applied "raw" learning algorithms, but often things are more complicated. At the very least, many learners have hyperparameters that need to be tuned to get sensible results. Reliable performance estimates can be obtained by nested resampling, i.e., by doing the tuning in an inner resampling loop while estimating the performance in an outer loop. Moreover, you might want to combine learners with pre-processing steps like imputation, scaling, outlier removal, dimensionality reduction or feature selection and so on. All this can be easily done using `mlr`'s wrapper functionality. The general principle is explained in the section about wrapper in the Advanced part of this tutorial. There are also several sections devoted to common pre-processing steps.
- Benchmark experiments can very quickly become computationally demanding. `mlr` offers some possibilities for parallelization.

2.8 Parallelization

R by default does not make use of parallelization. With the integration of `parallelMap()` into `mlr`, it becomes easy to activate the parallel computing capabilities already supported by `mlr`. `parallelMap()` works with all major parallelization backends: local multicore execution using `parallel()`, socket and MPI clusters using `snow()`, makeshift SSH-clusters using `BatchJobs()` and high performance computing clusters (managed by a scheduler like SLURM, Torque/PBS, SGE or LSF) also using `BatchJobs()`.

All you have to do is select a backend by calling one of the `parallelStart*` (`parallelMap::parallelStart()`) functions. The first loop `mlr` encounters which is marked as parallel executable will be automatically parallelized. It is good practice to call `parallelStop` (`parallelMap::parallelStop()`) at the end of your script.

```
library("parallelMap")
parallelStartSocket(2)
## Starting parallelization in mode=socket with cpus=2.
rdesc = makeResampleDesc("CV", iters = 3)
r = resample("classif.lda", iris.task, rdesc)
## Exporting objects to slaves for mode socket: .mlr.slave.options
## Resampling: cross-validation
## Measures:             mmce
## Mapping in parallel: mode = socket; level = mlr.resample; cpus = 2; elements = 3.
##
## Aggregated Result: mmce.test.mean=0.0200000
##
parallelStop()
## Stopped parallelization. All cleaned up.
```

On Linux or Mac OS X, you may want to use `parallelStartMulticore` (`parallelMap::parallelStart()`) instead.

2.8.1 Parallelization levels

We offer different parallelization levels for fine grained control over the parallelization. E.g., if you do not want to parallelize the `benchmark()` function because it has only very few iterations but want to parallelize the resampling (`resample()`) of each learner instead, you can specifically pass the `level "mlr.resample"` to the `parallelStart*` (`parallelMap::parallelStart()`) function. Currently the following levels are supported:

```
parallelGetRegisteredLevels()
## mlr: mlr.benchmark, mlr.resample, mlr.selectFeatures, mlr.tuneParams, mlr.ensemble
```

For further details please see the `parallelization()` documentation page.

2.8.2 Custom learners and parallelization

If you have implemented a custom learner yourself, locally, you currently need to export this to the slave. So if you see an error after calling, e.g., a parallelized version of `resample()` like this:

```
no applicable method for 'trainLearner' applied to an object of class <my_new_learner>
```

simply add the following line somewhere after calling `parallelMap::parallelStart()`.

```
parallelExport("trainLearner.<my_new_learner>", "predictLearner.<my_new_learner>")
```

2.8.3 The end

For further details, consult the parallelMap tutorial and help (`?parallelMap()`).

2.9 Visualization

2.9.1 Generation and plotting functions

`mlr`'s visualization capabilities rely on *generation functions* which generate data for plots, and *plotting functions* which plot this output using either `ggplot2::ggplot2()` or `ggvis::ggvis()` (the latter being currently experimental).

This separation allows users to easily make custom visualizations by taking advantage of the generation functions. The only data transformation that is handled inside plotting functions is reshaping. The reshaped data is also accessible by calling the plotting functions and then extracting the data from the `ggplot2::ggplot()` object.

The functions are named accordingly.

- Names of generation functions start with `generate` and are followed by a title-case description of their `FunctionPurpose`, followed by `Data`, i.e., `generateFunctionPurposeData`. These functions output objects of class `FunctionPurposeData`.
- Plotting functions are prefixed by `plot` followed by their purpose, i.e., `plotFunctionPurpose`.
- `ggvis::ggvis()` plotting functions have an additional suffix `GGVIS`, i.e., `plotFunctionPurposeGGVIS`.

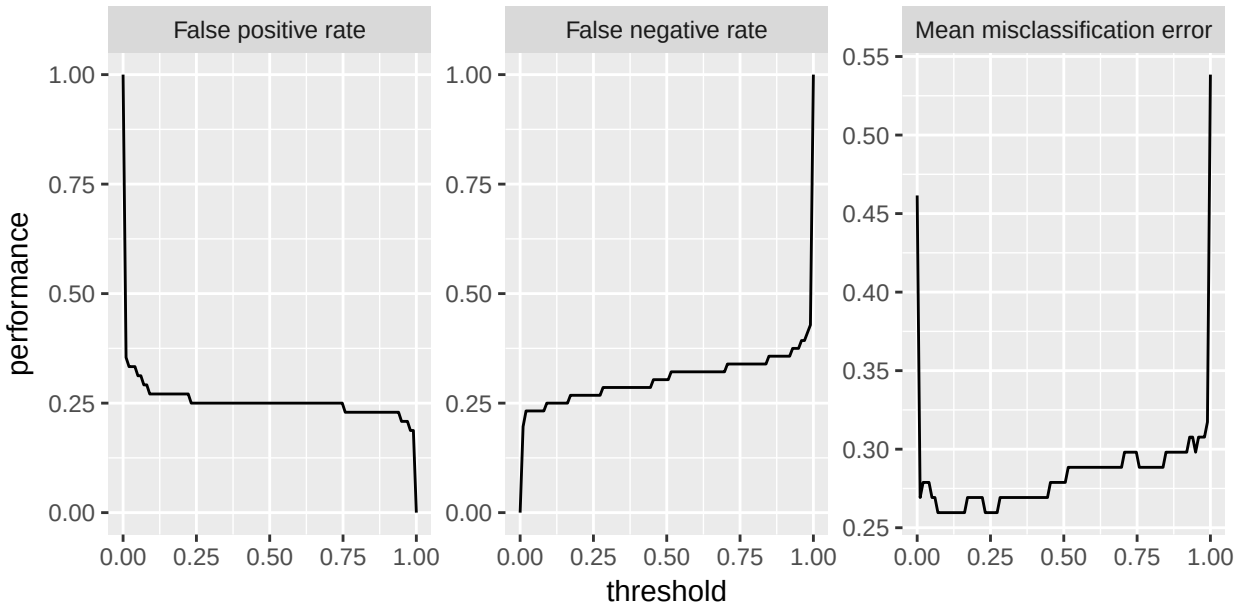
2.9.1.1 Some examples

In the example below we create a plot of classifier performance as function of the decision threshold for the binary classification problem `sonar.task`. The generation function `generateThreshVsPerfData()` creates an object of class `ThreshVsPerfData` which contains the data for the plot in slot `$data`.

```
lrn = makeLearner("classif.lda", predict.type = "prob")
n = getTaskSize(sonar.task)
mod = train(lrn, task = sonar.task, subset = seq(1, n, by = 2))
pred = predict(mod, task = sonar.task, subset = seq(2, n, by = 2))
d = generateThreshVsPerfData(pred, measures = list(fpr, fnr, mmce))

class(d)
## [1] "ThreshVsPerfData"
head(d$data)
##         fpr       fnr      mmce  threshold
## 1 1.0000000 0.0000000 0.4615385 0.00000000
## 2 0.3541667 0.1964286 0.2692308 0.01010101
## 3 0.3333333 0.2321429 0.2788462 0.02020202
## 4 0.3333333 0.2321429 0.2788462 0.03030303
## 5 0.3333333 0.2321429 0.2788462 0.04040404
## 6 0.3125000 0.2321429 0.2692308 0.05050505
```

For plotting we can use the built-in `mlr` function `plotThreshVsPerf()`.

```
plotThreshVsPerf(d)
```



Note that by default the `Measure` `name`s are used to annotate the panels.

```
fpr$name
## [1] "False positive rate"
fpr$id
## [1] "fpr"
```

This does not only apply to `plotThreshVsPerf()`, but to other plot functions that show performance measures as well, for example `plotLearningCurve()`. You can use the `id`s instead of the names by setting `pretty.names = FALSE`.

2.9.1.2 Customizing plots

As mentioned above it is easily possible to customize the built-in plots or making your own visualizations from scratch based on the generated data.

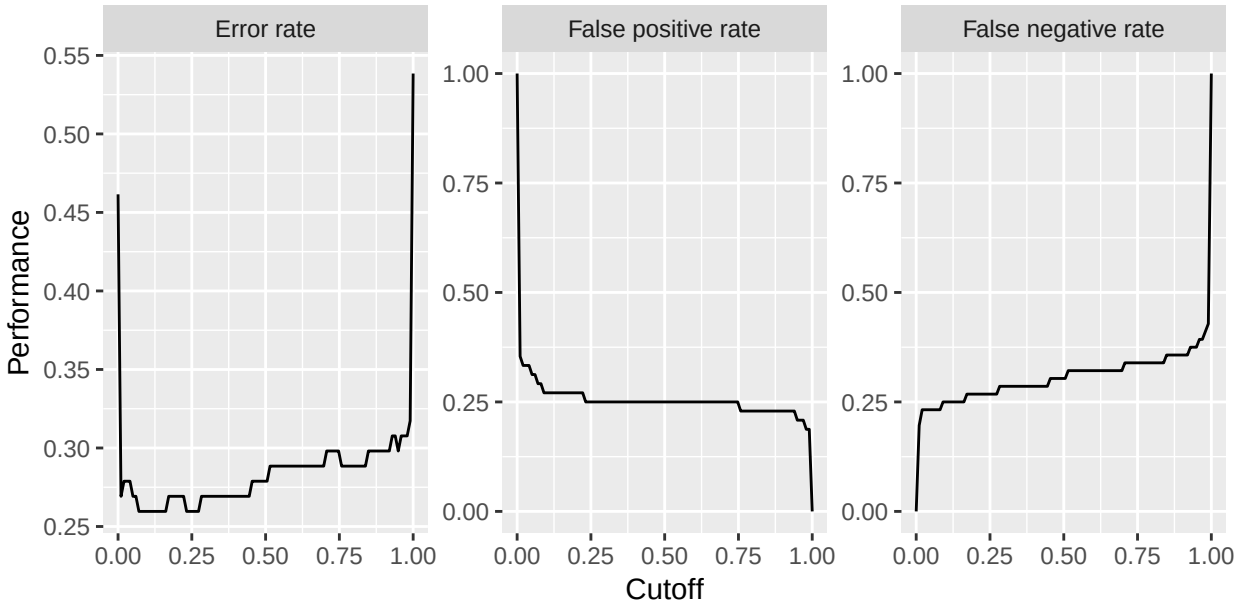
What will probably come up most often is changing labels and annotations. Generally, this can be done by manipulating the `ggplot2::ggplot()` object, in this example the object returned by `plotThreshVsPerf()`, using the usual `ggplot2::ggplot2()` functions like `ggplot2::labs()` or `ggplot2::labeller()`. Moreover, you can change the underlying data, either `d$data` (resulting from `generateThreshVsPerfData()` or the possibly reshaped data contained in the `ggplot2::ggplot()` object (resulting from `plotThreshVsPerf()`, most often by renaming columns or factor levels.

Below are two examples of how to alter the axis and panel labels of the above plot.

Imagine you want to change the order of the panels and also are not satisfied with the panel names, for example you find that "Mean misclassification error" is too long and you prefer "Error rate" instead. Moreover, you want the error rate to be displayed first.

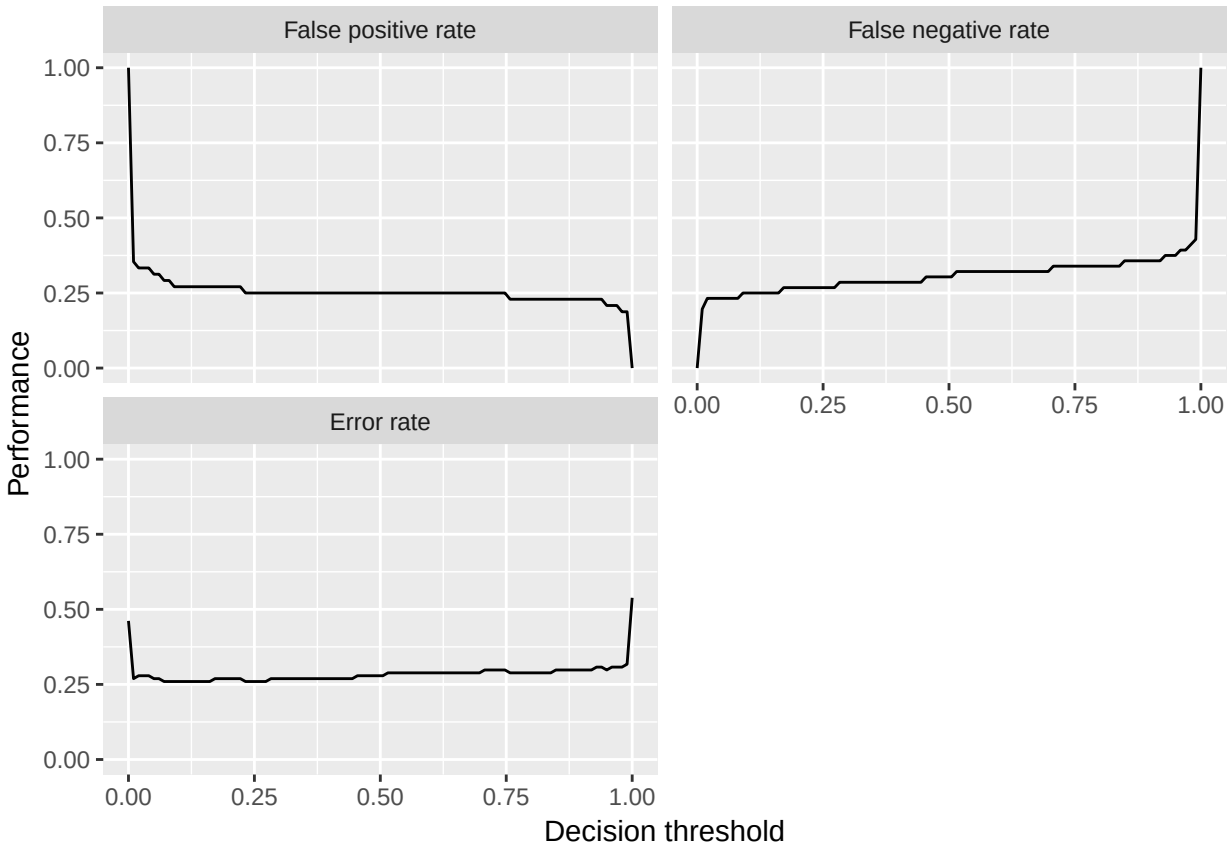
```
plt = plotThreshVsPerf(d, pretty.names = FALSE)

### Reshaped version of the underlying data d
head(plt$data)
##    threshold measure performance
## 1 0.00000000     fpr   1.0000000
## 2 0.01010101     fpr   0.3541667
## 3 0.02020202     fpr   0.3333333
```

```
## 4 0.03030303     fpr   0.3333333
## 5 0.04040404     fpr   0.3333333
## 6 0.05050505     fpr   0.3125000
levels(plt$data$measure)
## [1] "fpr"  "fnr"  "mmce"
### Rename and reorder factor levels
plt$data$measure = factor(plt$data$measure, levels = c("mmce", "fpr", "fnr"),
  labels = c("Error rate", "False positive rate", "False negative rate"))
plt = plt + xlab("Cutoff") + ylab("Performance")
plt
```



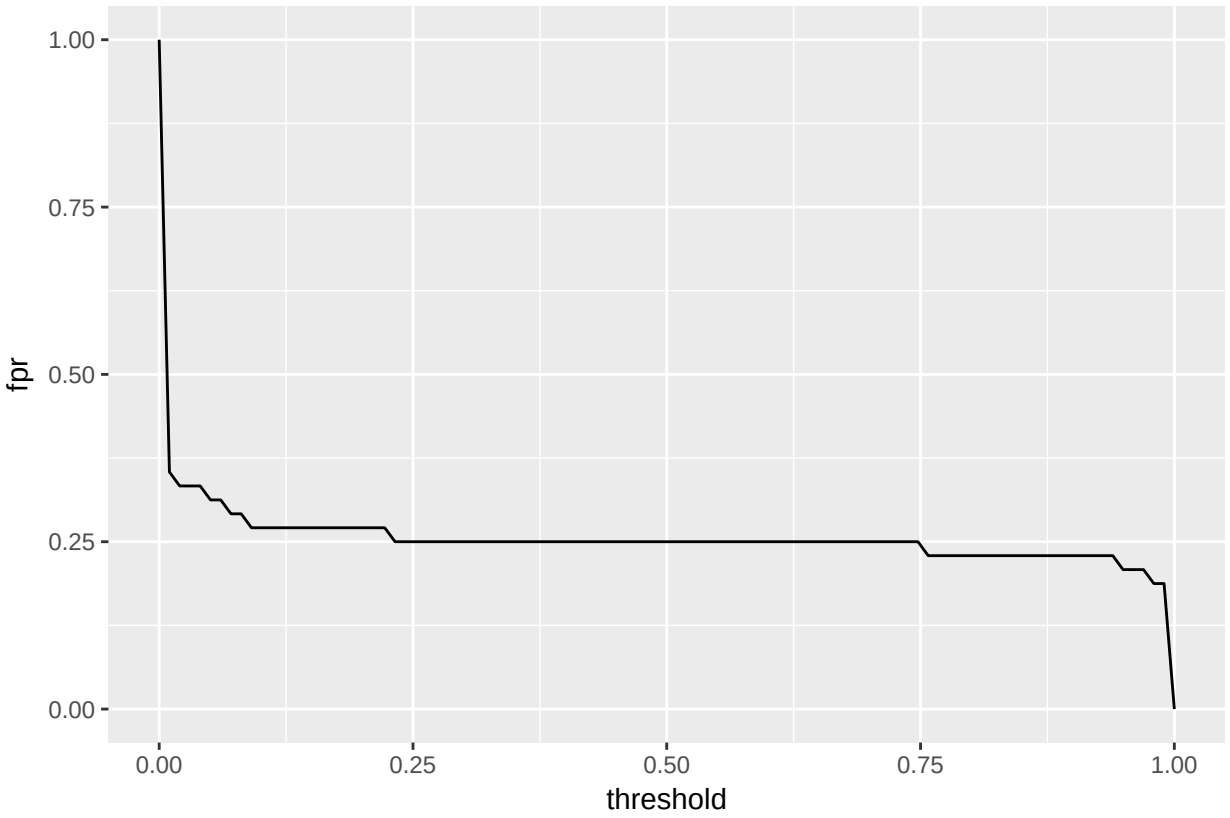
Using the `ggplot2::labeller()` function requires calling `ggplot2::facet_wrap()` (or `ggplot2::facet_grid()`), which can be useful if you want to change how the panels are positioned (number of rows and columns) or influence the axis limits.

```
plt = plotThreshVsPerf(d, pretty.names = FALSE)

measure_names = c(
  fpr = "False positive rate",
  fnr = "False negative rate",
  mmce = "Error rate"
)
### Manipulate the measure names via the labeller function and
### arrange the panels in two columns and choose common axis limits for all panels
plt = plt + facet_wrap( ~ measure, labeller = labeller(measure = measure_names), ncol = 2)
plt = plt + xlab("Decision threshold") + ylab("Performance")
plt
```



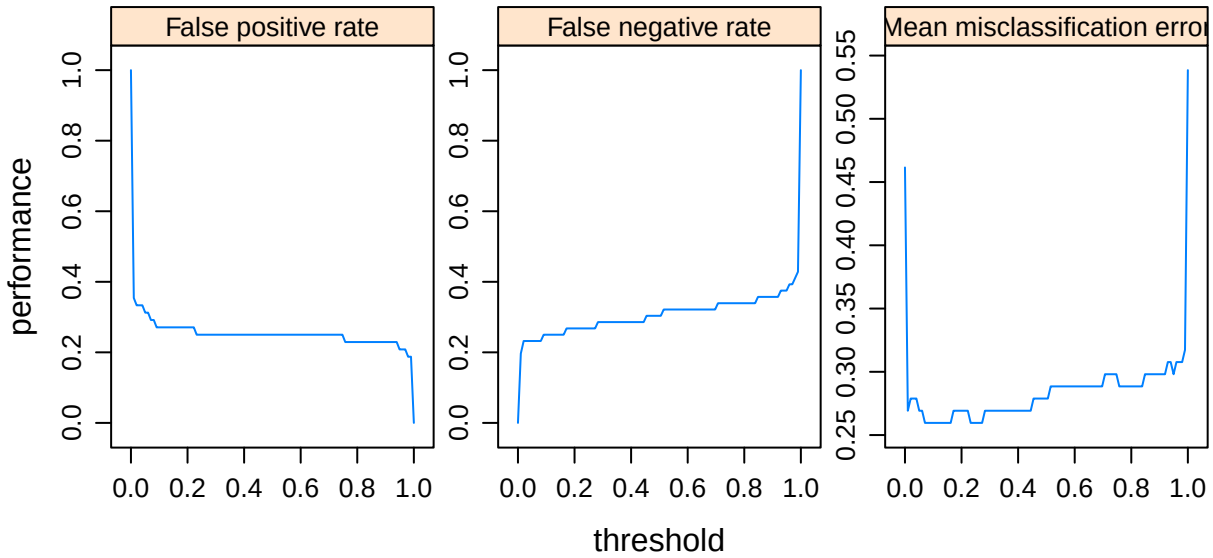
Instead of using the built-in function `plotThreshVsPerf()` we could also manually create the plot based on the output of `generateThreshVsPerfData()`: In this case to plot only one measure.

```
ggplot(d$data, aes(threshold, fpr)) + geom_line()
```



The decoupling of generation and plotting functions is especially practical if you prefer traditional `graphics::graphics()` or `lattice::lattice()`. Here is a `lattice::lattice()` plot which gives a result similar to that of `plotThreshVsPerf()`.

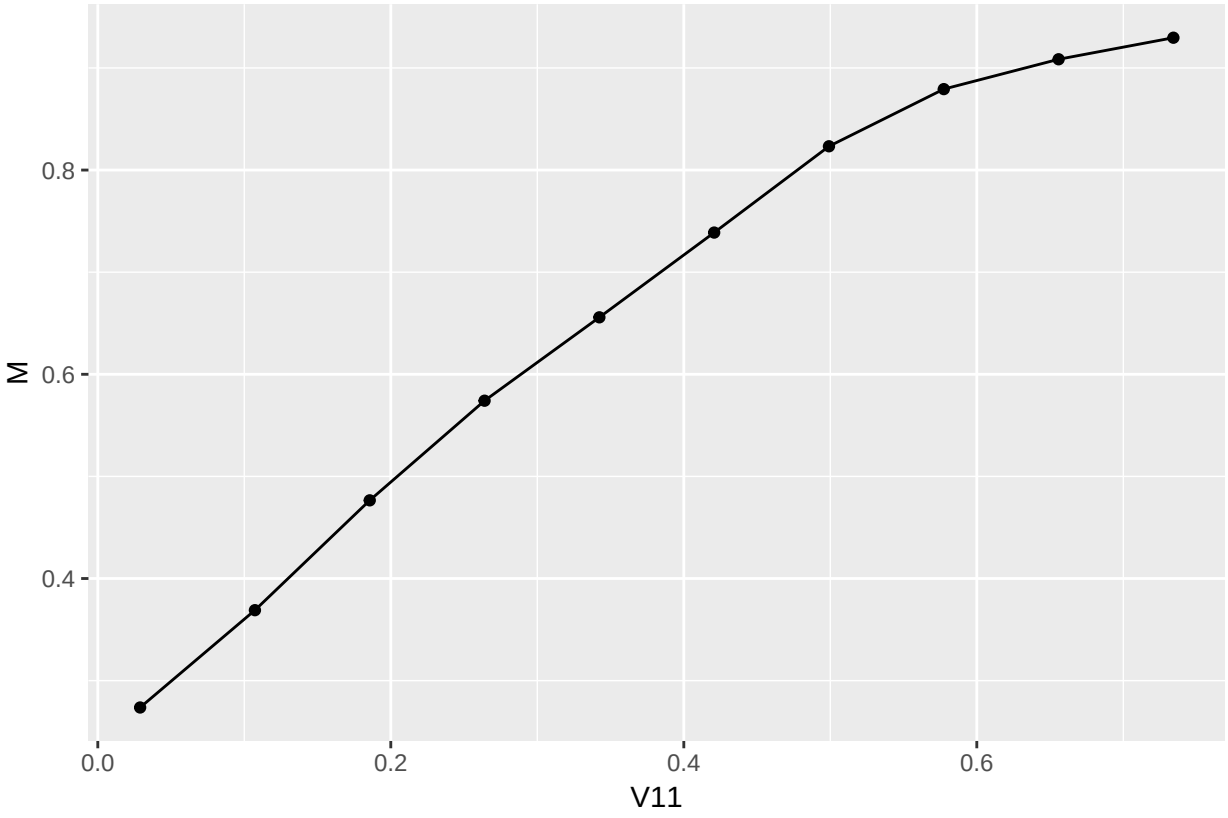
```
lattice::xyplot(fpr + fnr + mmce ~ threshold, data = d$data, type = "l", ylab = "performance",
  outer = TRUE, scales = list(relation = "free"),
  strip = strip.custom(factor.levels = sapply(d$measures, function(x) x$name),
    par.strip.text = list(cex = 0.8)))
```



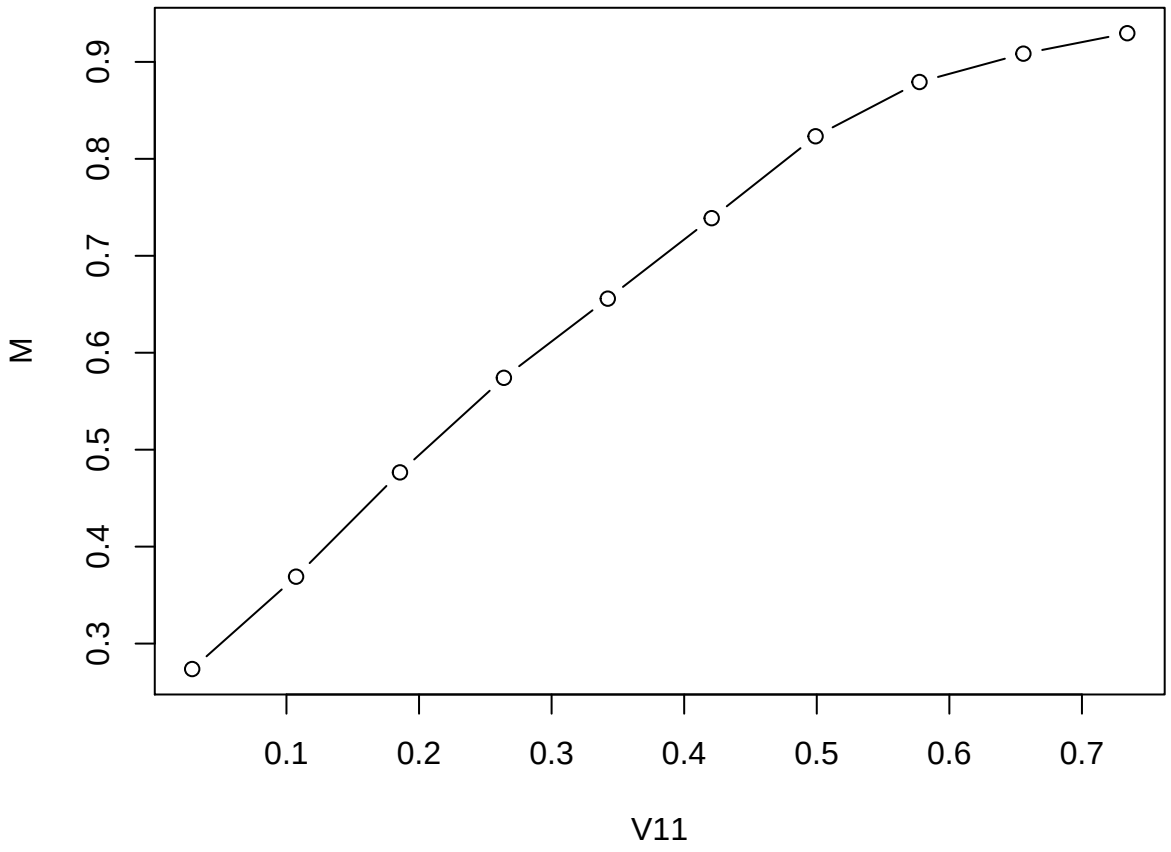
Let's conclude with a brief look on a second example. Here we use `plotPartialDependence()` but extract the data from the `ggplot2::ggplot()` object `plt` and use it to create a traditional `graphics::plot()`,

additional to the `ggplot2::ggplot()` plot.

```
sonar = getTaskData(sonar.task)
pd = generatePartialDependenceData(mod, sonar, "V11")
## Loading required package: mmpf
plt = plotPartialDependence(pd)
head(plt$data)
##           M Feature     Value
## 1 0.2737158     V11 0.0289000
## 2 0.3689970     V11 0.1072667
## 3 0.4765742     V11 0.1856333
## 4 0.5741233     V11 0.2640000
## 5 0.6557857     V11 0.3423667
## 6 0.7387962     V11 0.4207333
plt
```




```
plot(M ~ Value, data = plt$data, type = "b", xlab = plt$data$Feature[1])
```



2.9.2 Available generation and plotting functions

Below the currently available generation and plotting functions are listed and tutorial pages that provide in depth descriptions of the listed functions are referenced.

Note that some plots, e.g., `plotTuneMultiCritResult()` are not mentioned here since they lack a generation function. Both `plotThreshVsPerf()` and `plotROCCurves()` operate on the result of `generateThreshVsPerfData()`. Functions `plotPartialDependence()` and `plotPartialDependenceGGVIS()` can be applied to the results of both `generatePartialDependenceData()` and `generateFunctionalANOVAData()`.

The `ggvis::ggvis()` functions are experimental and are subject to change, though they should work. Most generate interactive `shiny::shiny()` applications, that automatically start and run locally.

generation function	ggplot2 plotting function	ggvis plotting function	tutorial pages
`generateThreshVsPerfData()`	`plotThreshVsPerf()`	`plotThreshVsPerfGGVIS()`	performance
	`plotROCCurves()`		ROC analysis
`generateCritDifferencesData()`	`plotCritDifferences()`		benchmark experiments
`generateHyperParsEffectData()`	`plotHyperParsEffect()`		tuning, hyperparameter tuning effects
`generateFilterValuesData()`	`plotFilterValues()`	`plotFilterValuesGGVIS()`	feature selection
`generateLearningCurveData()`	`plotLearningCurve()`	`plotLearningCurveGGVIS()`	learning curves
`generatePartialDependenceData()`	`plotPartialDependence()`	`plotPartialDependenceGGVIS()`	partial dependence
`generateFunctionalANOVAData()`			
`generateCalibrationData()`	`plotCalibration()`		classifier calibration

3 Advanced

3.1 Configuring mlr

`mlr` is designed to make usage errors due to typos or invalid parameter values as unlikely as possible. Occasionally, you might want to break those barriers and get full access, for example to reduce the amount of output on the console or to turn off checks. For all available options simply refer to the documentation of `configureMlr()`. In the following we show some common use cases.

Generally, function `configureMlr()` permits to set options globally for your current **R** session.

It is also possible to set options locally.

- All options referring to the behavior of learners (these are all options except `show.info`) can be set for an individual learner via the `config` argument of `makeLearner()`. The local precedes the global configuration.
- Some functions like `resample()`, `benchmark()`, `selectFeatures()`, `tuneParams()`, and `tuneParamsMultiCrit()` have a `show.info` flag that controls if progress messages are shown. The default value of `show.info` can be set by `configureMlr()`.

3.1.1 Example: Reducing the output on the console

You are bothered by all the output on the console like in this example?

```
rdesc = makeResampleDesc("Holdout")
r = resample("classif.multinom", iris.task, rdesc)
## Resampling: holdout
## Measures:             mmce
## # weights:  18 (10 variable)
## initial  value 109.861229
## iter  10 value 11.544965
## iter  20 value 5.816992
## iter  30 value 5.256034
## iter  40 value 5.236441
## iter  50 value 5.222550
## iter  60 value 5.218308
## iter  70 value 5.217042
## iter  80 value 5.216838
## final  value 5.216834
## converged
## [Resample] iter 1:    0.0000000
##
## Aggregated Result: mmce.test.mean=0.0000000
##
```

You can suppress the output for this Learner `makeLearner()` and this `resample()` call as follows:

```
lrn = makeLearner("classif.multinom", config = list(show.learner.output = FALSE))
r = resample(lrn, iris.task, rdesc, show.info = FALSE)
```

(Note that `nnet::multinom()` has a `trace` switch that can alternatively be used to turn off the progress messages.)

To globally suppress the output for all subsequent learners and calls to `resample()`, `benchmark()` etc. do the following:

```
configureMlr(show.learner.output = FALSE, show.info = FALSE)
r = resample("classif.multinom", iris.task, rdesc)
```

3.1.2 Accessing and resetting the configuration

Function `getMlrOptions()` returns a `base::list()` with the current configuration.

```
getMlrOptions()
## $show.info
## [1] FALSE
##
## $on.learner.error
## [1] "stop"
##
## $on.learner.warning
## [1] "warn"
##
## $on.par.without.desc
## [1] "stop"
##
## $on.par.out.of.bounds
## [1] "stop"
##
## $on.measure.not.applicable
## [1] "stop"
##
## $show.learner.output
## [1] FALSE
##
## $on.error.dump
## [1] FALSE
```

To restore the default configuration call `configureMlr()` with an empty argument list.

```
configureMlr()
getMlrOptions()
## $show.info
## [1] TRUE
##
## $on.learner.error
## [1] "stop"
##
## $on.learner.warning
## [1] "warn"
##
## $on.par.without.desc
## [1] "stop"
##
## $on.par.out.of.bounds
## [1] "stop"
##
## $on.measure.not.applicable
## [1] "stop"
##
```

```
## $show.learner.output
## [1] TRUE
##
## $on.error.dump
## [1] FALSE
```

3.1.3 Example: Turning off parameter checking

It might happen that you want to set a parameter of a Learner (`makeLearner()`, but the parameter is not registered in the learner's parameter set (`ParamHelpers::makeParamSet()`) yet. In this case you might want to contact us or open an issue as well! But until the problem is fixed you can turn off `mlr`'s parameter checking. The parameter setting will then be passed to the underlying function without further ado.

```
### Support Vector Machine with linear kernel and new parameter 'newParam'
lrn = makeLearner("classif.ksvm", kernel = "vanilladot", newParam = 3)
## Error in setHyperPars2.Learner(learner, insert(par.vals, args)): classif.ksvm: Setting parameter newP
## Did you mean one of these hyperparameters instead: degree scaled kernel
## You can switch off this check by using configureMlr!
### Turn off parameter checking completely
configureMlr(on.par.without.desc = "quiet")
lrn = makeLearner("classif.ksvm", kernel = "vanilladot", newParam = 3)
train(lrn, iris.task)
##  Setting default kernel parameters
## Model for learner.id=classif.ksvm; learner.class=classif.ksvm
## Trained on: task.id = iris-example; obs = 150; features = 4
## Hyperparameters: fit=FALSE,kernel=vanilladot,newParam=3
### Option "quiet" also masks typos
lrn = makeLearner("classif.ksvm", kernl = "vanilladot")
train(lrn, iris.task)
## Model for learner.id=classif.ksvm; learner.class=classif.ksvm
## Trained on: task.id = iris-example; obs = 150; features = 4
## Hyperparameters: fit=FALSE,kernl=vanilladot
### Alternatively turn off parameter checking, but still see warnings
configureMlr(on.par.without.desc = "warn")
lrn = makeLearner("classif.ksvm", kernl = "vanilladot", newParam = 3)
## Warning in setHyperPars2.Learner(learner, insert(par.vals, args)): classif.ksvm: Setting parameter ke
## Did you mean one of these hyperparameters instead: kernel nu degree
## You can switch off this check by using configureMlr!
## Warning in setHyperPars2.Learner(learner, insert(par.vals, args)): classif.ksvm: Setting parameter ne
## Did you mean one of these hyperparameters instead: degree scaled kernel
## You can switch off this check by using configureMlr!
train(lrn, iris.task)
## Model for learner.id=classif.ksvm; learner.class=classif.ksvm
## Trained on: task.id = iris-example; obs = 150; features = 4
## Hyperparameters: fit=FALSE,kernl=vanilladot,newParam=3
```

3.1.4 Example: Handling errors in a learning method

If a learning method throws an error the default behavior of `mlr` is to generate an exception as well. However, in some situations, for example if you conduct a larger bechmark experiment with multiple data sets and learners, you usually don't want the whole experiment stopped due to one error. You can prevent this using the `on.learner.error` option of `configureMlr()`.

```
### This call gives an error caused by the low number of observations in class "virginica"
train("classif.qda", task = iris.task, subset = 1:104)
## Error in qda.default(x, grouping, ...): some group is too small for 'qda'
### Get a warning instead of an error
configureMlr(on.learner.error = "warn")
mod = train("classif.qda", task = iris.task, subset = 1:104)
## Warning in train("classif.qda", task = iris.task, subset = 1:104): Could not train learner classif.q
##   some group is too small for 'qda'
mod
## Model for learner.id=classif.qda; learner.class=classif.qda
## Trained on: task.id = iris-example; obs = 104; features = 4
## Hyperparameters:
## Training failed: Error in qda.default(x, grouping, ...) :
##   some group is too small for 'qda'
##
## Training failed: Error in qda.default(x, grouping, ...) :
##   some group is too small for 'qda'
### mod is an object of class FailureModel
isFailureModel(mod)
## [1] TRUE
### Retrieve the error message
getFailureModelMsg(mod)
## [1] "Error in qda.default(x, grouping, ...) : \n  some group is too small for 'qda'\n"
### predict and performance return NA's
pred = predict(mod, iris.task)
pred
## Prediction: 150 observations
## predict.type: response
## threshold:
## time: NA
##   id  truth response
## 1  1 setosa     <NA>
## 2  2 setosa     <NA>
## 3  3 setosa     <NA>
## 4  4 setosa     <NA>
## 5  5 setosa     <NA>
## 6  6 setosa     <NA>
## ... (#rows: 150, #cols: 3)
performance(pred)
## mmce
##   NA
```

If `on.learner.error = "warn"` a warning is issued instead of an exception and an object of class `FailureModel()` is created. You can extract the error message using function `getFailureModelMsg()`. All further steps like prediction and performance calculation work and return `NA's`.

3.2 Wrapper

Wrappers can be employed to extend integrated learners (`makeLearner()`) with new functionality. The broad scope of operations and methods which are implemented as wrappers underline the flexibility of the wrapping approach:

- Data preprocessing
- Imputation

- Bagging
- Tuning
- Feature selection
- Cost-sensitive classification
- Over- and undersampling for imbalanced classification problems
- Multiclass extension (`makeMulticlassWrapper()`) for binary-class learners
- Multilabel classification

All these operations and methods have a few things in common: First, they all wrap around `mlr` learners (`makeLearner()`) and they return a new learner. Therefore learners can be wrapped multiple times. Second, they are implemented using a *train* (pre-model hook) and *predict* (post-model hook) method.

3.2.1 Example: Bagging wrapper

In this section we exemplary describe the bagging wrapper to create a random forest which supports weights. To achieve that we combine several decision trees from the `rpart` package to create our own custom random forest.

First, we create a weighted toy task.

```
data(iris)
task = makeClassifTask(data = iris, target = "Species", weights = as.integer(iris$Species))
```

Next, we use `makeBaggingWrapper()` to create the base learners and the bagged learner. We choose to set equivalents of `ntree` (100 base learners) and `mtry` (proportion of randomly selected features).

```
base.lrn = makeLearner("classif.rpart")
wrapped.lrn = makeBaggingWrapper(base.lrn, bw.iters = 100, bw.feats = 0.5)
print(wrapped.lrn)
## Learner classif.rpart.bagged from package rpart
## Type: classif
## Name: ; Short name:
## Class: BaggingWrapper
## Properties: twoclass,multiclass,missings,numerics,factors,ordered,prob,weights,featimp
## Predict-Type: response
## Hyperparameters: xval=0,bw.iters=100,bw.feats=0.5
```

As we can see in the output, the wrapped learner inherited all properties from the base learner, especially the "weights" attribute is still present. We can use this newly constructed learner like all base learners, i.e. we can use it in `train()`, `benchmark()`, `resample()`, etc.

```
benchmark(tasks = task, learners = list(base.lrn, wrapped.lrn))
## Task: iris, Learner: classif.rpart
## Resampling: cross-validation
## Measures:             mmce
## [Resample] iter 1:    0.0666667
## [Resample] iter 2:    0.2000000
## [Resample] iter 3:    0.0666667
## [Resample] iter 4:    0.1333333
## [Resample] iter 5:    0.0000000
## [Resample] iter 6:    0.0000000
## [Resample] iter 7:    0.1333333
## [Resample] iter 8:    0.1333333
## [Resample] iter 9:    0.0000000
## [Resample] iter 10:   0.0666667
##
```

```
## Aggregated Result: mmce.test.mean=0.0800000
##
## Task: iris, Learner: classif.rpart.bagged
## Resampling: cross-validation
## Measures:             mmce
## [Resample] iter 1:    0.0666667
## [Resample] iter 2:    0.2000000
## [Resample] iter 3:    0.0666667
## [Resample] iter 4:    0.0000000
## [Resample] iter 5:    0.0000000
## [Resample] iter 6:    0.0000000
## [Resample] iter 7:    0.1333333
## [Resample] iter 8:    0.1333333
## [Resample] iter 9:    0.0000000
## [Resample] iter 10:   0.0666667
##
## Aggregated Result: mmce.test.mean=0.0666667
##
##   task.id           learner.id mmce.test.mean
## 1    iris        classif.rpart     0.08000000
## 2    iris classif.rpart.bagged     0.06666667
```

That far we are quite happy with our new learner. But we hope for a better performance by tuning some hyperparameters of both the decision trees and bagging wrapper. Let's have a look at the available hyperparameters of the fused learner:

```
getParamSet(wrapped.lrn)
##                     Type len   Def   Constr Req Tunable Trafo
## bw.iters         integer   -    10 1 to Inf   -    TRUE     -
## bw.replace       logical   -  TRUE        -   -    TRUE     -
## bw.size          numeric   -     -   0 to 1   -    TRUE     -
## bw.feats         numeric   - 0.667   0 to 1   -    TRUE     -
## minsplit         integer   -    20 1 to Inf   -    TRUE     -
## minbucket        integer   -     - 1 to Inf   -    TRUE     -
## cp               numeric   -  0.01   0 to 1   -    TRUE     -
## maxcompete       integer   -     4 0 to Inf   -    TRUE     -
## maxsurrogate     integer   -     5 0 to Inf   -    TRUE     -
## usesurrogate    discrete   -     2    0,1,2   -    TRUE     -
## surrogatestyle  discrete   -     0      0,1   -    TRUE     -
## maxdepth         integer   -    30  1 to 30   -    TRUE     -
## xval             integer   -    10 0 to Inf   -   FALSE     -
## parms            untyped   -     -        -   -    TRUE     -
```

We choose to tune the parameters `minsplit` and `bw.feats` for the mmce using a random search (`TuneControl()`) in a 3-fold CV:

```
ctrl = makeTuneControlRandom(maxit = 10)
rdesc = makeResampleDesc("CV", iters = 3)
par.set = makeParamSet(
  makeIntegerParam("minsplit", lower = 1, upper = 10),
  makeNumericParam("bw.feats", lower = 0.25, upper = 1)
)
tuned.lrn = makeTuneWrapper(wrapped.lrn, rdesc, mmce, par.set, ctrl)
print(tuned.lrn)
## Learner classif.rpart.bagged.tuned from package rpart
```

```
## Type: classif
## Name: ; Short name:
## Class: TuneWrapper
## Properties: numerics,factors,ordered,missings,weights,prob,twoclass,multiclass,featimp
## Predict-Type: response
## Hyperparameters: xval=0,bw.iters=100,bw.feats=0.5
```

Calling the train method of the newly constructed learner performs the following steps:

1. The tuning wrapper sets parameters for the underlying model in slot `$next.learner` and calls its train method.
2. Next learner is the bagging wrapper. The passed down argument `bw.feats` is used in the bagging wrapper training function, the argument `minsplit` gets passed down to `$next.learner`. The base wrapper function calls the base learner `bw.iters` times and stores the resulting models.
3. The bagged models are evaluated using the mean mmce (default aggregation for this performance measure) and new parameters are selected using the tuning method.
4. This is repeated until the tuner terminates. Output is a tuned bagged learner.

```
lrn = train(tuned.lrn, task = task)
## [Tune] Started tuning learner classif.rpart.bagged for parameter set:
##             Type len Def    Constr Req Tunable Trafo
## minsplit integer   -   -   1 to 10   -    TRUE     -
## bw.feats numeric   -   - 0.25 to 1   -    TRUE     -
## With control class: TuneControlRandom
## Imputation value: 1
## [Tune-x] 1: minsplit=4; bw.feats=0.481
## [Tune-y] 1: mmce.test.mean=0.0533333; time: 0.1 min
## [Tune-x] 2: minsplit=9; bw.feats=0.662
## [Tune-y] 2: mmce.test.mean=0.0466667; time: 0.1 min
## [Tune-x] 3: minsplit=9; bw.feats=0.915
## [Tune-y] 3: mmce.test.mean=0.0466667; time: 0.1 min
## [Tune-x] 4: minsplit=2; bw.feats=0.573
## [Tune-y] 4: mmce.test.mean=0.0466667; time: 0.1 min
## [Tune-x] 5: minsplit=6; bw.feats=0.921
## [Tune-y] 5: mmce.test.mean=0.0466667; time: 0.1 min
## [Tune-x] 6: minsplit=2; bw.feats=0.526
## [Tune-y] 6: mmce.test.mean=0.0533333; time: 0.1 min
## [Tune-x] 7: minsplit=9; bw.feats=0.296
## [Tune-y] 7: mmce.test.mean=0.0866667; time: 0.1 min
## [Tune-x] 8: minsplit=3; bw.feats=0.281
## [Tune-y] 8: mmce.test.mean=0.0933333; time: 0.1 min
## [Tune-x] 9: minsplit=9; bw.feats=0.426
## [Tune-y] 9: mmce.test.mean=0.0733333; time: 0.1 min
## [Tune-x] 10: minsplit=2; bw.feats=0.539
## [Tune-y] 10: mmce.test.mean=0.0400000; time: 0.1 min
## [Tune] Result: minsplit=2; bw.feats=0.539 : mmce.test.mean=0.0400000
print(lrn)
## Model for learner.id=classif.rpart.bagged.tuned; learner.class=TuneWrapper
## Trained on: task.id = iris; obs = 150; features = 4
## Hyperparameters: xval=0,bw.iters=100,bw.feats=0.5
```

3.3 Data Preprocessing

Data preprocessing refers to any transformation of the data done before applying a learning algorithm. This comprises for example finding and resolving inconsistencies, imputation of missing values, identifying, removing or replacing outliers, discretizing numerical data or generating numerical dummy variables for categorical data, any kind of transformation like standardization of predictors or Box-Cox, dimensionality reduction and feature extraction and/or selection.

`mlr` offers several options for data preprocessing. Some of the following simple methods to change a `Task()` (or `data.frame`) were already mentioned on the page about learning tasks:

- `capLargeValues()`: Convert large/infinite numeric values.
- `createDummyFeatures()`: Generate dummy variables for factor features.
- `dropFeatures()`: Remove selected features.
- `joinClassLevels()`: Only for classification: Merge existing classes to new, larger classes.
- `mergeSmallFactorLevels()`: Merge infrequent levels of factor features.
- `normalizeFeatures()`: Normalize features by different methods, e.g., standardization or scaling to a certain range.
- `removeConstantFeatures()`: Remove constant features.
- `subsetTask()`: Remove observations and/or features from a `Task()`.

Moreover, there are tutorial pages devoted to

- Feature selection and
- Imputation of missing values.

3.3.1 Fusing learners with preprocessing

`mlr`'s wrapper functionality permits to combine learners with preprocessing steps. This means that the preprocessing "belongs" to the learner and is done any time the learner is trained or predictions are made.

This is, on the one hand, very practical. You don't need to change any data or learning `Task()`s and it's quite easy to combine different learners with different preprocessing steps.

On the other hand this helps to avoid a common mistake in evaluating the performance of a learner with preprocessing: Preprocessing is often seen as completely independent of the later applied learning algorithms. When estimating the performance of the a learner, e.g., by cross-validation all preprocessing is done beforehand on the full data set and only training/predicting the learner is done on the train/test sets. Depending on what exactly is done as preprocessing this can lead to overoptimistic results. For example if imputation by the mean is done on the whole data set before evaluating the learner performance you are using information from the test data during training, which can cause overoptimistic performance results.

To clarify things one should distinguish between *data-dependent* and *data-independent* preprocessing steps: Data-dependent steps in some way learn from the data and give different results when applied to different data sets. Data-independent steps always lead to the same results. Clearly, correcting errors in the data or removing data columns like Ids that should not be used for learning, is data-independent. Imputation of missing values by the mean, as mentioned above, is data-dependent. Imputation by a fixed constant, however, is not.

To get a honest estimate of learner performance combined with preprocessing, all data-dependent preprocessing steps must be included in the resampling. This is automatically done when fusing a learner with preprocessing.

To this end `mlr` provides two wrappers:

- `makePreprocWrapperCaret()` is an interface to all preprocessing options offered by `caret`'s `caret::preProcess()` function.
- `makePreprocWrapper()` permits to write your own custom preprocessing methods by defining the actions to be taken before training and before prediction.

As mentioned above the specified preprocessing steps then "belong" to the wrapped Learner (`makeLearner()`). In contrast to the preprocessing options listed above like `normalizeFeatures()`

- the `Task()` itself remains unchanged,
- the preprocessing is not done globally, i.e., for the whole data set, but for every pair of training/test data sets in, e.g., resampling,
- any parameters controlling the preprocessing as, e.g., the percentage of outliers to be removed can be tuned together with the base learner parameters.

We start with some examples for `makePreprocWrapperCaret()`.

3.3.2 Preprocessing with makePreprocWrapperCaret

`makePreprocWrapperCaret()` is an interface to `caret`'s `caret::preProcess()` function that provides many different options like imputation of missing values, data transformations as scaling the features to a certain range or Box-Cox and dimensionality reduction via Independent or Principal Component Analysis. For all possible options see the help page of function `caret::preProcess()`.

Note that the usage of `makePreprocWrapperCaret()` is slightly different than that of `caret::preProcess()`.

- `makePreprocWrapperCaret()` takes (almost) the same formal arguments as `caret:preProcess()`, but their names are prefixed by `ppc.`.
- The only exception: `makePreprocWrapperCaret()` does not have a `method` argument. Instead all preprocessing options that would be passed to `caret::preProcess()`'s `method` argument are given as individual logical parameters to `makePreprocWrapperCaret()`.

For example the following call to `caret::preProcess()`

```
preProcess(x, method = c("knnImpute", "pca"), pcaComp = 10)
```

with `x` being a `matrix` or `data.frame` would thus translate into

```
makePreprocWrapperCaret(learner, ppc.knnImpute = TRUE, ppc.pca = TRUE, ppc.pcaComp = 10)
```

where `learner` is a `mlr` Learner (`makeLearner()`) or the name of a learner class like `"classif.lda"`.

If you enable multiple preprocessing options (like knn imputation and principal component analysis above) these are executed in a certain order detailed on the help page of function `caret::preProcess()`.

In the following we show an example where principal components analysis (PCA) is used for dimensionality reduction. This should never be applied blindly, but can be beneficial with learners that get problems with high dimensionality or those that can profit from rotating the data.

We consider the `sonar.task()`, which poses a binary classification problem with 208 observations and 60 features.

```
sonar.task
## Supervised task: Sonar-example
## Type: classif
## Target: Class
## Observations: 208
## Features:
##    numerics     factors     ordered functionals
##          60           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
## Classes: 2
```

```
##   M   R
## 111  97
## Positive class: M
```

Below we fuse quadratic discriminant analysis (`MASS::qda()`) from package `MASS` with a principal components preprocessing step. The threshold is set to 0.9, i.e., the principal components necessary to explain a cumulative percentage of 90% of the total variance are kept. The data are automatically standardized prior to PCA.

```
lrn = makePreprocWrapperCaret("classif.qda", ppc.pca = TRUE, ppc.thresh = 0.9)
lrn
## Learner classif.qda.preproc from package MASS
## Type: classif
## Name: ; Short name:
## Class: PreprocWrapperCaret
## Properties: twoclass,multiclass,numerics,factors,prob
## Predict-Type: response
## Hyperparameters: ppc.BoxCox=FALSE,ppc.YeoJohnson=FALSE,ppc.expoTrans=FALSE,ppc.center=TRUE,ppc.scale=
```

The wrapped learner is trained on the `sonar.task()`. By inspecting the underlying `MASS::qda()` model, we see that the first 22 principal components have been used for training.

```
mod = train(lrn, sonar.task)
mod
## Model for learner.id=classif.qda.preproc; learner.class=PreprocWrapperCaret
## Trained on: task.id = Sonar-example; obs = 208; features = 60
## Hyperparameters: ppc.BoxCox=FALSE,ppc.YeoJohnson=FALSE,ppc.expoTrans=FALSE,ppc.center=TRUE,ppc.scale=
getLearnerModel(mod)
## Model for learner.id=classif.qda; learner.class=classif.qda
## Trained on: task.id = Sonar-example; obs = 208; features = 22
## Hyperparameters:
getLearnerModel(mod, more.unwrap = TRUE)
## Call:
## qda(f, data = getTaskData(.task, .subset, recode.target = "drop.levels"))
##
## Prior probabilities of groups:
##         M         R
## 0.5336538 0.4663462
##
## Group means:
##          PC1        PC2        PC3         PC4         PC5         PC6
## M  0.5976122 -0.8058235  0.9773518  0.03794232 -0.04568166 -0.06721702
## R -0.6838655  0.9221279 -1.1184128 -0.04341853  0.05227489  0.07691845
##          PC7         PC8        PC9       PC10        PC11          PC12
## M  0.2278162 -0.01034406 -0.2530606 -0.1793157 -0.04084466 -0.0004789888
## R -0.2606969  0.01183702  0.2895848  0.2051963  0.04673977  0.0005481212
##          PC13       PC14        PC15        PC16        PC17        PC18
## M -0.06138758 -0.1057137  0.02808048  0.05215865 -0.07453265  0.03869042
## R  0.07024765  0.1209713 -0.03213333 -0.05968671  0.08528994 -0.04427460
##          PC19         PC20        PC21         PC22
## M -0.01192247  0.006098658  0.01263492 -0.001224809
## R  0.01364323 -0.006978877 -0.01445851  0.001401586
```

Below the performances of `MASS::qda()` with and without PCA preprocessing are compared in a benchmark experiment. Note that we use stratified resampling to prevent errors in `MASS::qda()` due to a too small number of observations from either class.

```
rin = makeResampleInstance("CV", iters = 3, stratify = TRUE, task = sonar.task)
res = benchmark(list("classif.qda", lrn), sonar.task, rin, show.info = FALSE)
res
##         task.id          learner.id mmce.test.mean
## 1 Sonar-example         classif.qda       0.389648
## 2 Sonar-example classif.qda.preproc       0.273844
```

PCA preprocessing in this case turns out to be really beneficial for the performance of Quadratic Discriminant Analysis.

3.3.2.1 Joint tuning of preprocessing options and learner parameters

Let's see if we can optimize this a bit. The threshold value of 0.9 above was chosen arbitrarily and led to 22 out of 60 principal components. But maybe a lower or higher number of principal components should be used. Moreover, `qda` (`MASS::qda()`) has several options that control how the class covariance matrices or class probabilities are estimated.

Those preprocessing and learner parameters can be tuned jointly. Before doing this let's first get an overview of all the parameters of the wrapped learner using function `getParamSet()`.

```
getParamSet(lrn)
##                      Type len     Def                      Constr Req
## ppc.BoxCox        logical   -   FALSE                           -   -
## ppc.YeoJohnson    logical   -   FALSE                           -   -
## ppc.expoTrans     logical   -   FALSE                           -   -
## ppc.center        logical   -    TRUE                           -   -
## ppc.scale         logical   -    TRUE                           -   -
## ppc.range         logical   -   FALSE                           -   -
## ppc.knnImpute     logical   -   FALSE                           -   -
## ppc.bagImpute     logical   -   FALSE                           -   -
## ppc.medianImpute  logical   -   FALSE                           -   -
## ppc.pca           logical   -   FALSE                           -   -
## ppc.ica           logical   -   FALSE                           -   -
## ppc.spatialSign   logical   -   FALSE                           -   -
## ppc.corr          logical   -   FALSE                           -   -
## ppc.zv            logical   -   FALSE                           -   -
## ppc.nzv           logical   -   FALSE                           -   -
## ppc.thresh        numeric   -    0.95                  0 to Inf   -
## ppc.pcaComp       integer   -       -                  1 to Inf   -
## ppc.na.remove     logical   -    TRUE                           -   -
## ppc.k             integer   -       5                  1 to Inf   -
## ppc.fudge         numeric   -     0.2                  0 to Inf   -
## ppc.numUnique     integer   -       3                  1 to Inf   -
## ppc.n.comp        integer   -       -                  1 to Inf   -
## ppc.cutoff        numeric   -     0.9                    0 to 1   -
## ppc.freqCut       numeric   -      19                  1 to Inf   -
## ppc.uniqueCut     numeric   -      10                  0 to Inf   -
## method           discrete   -  moment           moment,mle,mve,t   -
## nu                numeric   -       5                  2 to Inf   Y
## predict.method   discrete   - plug-in plug-in,predictive,debiased   -
##                  Tunable Trafo
## ppc.BoxCox          TRUE     -
## ppc.YeoJohnson      TRUE     -
## ppc.expoTrans       TRUE     -
```

```
## ppc.center          TRUE     -
## ppc.scale           TRUE     -
## ppc.range           TRUE     -
## ppc.knnImpute       TRUE     -
## ppc.bagImpute       TRUE     -
## ppc.medianImpute    TRUE     -
## ppc.pca             TRUE     -
## ppc.ica             TRUE     -
## ppc.spatialSign     TRUE     -
## ppc.corr            TRUE     -
## ppc.zv              TRUE     -
## ppc.nzv             TRUE     -
## ppc.thresh          TRUE     -
## ppc.pcaComp         TRUE     -
## ppc.na.remove       TRUE     -
## ppc.k               TRUE     -
## ppc.fudge           TRUE     -
## ppc.numUnique       TRUE     -
## ppc.n.comp          TRUE     -
## ppc.cutoff          TRUE     -
## ppc.freqCut         TRUE     -
## ppc.uniqueCut       TRUE     -
## method              TRUE     -
## nu                  TRUE     -
## predict.method      TRUE     -
```

The parameters prefixed by `ppc.` belong to preprocessing. `method`, `nu` and `predict.method` are `MASS::qda()` parameters.

Instead of tuning the PCA threshold (`ppc.thresh`) we tune the number of principal components (`ppc.pcaComp`) directly. Moreover, for `MASS::qda()` we try two different ways to estimate the posterior probabilities (parameter `predict.method`): the usual plug-in estimates and unbiased estimates.

We perform a grid search and set the resolution to 10. This is for demonstration. You might want to use a finer resolution.

```
ps = makeParamSet(
  makeIntegerParam("ppc.pcaComp", lower = 1, upper = getTaskNFeats(sonar.task)),
  makeDiscreteParam("predict.method", values = c("plug-in", "debiased"))
)
ctrl = makeTuneControlGrid(resolution = 10)
res = tuneParams(lrn, sonar.task, rin, par.set = ps, control = ctrl, show.info = FALSE)
res
## Tune result:
## Op. pars: ppc.pcaComp=14; predict.method=plug-in
## mmce.test.mean=0.2400276
as.data.frame(res$opt.path)[1:3]
##    ppc.pcaComp predict.method mmce.test.mean
## 1            1        plug-in      0.4713596
## 2            8        plug-in      0.2494824
## 3           14        plug-in      0.2400276
## 4           21        plug-in      0.2690131
## 5           27        plug-in      0.2834369
## 6           34        plug-in      0.2882678
## 7           40        plug-in      0.2835059
```

```
## 8           47        plug-in      0.2737060
## 9           53        plug-in      0.3031056
## 10          60        plug-in      0.3896480
## 11           1       debiased      0.4807453
## 12           8       debiased      0.2541063
## 13          14       debiased      0.3168392
## 14          21       debiased      0.3312629
## 15          27       debiased      0.3216701
## 16          34       debiased      0.3120083
## 17          40       debiased      0.3120083
## 18          47       debiased      0.2932367
## 19          53       debiased      0.2977916
## 20          60       debiased      0.3942719
```

There seems to be a preference for a lower number of principal components (<27) for both `"plug-in"` and `"debiased"` with `"plug-in"` achieving slightly lower error rates.

3.3.3 Writing a custom preprocessing wrapper

If the options offered by `makePreprocWrapperCaret()` are not enough, you can write your own preprocessing wrapper using function `makePreprocWrapper()`.

As described in the tutorial section about wrapped learners wrappers are implemented using a *train* and a *predict* method. In case of preprocessing wrappers these methods specify how to transform the data before training and before prediction and are *completely user-defined*.

Below we show how to create a preprocessing wrapper that centers and scales the data before training/predicting. Some learning methods as, e.g., k nearest neighbors, support vector machines or neural networks usually require scaled features. Many, but not all, have a built-in scaling option where the training data set is scaled before model fitting and the test data set is scaled accordingly, that is by using the scaling parameters from the training stage, before making predictions. In the following we show how to add a scaling option to a Learner (`makeLearner()`) by coupling it with function `base::scale()`.

Note that we chose this simple example for demonstration. Centering/scaling the data is also possible with `makePreprocWrapperCaret()`.

3.3.3.1 Specifying the train function

The *train* function has to be a function with the following arguments:

- `data` is a `data.frame` with columns for all features and the target variable.
- `target` is a string and denotes the name of the target variable in `data`.
- `args` is a `list` of further arguments and parameters that influence the preprocessing.

It must return a `list` with elements `$data` and `$control`, where `$data` is the preprocessed data set and `$control` stores all information required to preprocess the data before prediction.

The *train* function for the scaling example is given below. It calls `base::scale()` on the numerical features and returns the scaled training data and the corresponding scaling parameters.

`args` contains the `center` and `scale` arguments of function `base::scale()` and slot `$control` stores the scaling parameters to be used in the prediction stage.

Regarding the latter note that the `center` and `scale` arguments of `base::scale()` can be either a logical value or a numeric vector of length equal to the number of the numeric columns in `data`, respectively. If a logical value was passed to `args` we store the column means and standard deviations/root mean squares in the `$center` and `$scale` slots of the returned `$control` object.

```
trainfun = function(data, target, args = list(center, scale)) {
  ### Identify numerical features
  cns = colnames(data)
  nums = setdiff(cns[sapply(data, is.numeric)], target)
  ### Extract numerical features from the data set and call scale
  x = as.matrix(data[, nums, drop = FALSE])
  x = scale(x, center = args$center, scale = args$scale)
  ### Store the scaling parameters in control
  ### These are needed to preprocess the data before prediction
  control = args
  if (is.logical(control$center) && control$center)
    control$center = attr(x, "scaled:center")
  if (is.logical(control$scale) && control$scale)
    control$scale = attr(x, "scaled:scale")
  ### Recombine the data
  data = data[, setdiff(cns, nums), drop = FALSE]
  data = cbind(data, as.data.frame(x))
  return(list(data = data, control = control))
}
```

3.3.3.2 Specifying the predict function

The *predict* function has the following arguments:

- `data` is a `data.frame` containing *only* feature values (as for prediction the target values naturally are not known).
- `target` is a string indicating the name of the target variable.
- `args` are the `args` that were passed to the *train* function.
- `control` is the object returned by the *train* function.

It returns the preprocessed data.

In our scaling example the *predict* function scales the numerical features using the parameters from the training stage stored in `control`.

```
predictfun = function(data, target, args, control) {
  ### Identify numerical features
  cns = colnames(data)
  nums = cns[sapply(data, is.numeric)]
  ### Extract numerical features from the data set and call scale
  x = as.matrix(data[, nums, drop = FALSE])
  x = scale(x, center = control$center, scale = control$scale)
  ### Recombine the data
  data = data[, setdiff(cns, nums), drop = FALSE]
  data = cbind(data, as.data.frame(x))
  return(data)
}
```

3.3.3.3 Creating the preprocessing wrapper

Below we create a preprocessing wrapper with a regression neural network (`nnet::nnet()`) (which itself does not have a scaling option) as base learner.

The *train* and *predict* functions defined above are passed to `makePreprocWrapper()` via the `train` and `predict` arguments. `par.vals` is a `list` of parameter values that is relayed to the `args` argument of the

train function.

```
lrn = makeLearner("regr.nnet", trace = FALSE, decay = 1e-02)
lrn = makePreprocWrapper(lrn, train = trainfun, predict = predictfun,
  par.vals = list(center = TRUE, scale = TRUE))
lrn
## Learner regr.nnet.preproc from package nnet
## Type: regr
## Name: ; Short name:
## Class: PreprocWrapper
## Properties: numerics,factors,weights
## Predict-Type: response
## Hyperparameters: size=3,trace=FALSE,decay=0.01
```

Let's compare the cross-validated mean squared error (mse) on the Boston Housing data set (`mlbench::BostonHousing()`) with and without scaling.

```
rdesc = makeResampleDesc("CV", iters = 3)

r = resample(lrn, bh.task, resampling = rdesc, show.info = FALSE)
r
## Resample Result
## Task: BostonHousing-example
## Learner: regr.nnet.preproc
## Aggr perf: mse.test.mean=22.1631331
## Runtime: 0.192447
lrn = makeLearner("regr.nnet", trace = FALSE, decay = 1e-02)
r = resample(lrn, bh.task, resampling = rdesc, show.info = FALSE)
r
## Resample Result
## Task: BostonHousing-example
## Learner: regr.nnet
## Aggr perf: mse.test.mean=34.4322951
## Runtime: 0.118722
```

3.3.3.4 Joint tuning of preprocessing and learner parameters

Often it's not clear which preprocessing options work best with a certain learning algorithm. As already shown for the number of principal components in `makePreprocWrapperCaret()` we can tune them easily together with other hyperparameters of the learner.

In our scaling example we can try if `nnet::nnet()` works best with both centering and scaling the data or if it's better to omit one of the two operations or do no preprocessing at all. In order to tune `center` and `scale` we have to add appropriate `LearnerParam` (`ParamHelpers::LearnerParam()`)s to the parameter set (`ParamHelpers::ParamSet()`) of the wrapped learner.

As mentioned above `base::scale()` allows for numeric and logical `center` and `scale` arguments. As we want to use the latter option we declare `center` and `scale` as logical learner parameters.

```
lrn = makeLearner("regr.nnet", trace = FALSE)
lrn = makePreprocWrapper(lrn, train = trainfun, predict = predictfun,
  par.set = makeParamSet(
    makeLogicalLearnerParam("center"),
    makeLogicalLearnerParam("scale")
  ),
  par.vals = list(center = TRUE, scale = TRUE))
```

```
lrn
## Learner regr.nnet.preproc from package nnet
## Type: regr
## Name: ; Short name:
## Class: PreprocWrapper
## Properties: numerics,factors,weights
## Predict-Type: response
## Hyperparameters: size=3,trace=FALSE,center=TRUE,scale=TRUE
getParamSet(lrn)
##             Type len    Def      Constr Req Tunable Trafo
## center   logical   -      -           -   -    TRUE     -
## scale    logical   -      -           -   -    TRUE     -
## size     integer   -      3    0 to Inf   -    TRUE     -
## maxit    integer   -    100    1 to Inf   -    TRUE     -
## linout   logical   -  FALSE           -   Y    TRUE     -
## entropy  logical   -  FALSE           -   Y    TRUE     -
## softmax  logical   -  FALSE           -   Y    TRUE     -
## censored logical   -  FALSE           -   Y    TRUE     -
## skip     logical   -  FALSE           -   -    TRUE     -
## rang     numeric   -    0.7 -Inf to Inf   -    TRUE     -
## decay    numeric   -      0    0 to Inf   -    TRUE     -
## Hess     logical   -  FALSE           -   -    TRUE     -
## trace    logical   -   TRUE           -   -   FALSE     -
## MaxNWts  integer   -   1000    1 to Inf   -   FALSE     -
## abstol   numeric   - 0.0001 -Inf to Inf   -    TRUE     -
## reltol   numeric   -  1e-08 -Inf to Inf   -    TRUE     -
```

Now we do a simple grid search for the `decay` parameter of `nnet::nnet()` and the `center` and `scale` parameters.

```
rdesc = makeResampleDesc("Holdout")
ps = makeParamSet(
  makeDiscreteParam("decay", c(0, 0.05, 0.1)),
  makeLogicalParam("center"),
  makeLogicalParam("scale")
)
ctrl = makeTuneControlGrid()
res = tuneParams(lrn, bh.task, rdesc, par.set = ps, control = ctrl, show.info = FALSE)

res
## Tune result:
## Op. pars: decay=0.05; center=TRUE; scale=TRUE
## mse.test.mean=17.1516485
as.data.frame(res$opt.path)
##    decay center scale mse.test.mean dob eol error.message exec.time
## 1      0   TRUE  TRUE      32.27409   1  NA          <NA>     0.052
## 2   0.05   TRUE  TRUE      17.15165   2  NA          <NA>     0.058
## 3    0.1   TRUE  TRUE      23.25944   3  NA          <NA>     0.059
## 4      0  FALSE  TRUE      32.15794   4  NA          <NA>     0.055
## 5   0.05  FALSE  TRUE      20.67869   5  NA          <NA>     0.049
## 6    0.1  FALSE  TRUE      22.66738   6  NA          <NA>     0.051
## 7      0   TRUE FALSE      63.02205   7  NA          <NA>     0.042
## 8   0.05   TRUE FALSE      47.76516   8  NA          <NA>     0.062
## 9    0.1   TRUE FALSE      44.63313   9  NA          <NA>     0.050
```

```
## 10     0  FALSE FALSE      75.73861  10  NA          <NA>     0.027
## 11  0.05  FALSE FALSE      26.78360  11  NA          <NA>     0.048
## 12   0.1  FALSE FALSE      34.86995  12  NA          <NA>     0.054
```

3.3.3.5 Preprocessing wrapper functions

If you have written a preprocessing wrapper that you might want to use from time to time it's a good idea to encapsulate it in an own function as shown below. If you think your preprocessing method is something others might want to use as well and should be integrated into `mlr` just contact us.

```
makePreprocWrapperScale = function(learner, center = TRUE, scale = TRUE) {
  trainfun = function(data, target, args = list(center, scale)) {
    cns = colnames(data)
    nums = setdiff(cns[sapply(data, is.numeric)], target)
    x = as.matrix(data[, nums, drop = FALSE])
    x = scale(x, center = args$center, scale = args$scale)
    control = args
    if (is.logical(control$center) && control$center)
      control$center = attr(x, "scaled:center")
    if (is.logical(control$scale) && control$scale)
      control$scale = attr(x, "scaled:scale")
    data = data[, setdiff(cns, nums), drop = FALSE]
    data = cbind(data, as.data.frame(x))
    return(list(data = data, control = control))
  }
  predictfun = function(data, target, args, control) {
    cns = colnames(data)
    nums = cns[sapply(data, is.numeric)]
    x = as.matrix(data[, nums, drop = FALSE])
    x = scale(x, center = control$center, scale = control$scale)
    data = data[, setdiff(cns, nums), drop = FALSE]
    data = cbind(data, as.data.frame(x))
    return(data)
  }
  makePreprocWrapper(
    learner,
    train = trainfun,
    predict = predictfun,
    par.set = makeParamSet(
      makeLogicalLearnerParam("center"),
      makeLogicalLearnerParam("scale")
    ),
    par.vals = list(center = center, scale = scale)
  )
}

lrn = makePreprocWrapperScale("classif.lda")
train(lrn, iris.task)
## Model for learner.id=classif.lda.preproc; learner.class=PreprocWrapper
## Trained on: task.id = iris-example; obs = 150; features = 4
## Hyperparameters: center=TRUE,scale=TRUE
```

3.4 Imputation of Missing Values

`mlr` provides several imputation methods which are listed on the help page `imputations()`. These include standard techniques as imputation by a constant value (like a fixed constant, the mean, median or mode) and random numbers (either from the empirical distribution of the feature under consideration or a certain distribution family). Moreover, missing values in one feature can be replaced based on the other features by predictions from any supervised Learner (`makeLearner()`) integrated into `mlr`.

If your favourite option is not implemented in `mlr` yet, you can easily create your own imputation method.

Also note that some of the learning algorithms included in `mlr` can deal with missing values in a sensible way, i.e., other than simply deleting observations with missing values. Those Learner (`makeLearner()`)s have the property `"missings"` and thus can be identified using `listLearners()`.

```
### Regression learners that can deal with missing values
listLearners("regr", properties = "missings")[c("class", "package")]
## Warning in listLearners.character("regr", properties = "missings"): The following learners could not
## classif.mxff,regr.mxff
## Check ?learners to see which packages you need or install mlr with all suggestions.
##              class      package
## 1 regr.bartMachine  bartMachine
## 2  regr.blackboost mboost,party
## 3     regr.cforest        party
## 4       regr.ctree        party
## 5      regr.cubist       Cubist
## 6 regr.featureless          mlr
## ... (#rows: 14, #cols: 2)
```

See also the list of integrated learners in the Appendix.

3.4.1 Imputation and reimputation

Imputation can be done by function `impute()`. You can specify an imputation method for each feature individually or for classes of features like numerics or factors. Moreover, you can generate dummy variables that indicate which values are missing, also either for classes of features or for individual features. These allow to identify the patterns and reasons for missing data and permit to treat imputed and observed values differently in a subsequent analysis.

Let's have a look at the airquality (`datasets::airquality()`) data set.

```
data(airquality)
summary(airquality)
##      Ozone           Solar.R           Wind             Temp
##  Min.   :  1.00   Min.   :  7.0   Min.   : 1.700   Min.   :56.00
##  1st Qu.: 18.00   1st Qu.:115.8   1st Qu.: 7.400   1st Qu.:72.00
##  Median : 31.50   Median :205.0   Median : 9.700   Median :79.00
##  Mean   : 42.13   Mean   :185.9   Mean   : 9.958   Mean   :77.88
##  3rd Qu.: 63.25   3rd Qu.:258.8   3rd Qu.:11.500   3rd Qu.:85.00
##  Max.   :168.00   Max.   :334.0   Max.   :20.700   Max.   :97.00
##  NA's   :37       NA's   :7
##      Month            Day
##  Min.   :5.000   Min.   : 1.0
##  1st Qu.:6.000   1st Qu.: 8.0
##  Median :7.000   Median :16.0
##  Mean   :6.993   Mean   :15.8
##  3rd Qu.:8.000   3rd Qu.:23.0
```

```
##  Max.   :9.000   Max.   :31.0
##
```

There are 37 `NA's` in variable `Ozone` (ozone pollution) and 7 `NA's` in variable `Solar.R` (solar radiation). For demonstration purposes we insert artificial `NA's` in column `Wind` (wind speed) and coerce it into a `factor`.

```
airq = airquality
ind = sample(nrow(airq), 10)
airq$Wind[ind] = NA
airq$Wind = cut(airq$Wind, c(0,8,16,24))
summary(airq)
##      Ozone           Solar.R           Wind         Temp
##  Min.   :  1.00   Min.   :  7.0   (0,8]  :49   Min.   :56.00
##  1st Qu.: 18.00   1st Qu.:115.8   (8,16] :88   1st Qu.:72.00
##  Median : 31.50   Median :205.0   (16,24]: 6   Median :79.00
##  Mean   : 42.13   Mean   :185.9   NA's   :10   Mean   :77.88
##  3rd Qu.: 63.25   3rd Qu.:258.8                3rd Qu.:85.00
##  Max.   :168.00   Max.   :334.0                Max.   :97.00
##  NA's   :37       NA's   :7
##      Month            Day
##  Min.   :5.000   Min.   : 1.0
##  1st Qu.:6.000   1st Qu.: 8.0
##  Median :7.000   Median :16.0
##  Mean   :6.993   Mean   :15.8
##  3rd Qu.:8.000   3rd Qu.:23.0
##  Max.   :9.000   Max.   :31.0
##
```

If you want to impute `NA's` in all integer features (these include `Ozone` and `Solar.R`) by the mean, in all factor features (`Wind`) by the mode and additionally generate dummy variables for all integer features, you can do this as follows:

```
imp = impute(airq, classes = list(integer = imputeMean(), factor = imputeMode()),
  dummy.classes = "integer")
```

`impute()` returns a `list` where slot `$data` contains the imputed data set. Per default, the dummy variables are factors with levels `"TRUE"` and `"FALSE"`. It is also possible to create numeric zero-one indicator variables.

```
head(imp$data, 10)
##       Ozone  Solar.R   Wind Temp Month Day Ozone.dummy Solar.R.dummy
## 1  41.00000 190.0000  (0,8]   67     5   1       FALSE         FALSE
## 2  36.00000 118.0000  (0,8]   72     5   2       FALSE         FALSE
## 3  12.00000 149.0000 (8,16]   74     5   3       FALSE         FALSE
## 4  18.00000 313.0000 (8,16]   62     5   4       FALSE         FALSE
## 5  42.12931 185.9315 (8,16]   56     5   5        TRUE          TRUE
## 6  28.00000 185.9315 (8,16]   66     5   6       FALSE          TRUE
## 7  23.00000 299.0000 (8,16]   65     5   7       FALSE         FALSE
## 8  19.00000  99.0000 (8,16]   59     5   8       FALSE         FALSE
## 9   8.00000  19.0000 (8,16]   61     5   9       FALSE         FALSE
## 10 42.12931 194.0000 (8,16]   69     5  10        TRUE         FALSE
```

Slot `$desc` is an `ImputationDesc` (`impute()`) object that stores all relevant information about the imputation. For the current example this includes the means and the mode computed on the non-missing data.

```
imp$desc
## Imputation description
## Target:
```

```
## Features: 6; Imputed: 6
## impute.new.levels: TRUE
## recode.factor.levels: TRUE
## dummy.type: factor
```

The imputation description shows the name of the target variable (not present), the number of features and the number of imputed features. Note that the latter number refers to the features for which an imputation method was specified (five integers plus one factor) and not to the features actually containing `NA's`. `dummy.type` indicates that the dummy variables are factors. For details on `impute.new.levels` and `recode.factor.levels` see the help page of function `impute()`.

Let's have a look at another example involving a target variable. A possible learning task associated with the airquality (`datasets::airquality()`) data is to predict the ozone pollution based on the meteorological features. Since we do not want to use columns `Day` and `Month` we remove them.

```
airq = subset(airq, select = 1:4)
```

The first 100 observations are used as training data set.

```
airq.train = airq[1:100,]
airq.test = airq[-c(1:100),]
```

In case of a supervised learning problem you need to pass the name of the target variable to `impute()`. This prevents imputation and creation of a dummy variable for the target variable itself and makes sure that the target variable is not used to impute the features.

In contrast to the example above we specify imputation methods for individual features instead of classes of features.

Missing values in `Solar.R` are imputed by random numbers drawn from the empirical distribution of the non-missing observations.

Function `imputeLearner` (`imputations()`) allows to use all supervised learning algorithms integrated into `mlr` for imputation. The type of the Learner (`makeLearner()`) (`regr`, `classif`) must correspond to the class of the feature to be imputed. The missing values in `Wind` are replaced by the predictions of a classification tree (`rpart::rpart()`). Per default, all available columns in `airq.train` except the target variable (`Ozone`) and the variable to be imputed (`Wind`) are used as features in the classification tree, here `Solar.R` and `Temp`. You can also select manually which columns to use. Note that `rpart::rpart()` can deal with missing feature values, therefore the `NA's` in column `Solar.R` do not pose a problem.

```
imp = impute(airq.train, target = "Ozone", cols = list(Solar.R = imputeHist(),
  Wind = imputeLearner("classif.rpart")), dummy.cols = c("Solar.R", "Wind"))
summary(imp$data)
##      Ozone           Solar.R          Wind         Temp
##  Min.   :  1.00   Min.   :  7.0   (0,8]  :34   Min.   :56.00
##  1st Qu.: 16.00   1st Qu.:113.8   (8,16] :61   1st Qu.:69.00
##  Median : 34.00   Median :223.0   (16,24]: 5   Median :79.50
##  Mean   : 41.59   Mean   :194.5                Mean   :76.87
##  3rd Qu.: 63.00   3rd Qu.:275.0                3rd Qu.:84.00
##  Max.   :135.00   Max.   :334.0                Max.   :93.00
##  NA's   :31
##  Solar.R.dummy Wind.dummy
##  FALSE:93      FALSE:94
##  TRUE : 7      TRUE : 6
##
##
##
##
```

```
##
imp$desc
## Imputation description
## Target: Ozone
## Features: 3; Imputed: 2
## impute.new.levels: TRUE
## recode.factor.levels: TRUE
## dummy.type: factor
```

The `ImputationDesc` (`impute()`) object can be used by function `reimpute()` to impute the test data set the same way as the training data.

```
airq.test.imp = reimpute(airq.test, imp$desc)
head(airq.test.imp)
##   Ozone Solar.R   Wind Temp Solar.R.dummy Wind.dummy
## 1   110     207  (0,8]   90         FALSE      FALSE
## 2    NA     222 (8,16]   92         FALSE      FALSE
## 3    NA     137 (8,16]   86         FALSE      FALSE
## 4    44     192 (8,16]   86         FALSE      FALSE
## 5    28     273 (8,16]   82         FALSE      FALSE
## 6    65     157 (8,16]   80         FALSE      FALSE
```

Especially when evaluating a machine learning method by some resampling technique you might want that `impute()`/`reimpute()` are called automatically each time before training/prediction. This can be achieved by creating an imputation wrapper.

3.4.2 Fusing a learner with imputation

You can couple a Learner (`makeLearner()`) with imputation by function `makeImputeWrapper()` which basically has the same formal arguments as `impute()`. Like in the example above we impute `Solar.R` by random numbers from its empirical distribution, `Wind` by the predictions of a classification tree and generate dummy variables for both features.

```
lrn = makeImputeWrapper("regr.lm", cols = list(Solar.R = imputeHist(),
  Wind = imputeLearner("classif.rpart")), dummy.cols = c("Solar.R", "Wind"))
lrn
## Learner regr.lm.imputed from package stats
## Type: regr
## Name: ; Short name:
## Class: ImputeWrapper
## Properties: numerics,factors,se,weights,missings
## Predict-Type: response
## Hyperparameters:
```

Before training the resulting Learner (`makeLearner()`), `impute()` is applied to the training set. Before prediction `reimpute()` is called on the test set and the `ImputationDesc` (`impute()`) object from the training stage.

We again aim to predict the ozone pollution from the meteorological variables. In order to create the `Task()` we need to delete observations with missing values in the target variable.

```
airq = subset(airq, subset = !is.na(airq$Ozone))
task = makeRegrTask(data = airq, target = "Ozone")
```

In the following the 3-fold cross-validated mean squared error is calculated.

```
rdesc = makeResampleDesc("CV", iters = 3)
r = resample(lrn, task, resampling = rdesc, show.info = FALSE, models = TRUE)
r$aggr
## mse.test.mean
##      508.5436
lapply(r$models, getLearnerModel, more.unwrap = TRUE)
## [[1]]
##
## Call:
## stats::lm(formula = f, data = d)
##
## Coefficients:
##       (Intercept)            Solar.R         Wind(8,16]
##         -91.37242            0.06636           -16.94854
##       Wind(16,24]               Temp  Solar.R.dummyTRUE
##         -22.46501            1.67896            -5.33519
##    Wind.dummyTRUE
##          -5.16636
##
##
## [[2]]
##
## Call:
## stats::lm(formula = f, data = d)
##
## Coefficients:
##       (Intercept)            Solar.R         Wind(8,16]
##          -70.5833             0.0528           -29.2506
##       Wind(16,24]               Temp  Solar.R.dummyTRUE
##          -28.8062             1.5732             1.4098
##    Wind.dummyTRUE
##            4.4286
##
##
## [[3]]
##
## Call:
## stats::lm(formula = f, data = d)
##
## Coefficients:
##       (Intercept)            Solar.R         Wind(8,16]
##         -92.79663            0.07018           -23.20071
##       Wind(16,24]               Temp  Solar.R.dummyTRUE
##         -10.24567            1.76729           -19.96295
##    Wind.dummyTRUE
##          -0.80538
```

A second possibility to fuse a learner with imputation is provided by `makePreprocWrapperCaret()`, which is an interface to carets `caret::preProcess()` function. `caret::preProcess()` only works for numeric features and offers imputation by k-nearest neighbors, bagged trees, and by the median.

3.5 Generic Bagging

One reason why random forests perform so well is that they are using bagging as a technique to gain more stability. But why do you want to limit yourself to the classifiers already implemented in well known random forests when it is really easy to build your own with `mlr`?

Just bag an `mlr` learner already `makeBaggingWrapper()`.

As in a random forest, we need a Learner which is trained on a subset of the data during each iteration of the bagging process. The subsets are chosen according to the parameters given to `makeBaggingWrapper()`:

- `bw.iters` On how many subsets (samples) do we want to train our Learner?
- `bw.replace` Sample with replacement (also known as *bootstrapping*)?
- `bw.size` Percentage size of the samples. If `bw.replace = TRUE`, `bw.size = 1` is the default. This does not mean that one sample will contain all the observations as observations will occur multiple times in each sample.
- `bw.feats` Percentage size of randomly selected features for each iteration.

Of course we also need a Learner which we have to pass to `makeBaggingWrapper()`.

```
lrn = makeLearner("classif.rpart")
bag.lrn = makeBaggingWrapper(lrn, bw.iters = 50, bw.replace = TRUE,
  bw.size = 0.8, bw.feats = 3/4)
```

Now we can compare the performance with and without bagging. First let's try it without bagging:

```
rdesc = makeResampleDesc("CV", iters = 10)
r = resample(learner = lrn, task = sonar.task, resampling = rdesc, show.info = FALSE)
r$aggr
## mmce.test.mean
##      0.3038095
```

And now with bagging:

```
rdesc = makeResampleDesc("CV", iters = 10)
result = resample(learner = bag.lrn, task = sonar.task, resampling = rdesc, show.info = FALSE)
result$aggr
## mmce.test.mean
##      0.1961905
```

Training more learners takes more time, but can outperform pure learners on noisy data with many features.

3.5.1 Changing the type of prediction

In case of a *classification* problem the predicted class labels are determined by majority voting over the predictions of the individual models. Additionally, posterior probabilities can be estimated as the relative proportions of the predicted class labels. For this purpose you have to change the predict type of the *bagging learner* as follows.

```
bag.lrn = setPredictType(bag.lrn, predict.type = "prob")
```

Note that it is not relevant if the *base learner* itself can predict probabilities and that for this reason the predict type of the *base learner* always has to be `"response"`.

For *regression* the mean value across predictions is computed. Moreover, the standard deviation across predictions is estimated if the predict type of the bagging learner is changed to `"se"`. Below, we give a small example for regression.

```
n = getTaskSize(bh.task)
train.inds = seq(1, n, 3)
test.inds  = setdiff(1:n, train.inds)
lrn = makeLearner("regr.rpart")
bag.lrn = makeBaggingWrapper(lrn)
bag.lrn = setPredictType(bag.lrn, predict.type = "se")
mod = train(learner = bag.lrn, task = bh.task, subset = train.inds)
```

With function `getLearnerModel()`, you can access the models fitted in the individual iterations.

```
head(getLearnerModel(mod), 2)
## [[1]]
## Model for learner.id=regr.rpart; learner.class=regr.rpart
## Trained on: task.id = BostonHousing-example; obs = 169; features = 13
## Hyperparameters: xval=0
##
## [[2]]
## Model for learner.id=regr.rpart; learner.class=regr.rpart
## Trained on: task.id = BostonHousing-example; obs = 169; features = 13
## Hyperparameters: xval=0
```

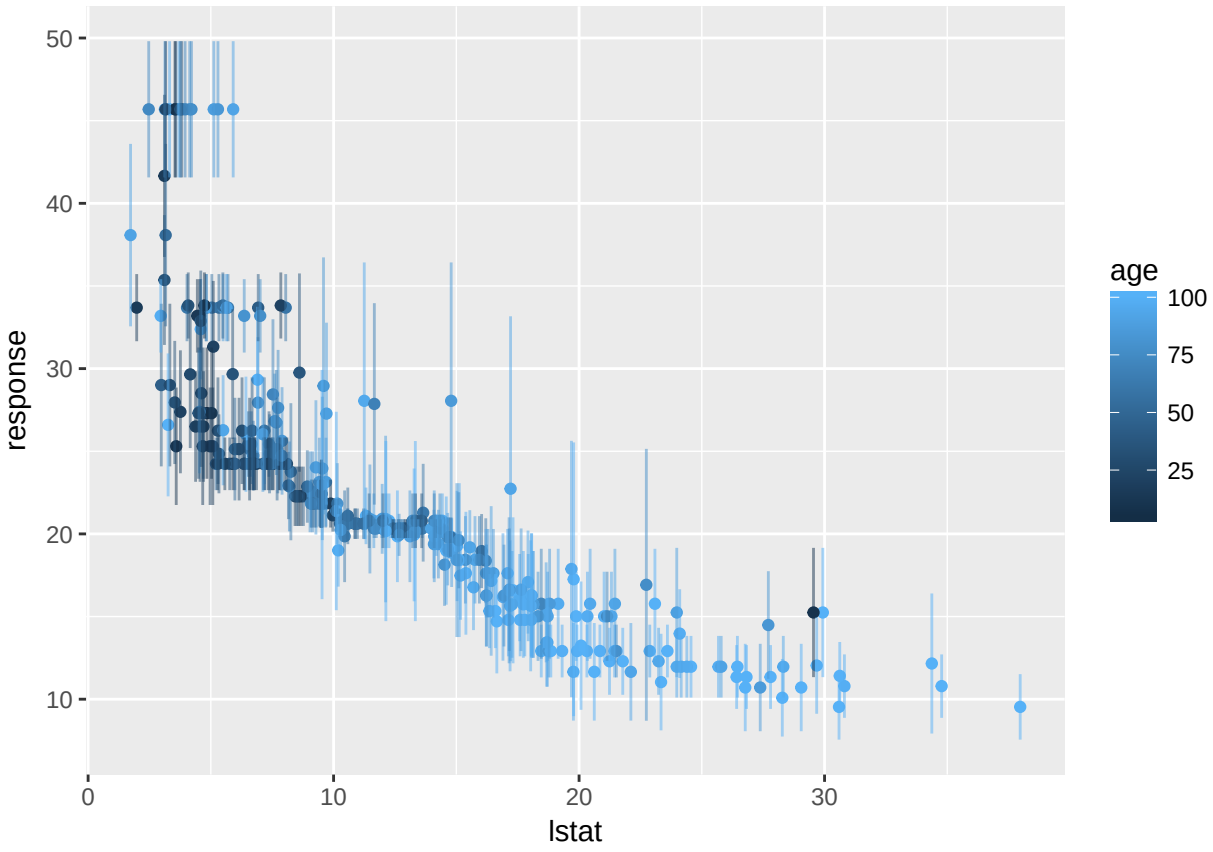
Predict the response and calculate the standard deviation:

```
pred = predict(mod, task = bh.task, subset = test.inds)
head(as.data.frame(pred))
##   id truth response       se
## 2  2  21.6 22.54522 2.445421
## 3  3  34.7 33.68849 2.031165
## 5  5  36.2 33.68849 2.031165
## 6  6  28.7 24.24084 1.592487
## 8  8  27.1 15.77341 3.327144
## 9  9  16.5 15.24625 3.910597
```

In the column labelled `se` the standard deviation for each prediction is given.

Let's visualise this a bit using `ggplot2::ggplot2()`. Here we plot the percentage of lower status of the population (`lstat`) against the prediction.

```
library("ggplot2")
library("reshape2")
data = cbind(as.data.frame(pred), getTaskData(bh.task, subset = test.inds))
g = ggplot(data, aes(x = lstat, y = response, ymin = response-se, ymax = response+se, col = age))
g + geom_point() + geom_linerange(alpha=0.5)
```



3.6 Iterated F-Racing for mixed spaces and dependencies

The package supports a larger number of tuning algorithms, which can all be looked up and selected via `TuneControl()`. One of the cooler algorithms is iterated F-racing from the `irace::irace()` package (technical description here). This not only works for arbitrary parameter types (numeric, integer, discrete, logical), but also for so-called dependent / hierarchical parameters:

```
ps = makeParamSet(
  makeNumericParam("C", lower = -12, upper = 12, trafo = function(x) 2^x),
  makeDiscreteParam("kernel", values = c("vanilladot", "polydot", "rbfdot")),
  makeNumericParam("sigma", lower = -12, upper = 12, trafo = function(x) 2^x,
    requires = quote(kernel == "rbfdot")),
  makeIntegerParam("degree", lower = 2L, upper = 5L,
    requires = quote(kernel == "polydot"))
)
ctrl = makeTuneControlIrace(maxExperiments = 200L)
rdesc = makeResampleDesc("Holdout")
res = tuneParams("classif.ksvm", iris.task, rdesc, par.set = ps, control = ctrl, show.info = FALSE)
print(head(as.data.frame(res$opt.path)))
##           C     kernel     sigma degree mmce.test.mean dob eol
## 1  3.935326 vanilladot        NA     NA           0.04   1  NA
## 2  2.097016     rbfdot 10.771499     NA           0.72   1  NA
## 3 -0.530357    polydot        NA      3           0.06   1  NA
## 4 -5.888312    polydot        NA      3           0.04   1  NA
## 5  2.528851    polydot        NA      3           0.04   1  NA
## 6 -3.190582     rbfdot -5.404658     NA           0.36   1  NA
```

```
##   error.message exec.time
## 1          <NA>     0.056
## 2          <NA>     0.026
## 3          <NA>     0.094
## 4          <NA>     0.045
## 5          <NA>     0.035
## 6          <NA>     0.058
```

See how we made the kernel parameters like `sigma` and `degree` dependent on the `kernel` selection parameters? This approach allows you to tune parameters of multiple kernels at once, efficiently concentrating on the ones which work best for your given data set.

3.6.1 Tuning across whole model spaces with ModelMultiplexer

We can now take the following example even one step further. If we use the `makeModelMultiplexer()` we can tune over different model classes at once, just as we did with the SVM kernels above.

```
base.learners = list(
  makeLearner("classif.ksvm"),
  makeLearner("classif.randomForest")
)
lrn = makeModelMultiplexer(base.learners)
```

Function `makeModelMultiplexerParamSet()` offers a simple way to construct a parameter set for tuning: The parameter names are prefixed automatically and the `requires` element is set, too, to make all parameters subordinate to `selected.learner`.

```
ps = makeModelMultiplexerParamSet(lrn,
  makeNumericParam("sigma", lower = -12, upper = 12, trafo = function(x) 2^x),
  makeIntegerParam("ntree", lower = 1L, upper = 500L)
)
print(ps)
##                               Type len Def
## selected.learner           discrete   -   -
## classif.ksvm.sigma          numeric   -   -
## classif.randomForest.ntree  integer   -   -
##                                                      Constr Req Tunable
## selected.learner           classif.ksvm,classif.randomForest   -    TRUE
## classif.ksvm.sigma                                -12 to 12   Y    TRUE
## classif.randomForest.ntree                         1 to 500   Y    TRUE
##                            Trafo
## selected.learner               -
## classif.ksvm.sigma             Y
## classif.randomForest.ntree     -
rdesc = makeResampleDesc("CV", iters = 2L)
ctrl = makeTuneControlIrace(maxExperiments = 200L)
res = tuneParams(lrn, iris.task, rdesc, par.set = ps, control = ctrl, show.info = FALSE)
print(head(as.data.frame(res$opt.path)))
##       selected.learner classif.ksvm.sigma classif.randomForest.ntree
## 1         classif.ksvm          -6.786569                          NA
## 2 classif.randomForest                 NA                          99
## 3         classif.ksvm           1.716710                          NA
## 4         classif.ksvm          -5.521533                          NA
## 5 classif.randomForest                 NA                         494
```

```
## 6 classif.randomForest                 NA                          485
##   mmce.test.mean dob eol error.message exec.time
## 1     0.21333333   1  NA          <NA>     0.052
## 2     0.05333333   1  NA          <NA>     0.047
## 3     0.08666667   1  NA          <NA>     0.051
## 4     0.08000000   1  NA          <NA>     0.052
## 5     0.06000000   1  NA          <NA>     0.070
## 6     0.05333333   1  NA          <NA>     0.071
```

3.6.2 Multi-criteria evaluation and optimization

During tuning you might want to optimize multiple, potentially conflicting, performance measures simultaneously.

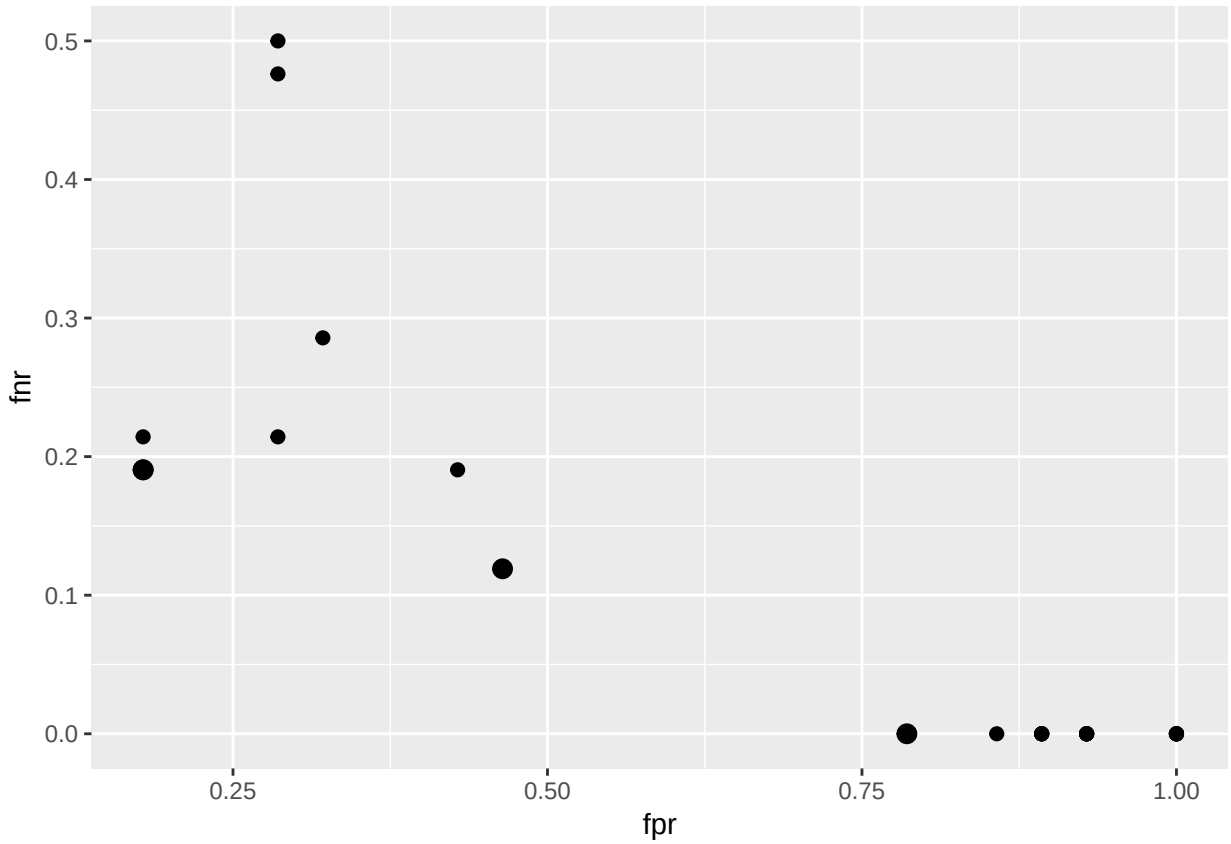
In the following example we aim to minimize both, the false positive and the false negative rates (`fpr` and `fnr`). We again tune the hyperparameters of an SVM (function `kernlab::ksvm()`) with a radial basis kernel and use `sonar.task()` for illustration. As search strategy we choose a random search.

For all available multi-criteria tuning algorithms see `TuneMultiCritControl()`.

```
ps = makeParamSet(
  makeNumericParam("C", lower = -12, upper = 12, trafo = function(x) 2^x),
  makeNumericParam("sigma", lower = -12, upper = 12, trafo = function(x) 2^x)
)
ctrl = makeTuneMultiCritControlRandom(maxit = 30L)
rdesc = makeResampleDesc("Holdout")
res = tuneParamsMultiCrit("classif.ksvm", task = sonar.task, resampling = rdesc, par.set = ps,
  measures = list(fpr, fnr), control = ctrl, show.info = FALSE)
res
## Tune multicrit result:
## Points on front: 4
head(as.data.frame(trafoOptPath(res$opt.path)))
##              C        sigma fpr.test.mean fnr.test.mean dob eol
## 1  2.604865405 7.179615e+01     0.8928571     0.0000000   1  NA
## 2 23.585674226 1.166616e-03     0.2857143     0.2142857   2  NA
## 3 23.888713641 7.922796e+01     0.8928571     0.0000000   3  NA
## 4  0.003545805 5.142143e+02     1.0000000     0.0000000   4  NA
## 5  0.054254630 5.453198e-04     0.2857143     0.5000000   5  NA
## 6  0.015666530 1.865058e-01     0.8571429     0.0000000   6  NA
##   error.message exec.time
## 1          <NA>     0.062
## 2          <NA>     0.061
## 3          <NA>     0.060
## 4          <NA>     0.061
## 5          <NA>     0.058
## 6          <NA>     0.048
```

The results can be visualized with function `plotTuneMultiCritResult()`. The plot shows the false positive and false negative rates for all parameter settings evaluated during tuning. Points on the Pareto front are slightly increased.

```
plotTuneMultiCritResult(res)
```



3.7 Feature Selection

Often, data sets include a large number of features. The technique of extracting a subset of relevant features is called feature selection. Feature selection can enhance the interpretability of the model, speed up the learning process and improve the learner performance. There exist different approaches to identify the relevant features. `mlr` supports *filter* and *wrapper methods*.

3.7.1 Filter methods

Filter methods assign an importance value to each feature. Based on these values the features can be ranked and a feature subset can be selected.

3.7.1.1 Calculating the feature importance

Different methods for calculating the feature importance are built into `mlr`'s function `generateFilterValuesData()` (`getFilterValues()` has been deprecated in favor of `generateFilterValuesData()`.). Currently, classification, regression and survival analysis tasks are supported. A table showing all available methods can be found in article filter methods.

Function `generateFilterValuesData()` requires the `Task()` and a character string specifying the filter method.

```
fv = generateFilterValuesData(iris.task, method = "information.gain")
fv
## FilterValues:
## Task: iris-example
```

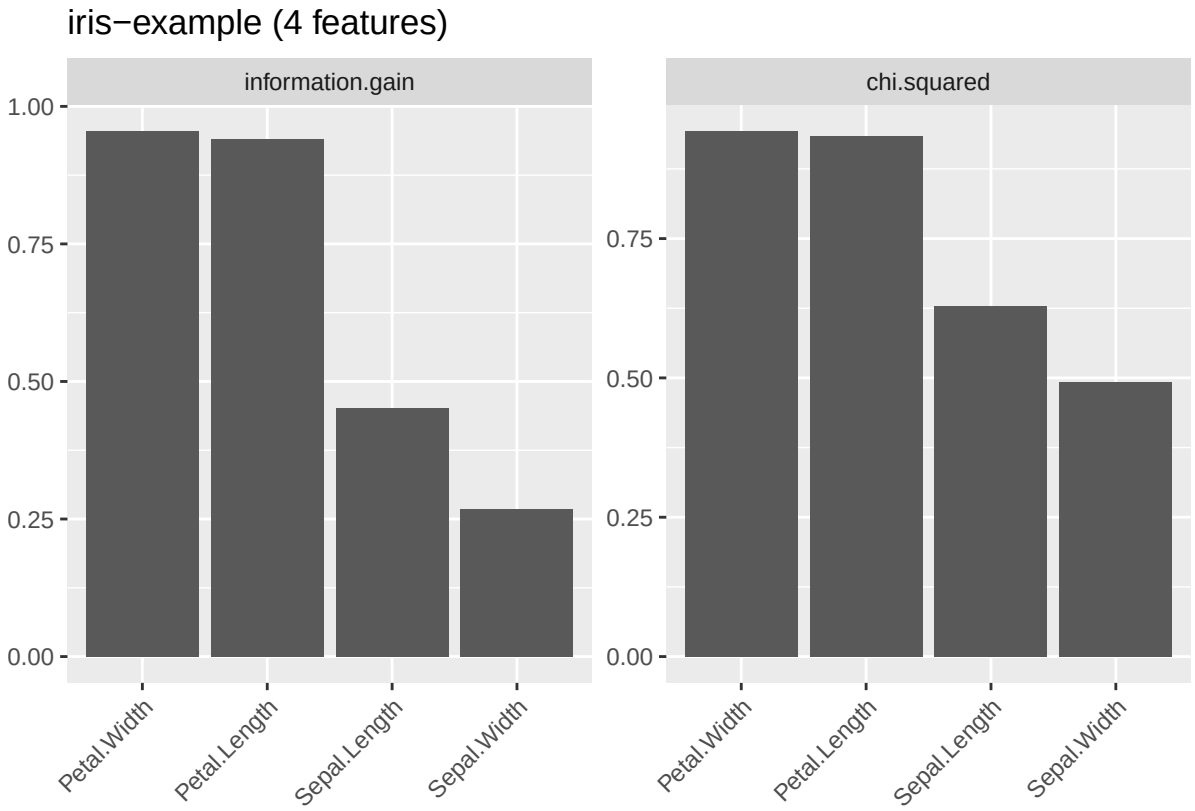
```
##           name    type information.gain
## 1 Sepal.Length numeric        0.4521286
## 2  Sepal.Width numeric        0.2672750
## 3 Petal.Length numeric        0.9402853
## 4  Petal.Width numeric        0.9554360
```

`fv` is a `FilterValues()` object and `fv$data` contains a `data.frame` that gives the importance values for all features. Optionally, a vector of filter methods can be passed.

```
fv2 = generateFilterValuesData(iris.task, method = c("information.gain", "chi.squared"))
fv2$data
##           name    type information.gain chi.squared
## 1 Sepal.Length numeric        0.4521286   0.6288067
## 2  Sepal.Width numeric        0.2672750   0.4922162
## 3 Petal.Length numeric        0.9402853   0.9346311
## 4  Petal.Width numeric        0.9554360   0.9432359
```

A bar plot of importance values for the individual features can be obtained using function `plotFilterValues()`.

```
plotFilterValues(fv2)
```



By default `plotFilterValues()` will create facetted subplots if multiple filter methods are passed as input to `generateFilterValuesData()`.

There is also an experimental `ggvis` plotting function, `plotFilterValuesGGVIS()`. This takes the same arguments as `plotFilterValues()` and produces a `shiny` application that allows the interactive selection of the displayed filter method, the number of features selected, and the sorting method (e.g., ascending or descending).

```
plotFilterValuesGGVIS(fv2)
```

According to the "information.gain" measure, Petal.Width and Petal.Length contain the most information about the target variable Species.

3.7.1.2 Selecting a feature subset

With mlr's function filterFeatures() you can create a new Task() by leaving out features of lower importance.

There are several ways to select a feature subset based on feature importance values:

- Keep a certain *absolute number* (abs) of features with highest importance.
- Keep a certain *percentage* (perc) of features with highest importance.
- Keep all features whose importance exceeds a certain *threshold value* (threshold).

Function filterFeatures() supports these three methods as shown in the following example. Moreover, you can either specify the method for calculating the feature importance or you can use previously computed importance values via argument fval.

```
### Keep the 2 most important features
filtered.task = filterFeatures(iris.task, method = "information.gain", abs = 2)

### Keep the 25% most important features
filtered.task = filterFeatures(iris.task, fval = fv, perc = 0.25)

### Keep all features with importance greater than 0.5
filtered.task = filterFeatures(iris.task, fval = fv, threshold = 0.5)
filtered.task
## Supervised task: iris-example
## Type: classif
## Target: Species
## Observations: 150
## Features:
##    numerics     factors     ordered functionals
##           2           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
## Classes: 3
##     setosa versicolor  virginica
##         50         50         50
## Positive class: NA
```

3.7.1.3 Fuse a learner with a filter method

Often feature selection based on a filter method is part of the data preprocessing and in a subsequent step a learning method is applied to the filtered data. In a proper experimental setup you might want to automate the selection of the features so that it can be part of the validation method of your choice. A Learner (makeLearner()) can be fused with a filter method by function makeFilterWrapper(). The resulting Learner (makeLearner()) has the additional class attribute FilterWrapper().

In the following example we calculate the 10-fold cross-validated error rate mmce of the k-nearest neighbor classifier (FNN::fnn()) with preceding feature selection on the iris (datasets::iris()) data set. We use "information.gain" as importance measure and select the 2 features with highest importance. In each resampling iteration feature selection is carried out on the corresponding training data set before fitting the learner.

```
lrn = makeFilterWrapper(learner = "classif.fnn", fw.method = "information.gain", fw.abs = 2)
rdesc = makeResampleDesc("CV", iters = 10)
r = resample(learner = lrn, task = iris.task, resampling = rdesc, show.info = FALSE, models = TRUE)
r$aggr
## mmce.test.mean
##     0.03333333
```

You may want to know which features have been used. Luckily, we have called `resample()` with the argument `models = TRUE`, which means that `r$models` contains a `list` of models (`makeWrappedModel()`) fitted in the individual resampling iterations. In order to access the selected feature subsets we can call `getFilteredFeatures()` on each model.

```
sfeats = sapply(r$models, getFilteredFeatures)
table(sfeats)
## sfeats
## Petal.Length  Petal.Width
##           10           10
```

The selection of features seems to be very stable. The features `Sepal.Length` and `Sepal.Width` did not make it into a single fold.

3.7.1.4 Tuning the size of the feature subset

In the above examples the number/percentage of features to select or the threshold value have been arbitrarily chosen. If filtering is a preprocessing step before applying a learning method optimal values with regard to the learner performance can be found by tuning.

In the following regression example we consider the `BostonHousing` (`mlbench::BostonHousing()`) data set. We use a linear regression model and determine the optimal percentage value for feature selection such that the 3-fold cross-validated mean squared error (`mse()`) of the learner is minimal. As search strategy for tuning a grid search is used.

```
lrn = makeFilterWrapper(learner = "regr.lm", fw.method = "chi.squared")
ps = makeParamSet(makeDiscreteParam("fw.perc", values = seq(0.2, 0.5, 0.05)))
rdesc = makeResampleDesc("CV", iters = 3)
res = tuneParams(lrn, task = bh.task, resampling = rdesc, par.set = ps,
  control = makeTuneControlGrid())
## [Tune] Started tuning learner regr.lm.filtered for parameter set:
##             Type len Def                          Constr Req Tunable Trafo
## fw.perc discrete   -   - 0.2,0.25,0.3,0.35,0.4,0.45,0.5   -    TRUE     -
## With control class: TuneControlGrid
## Imputation value: Inf
## [Tune-x] 1: fw.perc=0.2
## [Tune-y] 1: mse.test.mean=35.3053891; time: 0.0 min
## [Tune-x] 2: fw.perc=0.25
## [Tune-y] 2: mse.test.mean=35.3053891; time: 0.0 min
## [Tune-x] 3: fw.perc=0.3
## [Tune-y] 3: mse.test.mean=34.7691587; time: 0.0 min
## [Tune-x] 4: fw.perc=0.35
## [Tune-y] 4: mse.test.mean=32.1120799; time: 0.0 min
## [Tune-x] 5: fw.perc=0.4
## [Tune-y] 5: mse.test.mean=32.1120799; time: 0.0 min
## [Tune-x] 6: fw.perc=0.45
## [Tune-y] 6: mse.test.mean=30.9324145; time: 0.0 min
## [Tune-x] 7: fw.perc=0.5
## [Tune-y] 7: mse.test.mean=30.9324145; time: 0.0 min
```

```
## [Tune] Result: fw.perc=0.45 : mse.test.mean=30.9324145
res
## Tune result:
## Op. pars: fw.perc=0.45
## mse.test.mean=30.9324145
```

The performance of all percentage values visited during tuning is:

```
as.data.frame(res$opt.path)
##   fw.perc mse.test.mean dob eol error.message exec.time
## 1     0.2      35.30539   1  NA          <NA>     0.324
## 2    0.25      35.30539   2  NA          <NA>     0.328
## 3     0.3      34.76916   3  NA          <NA>     0.226
## 4    0.35      32.11208   4  NA          <NA>     0.308
## 5     0.4      32.11208   5  NA          <NA>     0.401
## 6    0.45      30.93241   6  NA          <NA>     0.247
## 7     0.5      30.93241   7  NA          <NA>     0.228
```

The optimal percentage and the corresponding performance can be accessed as follows:

```
res$x
## $fw.perc
## [1] 0.45
res$y
## mse.test.mean
##      30.93241
```

After tuning we can generate a new wrapped learner with the optimal percentage value for further use.

```
lrn = makeFilterWrapper(learner = "regr.lm", fw.method = "chi.squared", fw.perc = res$x$fw.perc)
mod = train(lrn, bh.task)
mod
## Model for learner.id=regr.lm.filtered; learner.class=FilterWrapper
## Trained on: task.id = BostonHousing-example; obs = 506; features = 13
## Hyperparameters: fw.method=chi.squared,fw.perc=0.45
getFilteredFeatures(mod)
## [1] "crim"  "zn"    "rm"    "dis"   "rad"   "lstat"
```

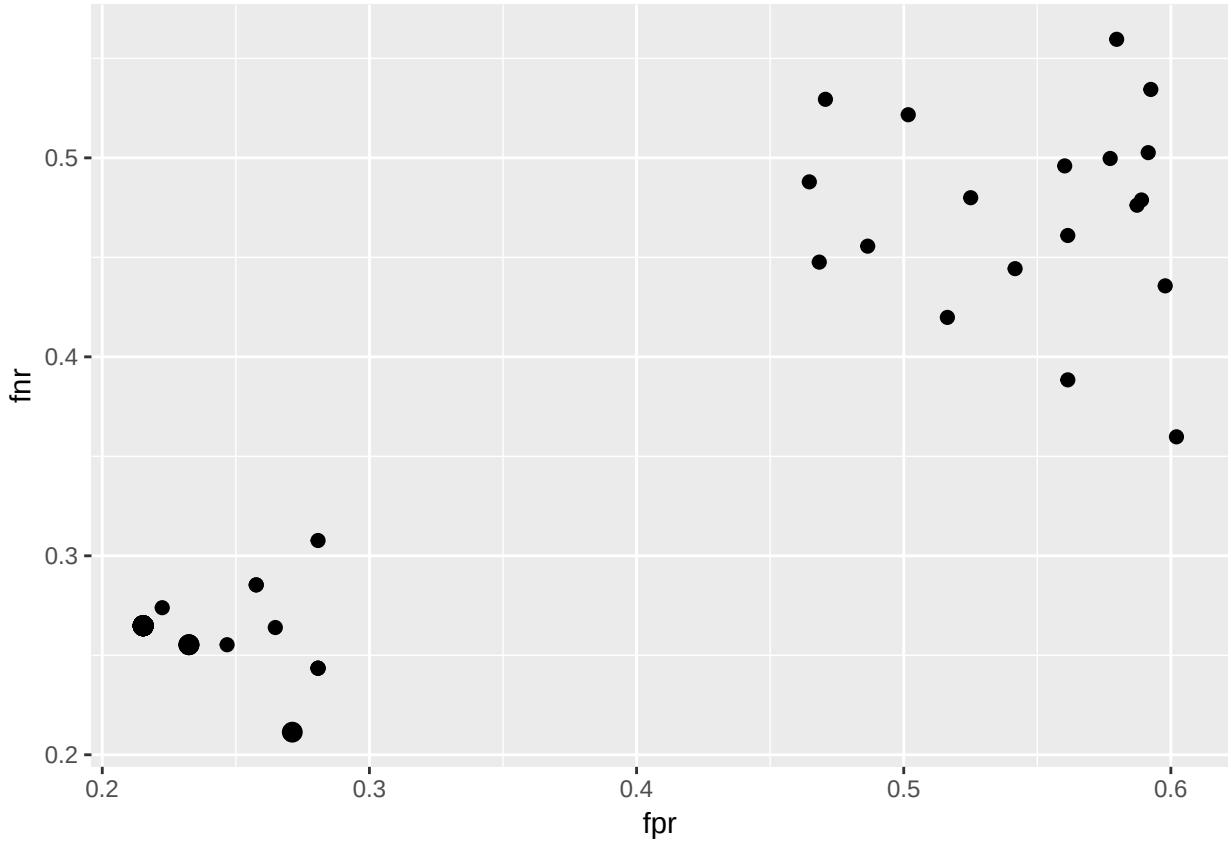
Here is another example using multi-criteria tuning. We consider linear discriminant analysis (`MASS::lda()`) with precedent feature selection based on the Chi-squared statistic of independence (`"chi.squared"`) on the `Sonar` (`mlbench::sonar()`) data set and tune the threshold value. During tuning both, the false positive and the false negative rate fpr and fnr), are minimized. As search strategy we choose a random search (see `makeTuneMultiCritControlRandom` (`?TuneMultiCritControl()`).

```
lrn = makeFilterWrapper(learner = "classif.lda", fw.method = "chi.squared")
ps = makeParamSet(makeNumericParam("fw.threshold", lower = 0.1, upper = 0.9))
rdesc = makeResampleDesc("CV", iters = 10)
res = tuneParamsMultiCrit(lrn, task = sonar.task, resampling = rdesc, par.set = ps,
  measures = list(fpr, fnr), control = makeTuneMultiCritControlRandom(maxit = 50L),
  show.info = FALSE)
res
## Tune multicrit result:
## Points on front: 22
head(as.data.frame(res$opt.path))
##   fw.threshold fpr.test.mean fnr.test.mean dob eol error.message exec.time
## 1    0.8763312     0.5602597     0.4959668   1  NA          <NA>     2.037
## 2    0.7748634     0.5915260     0.5026335   2  NA          <NA>     2.249
```

```
## 3    0.2485588     0.2152922     0.2648341   3  NA          <NA>     2.019
## 4    0.4636301     0.2647727     0.2639610   4  NA          <NA>     2.077
## 5    0.2700361     0.2224351     0.2739250   5  NA          <NA>     2.136
## 6    0.1788884     0.2152922     0.2648341   6  NA          <NA>     1.980
```

The results can be visualized with function `plotTuneMultiCritResult()`. The plot shows the false positive and false negative rates for all parameter values visited during tuning. The size of the points on the Pareto front is slightly increased.

```
plotTuneMultiCritResult(res)
```



3.7.2 Wrapper methods

Wrapper methods use the performance of a learning algorithm to assess the usefulness of a feature set. In order to select a feature subset a learner is trained repeatedly on different feature subsets and the subset which leads to the best learner performance is chosen.

In order to use the wrapper approach we have to decide:

- How to assess the performance: This involves choosing a performance measure that serves as feature selection criterion and a resampling strategy.
- Which learning method to use.
- How to search the space of possible feature subsets.

The search strategy is defined by functions following the naming convention `makeFeatSelControl<search_strategy>`. The following search strategies are available:

- Exhaustive search `makeFeatSelControlExhaustive` (`?FeatSelControl()`),
- Genetic algorithm `makeFeatSelControlGA` (`?FeatSelControl()`),

- Random search `makeFeatSelControlRandom` (`?FeatSelControl()`),
- Deterministic forward or backward search `makeFeatSelControlSequential` (`?FeatSelControl()`).

3.7.2.1 Select a feature subset

Feature selection can be conducted with function `selectFeatures()`.

In the following example we perform an exhaustive search on the `Wisconsin Prognostic Breast Cancer` (`TH.data::wpbc()`) data set. As learning method we use the `Cox proportional hazards model` (`survival::coxph()`). The performance is assessed by the holdout estimate of the concordance index cindex).

```
### Specify the search strategy
ctrl = makeFeatSelControlRandom(maxit = 20L)
ctrl
## FeatSel control: FeatSelControlRandom
## Same resampling instance: TRUE
## Imputation value: <worst>
## Max. features: <not used>
## Max. iterations: 20
## Tune threshold: FALSE
## Further arguments: prob=0.5
```

`ctrl` is a`FeatSelControl()` object that contains information about the search strategy and potential parameter values.

```
### Resample description
rdesc = makeResampleDesc("Holdout")

### Select features
sfeats = selectFeatures(learner = "surv.coxph", task = wpbc.task, resampling = rdesc,
  control = ctrl, show.info = FALSE)
sfeats
## FeatSel result:
## Features (20): mean_perimeter, mean_area, mean_compactness, mean_concavity, mean_symmetry, mean_frac
## cindex.test.mean=0.6396761
```

`sfeats`is a `FeatSelResult` (`selectFeatures()`) object. The selected features and the corresponding performance can be accessed as follows:

```
sfeats$x
##  [1] "mean_perimeter"    "mean_area"         "mean_compactness"
##  [4] "mean_concavity"    "mean_symmetry"     "mean_fractaldim"
##  [7] "SE_radius"         "SE_texture"        "SE_perimeter"
## [10] "SE_area"           "SE_concavepoints"  "SE_symmetry"
## [13] "SE_fractaldim"     "worst_texture"     "worst_perimeter"
## [16] "worst_area"        "worst_smoothness"  "worst_compactness"
## [19] "worst_concavity"   "worst_fractaldim"
sfeats$y
## cindex.test.mean
##        0.6396761
```

In a second example we fit a simple linear regression model to the `BostonHousing` (`mlbench::BostonHousing()`) data set and use a sequential search to find a feature set that minimizes the mean squared error mse). `method = "sfs"` indicates that we want to conduct a sequential forward search where features are added to the model until the performance cannot be improved anymore. See the documentation page

`makeFeatSelControlSequential` (`?FeatSelControl()`) for other available sequential search methods. The search is stopped if the improvement is smaller than `alpha = 0.02`.

```
### Specify the search strategy
ctrl = makeFeatSelControlSequential(method = "sfs", alpha = 0.02)

### Select features
rdesc = makeResampleDesc("CV", iters = 10)
sfeats = selectFeatures(learner = "regr.lm", task = bh.task, resampling = rdesc, control = ctrl,
  show.info = FALSE)
sfeats
## FeatSel result:
## Features (11): crim, zn, chas, nox, rm, dis, rad, tax, ptratio, b, lstat
## mse.test.mean=23.9648546
```

Further information about the sequential feature selection process can be obtained by function `analyzeFeatSelResult()`.

```
analyzeFeatSelResult(sfeats)
## Features         : 11
## Performance      : mse.test.mean=23.9648546
## crim, zn, chas, nox, rm, dis, rad, tax, ptratio, b, lstat
##
## Path to optimum:
## - Features:    0  Init   :                       Perf = 85.202  Diff: NA  *
## - Features:    1  Add    : lstat                 Perf = 38.959  Diff: 46.242  *
## - Features:    2  Add    : rm                    Perf = 31.509  Diff: 7.4505  *
## - Features:    3  Add    : ptratio               Perf = 28.134  Diff: 3.3751  *
## - Features:    4  Add    : dis                   Perf = 27.219  Diff: 0.91437  *
## - Features:    5  Add    : nox                   Perf = 25.891  Diff: 1.3289  *
## - Features:    6  Add    : b                     Perf = 25.421  Diff: 0.4696  *
## - Features:    7  Add    : zn                    Perf = 25.084  Diff: 0.3367  *
## - Features:    8  Add    : chas                  Perf = 24.815  Diff: 0.26966  *
## - Features:    9  Add    : rad                   Perf = 24.767  Diff: 0.047654  *
## - Features:   10  Add    : tax                   Perf = 24.297  Diff: 0.4698  *
## - Features:   11  Add    : crim                  Perf = 23.965  Diff: 0.3323  *
##
## Stopped, because no improving feature was found.
```

3.7.2.2 Fuse a learner with feature selection

A Learner (`makeLearner()`) can be fused with a feature selection strategy (i.e., a search strategy, a performance measure and a resampling strategy) by function `makeFeatSelWrapper()`. During training features are selected according to the specified selection scheme. Then, the learner is trained on the selected feature subset.

```
rdesc = makeResampleDesc("CV", iters = 3)
lrn = makeFeatSelWrapper("surv.coxph", resampling = rdesc,
  control = makeFeatSelControlRandom(maxit = 10), show.info = FALSE)
mod = train(lrn, task = wpbc.task)
mod
## Model for learner.id=surv.coxph.featsel; learner.class=FeatSelWrapper
## Trained on: task.id = wpbc-example; obs = 194; features = 32
## Hyperparameters:
```

The result of the feature selection can be extracted by function `getFeatSelResult()`.

```
sfeats = getFeatSelResult(mod)
sfeats
## FeatSel result:
## Features (16): mean_radius, mean_area, mean_compactness, mean_concavity, mean_concavepoints, mean_fra
## cindex.test.mean=0.6273841
```

The selected features are:

```
sfeats$x
##  [1] "mean_radius"        "mean_area"          "mean_compactness"
##  [4] "mean_concavity"     "mean_concavepoints" "mean_fractaldim"
##  [7] "SE_perimeter"       "SE_smoothness"      "SE_concavepoints"
## [10] "worst_radius"       "worst_perimeter"    "worst_smoothness"
## [13] "worst_symmetry"     "worst_fractaldim"   "tsize"
## [16] "pnodes"
```

The 5-fold cross-validated performance of the learner specified above can be computed as follows:

```
out.rdesc = makeResampleDesc("CV", iters = 5)

r = resample(learner = lrn, task = wpbc.task, resampling = out.rdesc, models = TRUE,
  show.info = FALSE)
r$aggr
## cindex.test.mean
##         0.599621
```

The selected feature sets in the individual resampling iterations can be extracted as follows:

```
lapply(r$models, getFeatSelResult)
## [[1]]
## FeatSel result:
## Features (14): mean_radius, mean_concavity, mean_concavepoints, mean_symmetry, mean_fractaldim, SE_ra
## cindex.test.mean=0.6787954
##
## [[2]]
## FeatSel result:
## Features (11): mean_radius, mean_texture, mean_perimeter, mean_symmetry, mean_fractaldim, SE_area, SE
## cindex.test.mean=0.7074560
##
## [[3]]
## FeatSel result:
## Features (15): mean_texture, mean_compactness, mean_concavity, mean_fractaldim, SE_radius, SE_smoothn
## cindex.test.mean=0.6660038
##
## [[4]]
## FeatSel result:
## Features (14): mean_texture, mean_perimeter, mean_compactness, mean_concavity, mean_fractaldim, SE_te
## cindex.test.mean=0.5975525
##
## [[5]]
## FeatSel result:
## Features (13): mean_area, mean_smoothness, mean_compactness, mean_concavity, mean_fractaldim, SE_text
## cindex.test.mean=0.6386685
```

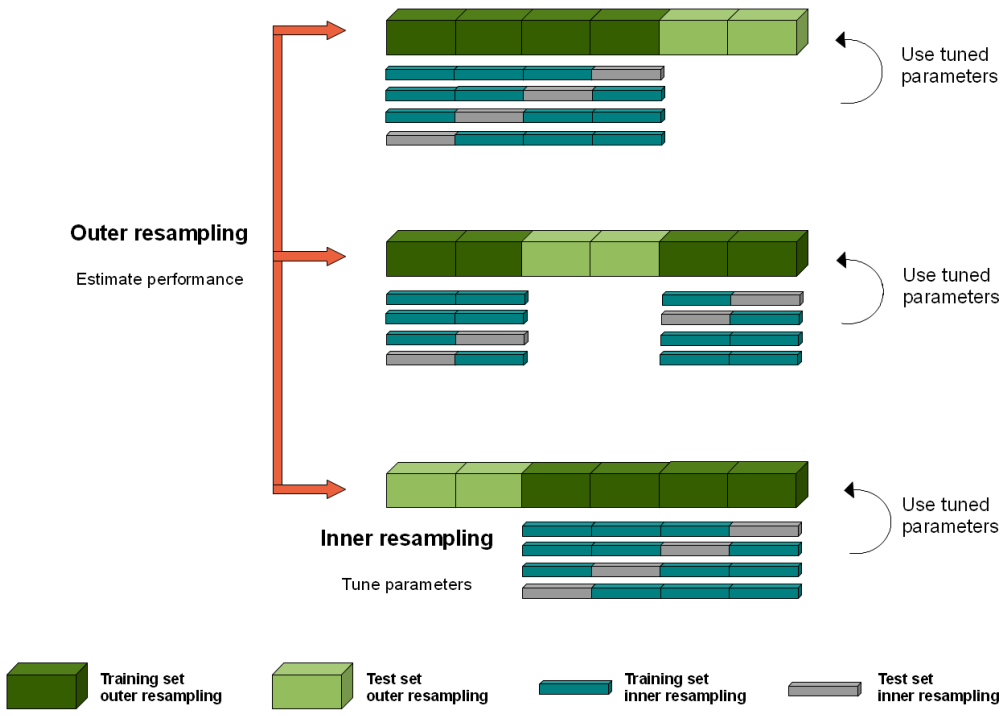


Figure 2: Nested Resampling Figure

3.8 Nested Resampling

In order to obtain honest performance estimates for a learner all parts of the model building like preprocessing and model selection steps should be included in the resampling, i.e., repeated for every pair of training/test data. For steps that themselves require resampling like parameter tuning or feature selection (via the wrapper approach) this results in two nested resampling loops.

The graphic above illustrates nested resampling for parameter tuning with 3-fold cross-validation in the outer and 4-fold cross-validation in the inner loop.

In the outer resampling loop, we have three pairs of training/test sets. On each of these outer training sets parameter tuning is done, thereby executing the inner resampling loop. This way, we get one set of selected hyperparameters for each outer training set. Then the learner is fitted on each outer training set using the corresponding selected hyperparameters and its performance is evaluated on the outer test sets.

In `mlr`, you can get nested resampling for free without programming any looping by using the wrapper functionality. This works as follows:

1. Generate a wrapped Learner (`makeLearner()`) via function `makeTuneWrapper()` or `makeFeatSelWrapper()`. Specify the inner resampling strategy using their `resampling` argument.
2. Call function `resample()` (see also the section about resampling and pass the outer resampling strategy to its `resampling` argument.

You can freely combine different inner and outer resampling strategies.

The outer strategy can be a resample description `ResampleDesc` (`makeResampleDesc()`)) or a resample instance (`makeResampleInstance()`)). A common setup is prediction and performance evaluation on a fixed outer test set. This can be achieved by using function `makeFixedHoldoutInstance()` to generate the outer resample instance(makeResampleInstance()‘).

The inner resampling strategy should preferably be a `ResampleDesc` (`makeResampleDesc()`), as the sizes of the outer training sets might differ. Per default, the inner resample description is instantiated once for every outer training set. This way during tuning/feature selection all parameter or feature sets are compared on the same inner training/test sets to reduce variance. You can also turn this off using the `same.resampling.instance` argument of `makeTuneControl*` (`TuneControl()`) or `makeFeatSelControl*` (`FeatSelControl()`).

Nested resampling is computationally expensive. For this reason in the examples shown below we use relatively small search spaces and a low number of resampling iterations. In practice, you normally have to increase both. As this is computationally intensive you might want to have a look at section parallelization.

3.8.1 Tuning

As you might recall from the tutorial page about tuning, you need to define a search space by function `ParamHelpers::makeParamSet()`, a search strategy by `makeTuneControl*(TuneControl())`, and a method to evaluate hyperparameter settings (i.e., the inner resampling strategy and a performance measure).

Below is a classification example. We evaluate the performance of a support vector machine (`kernlab::ksvm()`) with tuned cost parameter `C` and RBF kernel parameter `sigma`. We use 3-fold cross-validation in the outer and subsampling with 2 iterations in the inner loop. For tuing a grid search is used to find the hyperparameters with lowest error rate (mmce is the default measure for classification). The wrapped Learner (`makeLearner()`) is generated by calling `makeTuneWrapper()`.

Note that in practice the parameter set should be larger. A common recommendation is `2^(-12:12)` for both `C` and `sigma`.

```
### Tuning in inner resampling loop
ps = makeParamSet(
  makeDiscreteParam("C", values = 2^(-2:2)),
  makeDiscreteParam("sigma", values = 2^(-2:2))
)
ctrl = makeTuneControlGrid()
inner = makeResampleDesc("Subsample", iters = 2)
lrn = makeTuneWrapper("classif.ksvm", resampling = inner, par.set = ps, control = ctrl, show.info = FALS

### Outer resampling loop
outer = makeResampleDesc("CV", iters = 3)
r = resample(lrn, iris.task, resampling = outer, extract = getTuneResult, show.info = FALSE)

r
## Resample Result
## Task: iris-example
## Learner: classif.ksvm.tuned
## Aggr perf: mmce.test.mean=0.0533333
## Runtime: 4.00414
```

You can obtain the error rates on the 3 outer test sets by:

```
r$measures.test
##   iter mmce
## 1    1 0.08
## 2    2 0.04
## 3    3 0.04
```

3.8.1.1 Accessing the tuning result

We have kept the results of the tuning for further evaluations. For example one might want to find out, if the best obtained configurations vary for the different outer splits. As storing entire models may be expensive (but possible by setting `models = TRUE`) we used the `extract` option of `resample()`. Function `getTuneResult()` returns, among other things, the optimal hyperparameter values and the optimization path (`ParamHelpers::OptPath()`) for each iteration of the outer resampling loop. Note that the performance values shown when printing `r$extract` are the aggregated performances resulting from inner resampling on the outer training set for the best hyperparameter configurations (not to be confused with `r$measures.test` shown above).

```
r$extract
## [[1]]
## Tune result:
## Op. pars: C=2; sigma=0.25
## mmce.test.mean=0.0000000
##
## [[2]]
## Tune result:
## Op. pars: C=1; sigma=1
## mmce.test.mean=0.0735294
##
## [[3]]
## Tune result:
## Op. pars: C=4; sigma=1
## mmce.test.mean=0.0588235
names(r$extract[[1]])
## [1] "learner"   "control"   "x"         "y"         "threshold" "opt.path"
```

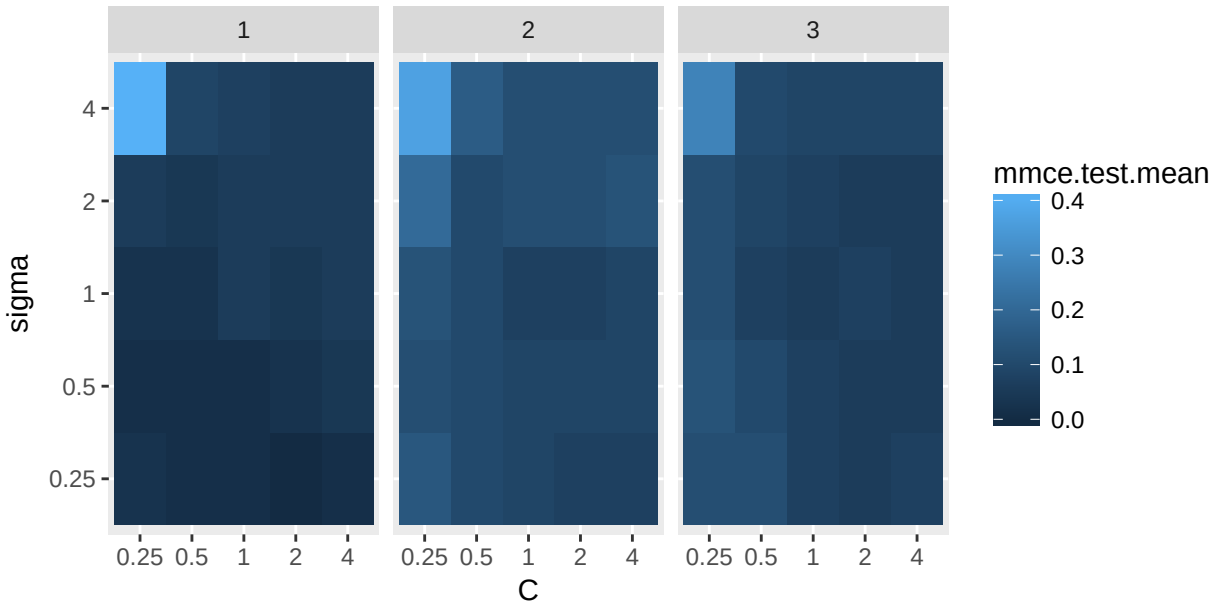
We can compare the optimal parameter settings obtained in the 3 resampling iterations. As you can see, the optimal configuration usually depends on the data. You may be able to identify a *range* of parameter settings that achieve good performance though, e.g., the values for `C` should be at least 1 and the values for `sigma` should be between 0 and 1.

With function `getNestedTuneResultsOptPathDf()` you can extract the optimization paths for the 3 outer cross-validation iterations for further inspection and analysis. These are stacked in one `data.frame` with column `iter` indicating the resampling iteration.

```
opt.paths = getNestedTuneResultsOptPathDf(r)
head(opt.paths, 10)
##       C sigma mmce.test.mean dob eol error.message exec.time iter
## 1  0.25  0.25     0.02941176   1  NA          <NA>     0.042    1
## 2   0.5  0.25     0.01470588   2  NA          <NA>     0.041    1
## 3     1  0.25     0.01470588   3  NA          <NA>     0.044    1
## 4     2  0.25     0.00000000   4  NA          <NA>     0.041    1
## 5     4  0.25     0.01470588   5  NA          <NA>     0.044    1
## 6  0.25   0.5     0.01470588   6  NA          <NA>     0.041    1
## 7   0.5   0.5     0.01470588   7  NA          <NA>     0.052    1
## 8     1   0.5     0.01470588   8  NA          <NA>     0.056    1
## 9     2   0.5     0.02941176   9  NA          <NA>     0.050    1
## 10    4   0.5     0.04411765  10  NA          <NA>     0.054    1
```

Below we visualize the `opt.paths` for the 3 outer resampling iterations.

```
g = ggplot(opt.paths, aes(x = C, y = sigma, fill = mmce.test.mean))
g + geom_tile() + facet_wrap(~ iter)
```



Another useful function is `getNestedTuneResultsX()`, which extracts the best found hyperparameter settings for each outer resampling iteration.

```
getNestedTuneResultsX(r)
##   C sigma
## 1 2  0.25
## 2 1  1.00
## 3 4  1.00
```

3.8.2 Feature selection

As you might recall from the section about feature selection, `mlr` supports the filter and the wrapper approach.

3.8.2.1 Wrapper methods

Wrapper methods use the performance of a learning algorithm to assess the usefulness of a feature set. In order to select a feature subset a learner is trained repeatedly on different feature subsets and the subset which leads to the best learner performance is chosen.

For feature selection in the inner resampling loop, you need to choose a search strategy (function `makeFeatSelControl*` (`FeatSelControl()`)), a performance measure and the inner resampling strategy. Then use function `makeFeatSelWrapper()` to bind everything together.

Below we use sequential forward selection with linear regression on the `BostonHousing` (`mlbench::BostonHousing()` data set (`bh.task()`).

```
### Feature selection in inner resampling loop
inner = makeResampleDesc("CV", iters = 3)
lrn = makeFeatSelWrapper("regr.lm", resampling = inner,
  control = makeFeatSelControlSequential(method = "sfs"), show.info = FALSE)

### Outer resampling loop
outer = makeResampleDesc("Subsample", iters = 2)
r = resample(learner = lrn, task = bh.task, resampling = outer, extract = getFeatSelResult,
  show.info = FALSE)
```

```
r
## Resample Result
## Task: BostonHousing-example
## Learner: regr.lm.featsel
## Aggr perf: mse.test.mean=30.4077041
## Runtime: 7.60017
r$measures.test
##   iter      mse
## 1    1 32.18191
## 2    2 28.63350
```

3.8.2.1.1 Accessing the selected features

The result of the feature selection can be extracted by function `getFeatSelResult()`. It is also possible to keep whole models (`makeWrappedModel()`) by setting `models = TRUE` when calling `resample()`.

```
r$extract
## [[1]]
## FeatSel result:
## Features (8): zn, chas, nox, rm, dis, ptratio, b, lstat
## mse.test.mean=20.7541688
##
## [[2]]
## FeatSel result:
## Features (5): nox, rm, dis, ptratio, lstat
## mse.test.mean=23.8121522
### Selected features in the first outer resampling iteration
r$extract[[1]]$x
## [1] "zn"      "chas"    "nox"     "rm"      "dis"     "ptratio" "b"
## [8] "lstat"
### Resampled performance of the selected feature subset on the first inner training set
r$extract[[1]]$y
## mse.test.mean
##      20.75417
```

As for tuning, you can extract the optimization paths. The resulting `data.frame`s contain, among others, binary columns for all features, indicating if they were included in the linear regression model, and the corresponding performances.

```
opt.paths = lapply(r$extract, function(x) as.data.frame(x$opt.path))
head(opt.paths[[1]])
##   crim zn indus chas nox rm age dis rad tax ptratio b lstat mse.test.mean
## 1    0  0     0    0   0  0   0   0   0   0       0 0     0      85.31576
## 2    1  0     0    0   0  0   0   0   0   0       0 0     0      70.08119
## 3    0  1     0    0   0  0   0   0   0   0       0 0     0      72.38628
## 4    0  0     1    0   0  0   0   0   0   0       0 0     0      62.29939
## 5    0  0     0    1   0  0   0   0   0   0       0 0     0      84.88730
## 6    0  0     0    0   1  0   0   0   0   0       0 0     0      67.81249
##   dob eol error.message exec.time
## 1   1   2          <NA>     0.024
## 2   2   2          <NA>     0.037
## 3   2   2          <NA>     0.035
## 4   2   2          <NA>     0.040
## 5   2   2          <NA>     0.047
## 6   2   2          <NA>     0.037
```

An easy-to-read version of the optimization path for sequential feature selection can be obtained with function `analyzeFeatSelResult()`.

```
analyzeFeatSelResult(r$extract[[1]])
## Features         : 8
## Performance      : mse.test.mean=20.7541688
## zn, chas, nox, rm, dis, ptratio, b, lstat
##
## Path to optimum:
## - Features:    0  Init   :                       Perf = 85.316  Diff: NA  *
## - Features:    1  Add    : lstat                 Perf = 37.193  Diff: 48.123  *
## - Features:    2  Add    : rm                    Perf = 28.013  Diff: 9.1801  *
## - Features:    3  Add    : ptratio               Perf = 24.876  Diff: 3.1371  *
## - Features:    4  Add    : b                     Perf = 22.454  Diff: 2.4219  *
## - Features:    5  Add    : dis                   Perf = 21.98  Diff: 0.47361  *
## - Features:    6  Add    : nox                   Perf = 21.013  Diff: 0.96787  *
## - Features:    7  Add    : chas                  Perf = 20.8  Diff: 0.21274  *
## - Features:    8  Add    : zn                    Perf = 20.754  Diff: 0.045669  *
##
## Stopped, because no improving feature was found.
```

3.8.2.2 Filter methods with tuning

Filter methods assign an importance value to each feature. Based on these values you can select a feature subset by either keeping all features with importance higher than a certain threshold or by keeping a fixed number or percentage of the highest ranking features. Often, neither the theshold nor the number or percentage of features is known in advance and thus tuning is necessary.

In the example below the threshold value (`fw.threshold`) is tuned in the inner resampling loop. For this purpose the base Learner (`makeLearner()`) `"regr.lm"` is wrapped two times. First, `makeFilterWrapper()` is used to fuse linear regression with a feature filtering preprocessing step. Then a tuning step is added by `makeTuneWrapper()`.

```
### Tuning of the percentage of selected filters in the inner loop
lrn = makeFilterWrapper(learner = "regr.lm", fw.method = "chi.squared")
ps = makeParamSet(makeDiscreteParam("fw.threshold", values = seq(0, 1, 0.2)))
ctrl = makeTuneControlGrid()
inner = makeResampleDesc("CV", iters = 3)
lrn = makeTuneWrapper(lrn, resampling = inner, par.set = ps, control = ctrl, show.info = FALSE)

### Outer resampling loop
outer = makeResampleDesc("CV", iters = 3)
r = resample(learner = lrn, task = bh.task, resampling = outer, models = TRUE, show.info = FALSE)
r
## Resample Result
## Task: BostonHousing-example
## Learner: regr.lm.filtered.tuned
## Aggr perf: mse.test.mean=23.9538769
## Runtime: 4.56361
```

3.8.2.2.1 Accessing the selected features and optimal percentage

In the above example we kept the complete model (`makeWrappedModel()`)s.

Below are some examples that show how to extract information from the model (`makeWrappedModel()`)s.

```
r$models
## [[1]]
## Model for learner.id=regr.lm.filtered.tuned; learner.class=TuneWrapper
## Trained on: task.id = BostonHousing-example; obs = 337; features = 13
## Hyperparameters: fw.method=chi.squared
##
## [[2]]
## Model for learner.id=regr.lm.filtered.tuned; learner.class=TuneWrapper
## Trained on: task.id = BostonHousing-example; obs = 338; features = 13
## Hyperparameters: fw.method=chi.squared
##
## [[3]]
## Model for learner.id=regr.lm.filtered.tuned; learner.class=TuneWrapper
## Trained on: task.id = BostonHousing-example; obs = 337; features = 13
## Hyperparameters: fw.method=chi.squared
```

The result of the feature selection can be extracted by function `getFilteredFeatures()`. Almost always all 13 features are selected.

```
lapply(r$models, function(x) getFilteredFeatures(x$learner.model$next.model))
## [[1]]
##  [1] "crim"    "zn"      "indus"   "nox"     "rm"      "age"     "dis"
##  [8] "rad"     "tax"     "ptratio" "b"       "lstat"
##
## [[2]]
##  [1] "crim"    "zn"      "indus"   "chas"    "nox"     "rm"      "age"
##  [8] "dis"     "rad"     "tax"     "ptratio" "b"       "lstat"
##
## [[3]]
##  [1] "crim"    "zn"      "indus"   "chas"    "nox"     "rm"      "age"
##  [8] "dis"     "rad"     "tax"     "ptratio" "b"       "lstat"
```

Below the tune results (`TuneResult()`) and optimization paths (`ParamHelpers::OptPath()`) are accessed.

```
res = lapply(r$models, getTuneResult)
res
## [[1]]
## Tune result:
## Op. pars: fw.threshold=0.2
## mse.test.mean=23.9887628
##
## [[2]]
## Tune result:
## Op. pars: fw.threshold=0
## mse.test.mean=25.7718103
##
## [[3]]
## Tune result:
## Op. pars: fw.threshold=0
## mse.test.mean=24.4980718
opt.paths = lapply(res, function(x) as.data.frame(x$opt.path))
opt.paths[[1]]
##   fw.threshold mse.test.mean dob eol error.message exec.time
## 1            0      24.74447   1  NA          <NA>     0.238
## 2          0.2      23.98876   2  NA          <NA>     0.246
```

```
## 3          0.4      23.98876   3  NA          <NA>     0.228
## 4          0.6      36.20027   4  NA          <NA>     0.226
## 5          0.8      82.64427   5  NA          <NA>     0.219
## 6            1      88.33096   6  NA          <NA>     0.211
```

3.8.3 Benchmark experiments

In a benchmark experiment multiple learners are compared on one or several tasks (see also the section about benchmarking. Nested resampling in benchmark experiments is achieved the same way as in resampling:

- First, use `makeTuneWrapper()` or `makeFeatSelWrapper()` to generate wrapped Learner (`makeLearner()`)s with the inner resampling strategies of your choice.
- Second, call `benchmark()` and specify the outer resampling strategies for all tasks.

The inner resampling strategies should be resample descriptions (`makeResampleDesc()`). You can use different inner resampling strategies for different wrapped learners. For example it might be practical to do fewer subsampling or bootstrap iterations for slower learners.

If you have larger benchmark experiments you might want to have a look at the section about parallelization.

As mentioned in the section about benchmark experiments you can also use different resampling strategies for different learning tasks by passing a `list` of resampling descriptions or instances to `benchmark()`.

We will see three examples to show different benchmark settings:

1. Two data sets + two classification algorithms + tuning
2. One data set + two regression algorithms + feature selection
3. One data set + two regression algorithms + feature filtering + tuning

3.8.3.1 Example 1: Two tasks, two learners, tuning

Below is a benchmark experiment with two data sets, `datasets::iris()` and `mlbench::sonar()`, and two Learner (`makeLearner()`)s, `kernlab::ksvm()` and `kknn::kknn()`, that are both tuned.

As inner resampling strategies we use holdout for `kernlab::ksvm()` and subsampling with 3 iterations for `kknn::kknn()`. As outer resampling strategies we take holdout for the `datasets::iris()` and bootstrap with 2 iterations for the `mlbench::sonar()` data (`sonar.task()`). We consider the accuracy (acc), which is used as tuning criterion, and also calculate the balanced error rate (ber).

```
### List of learning tasks
tasks = list(iris.task, sonar.task)

### Tune svm in the inner resampling loop
ps = makeParamSet(
  makeDiscreteParam("C", 2^(-1:1)),
  makeDiscreteParam("sigma", 2^(-1:1)))
ctrl = makeTuneControlGrid()
inner = makeResampleDesc("Holdout")
lrn1 = makeTuneWrapper("classif.ksvm", resampling = inner, par.set = ps, control = ctrl,
  show.info = FALSE)

### Tune k-nearest neighbor in inner resampling loop
ps = makeParamSet(makeDiscreteParam("k", 3:5))
ctrl = makeTuneControlGrid()
inner = makeResampleDesc("Subsample", iters = 3)
lrn2 = makeTuneWrapper("classif.kknn", resampling = inner, par.set = ps, control = ctrl,
  show.info = FALSE)
```

```
## Loading required package: kknn
### Learners
lrns = list(lrn1, lrn2)

### Outer resampling loop
outer = list(makeResampleDesc("Holdout"), makeResampleDesc("Bootstrap", iters = 2))
res = benchmark(lrns, tasks, outer, measures = list(acc, ber), show.info = FALSE)
res
##         task.id         learner.id acc.test.mean ber.test.mean
## 1  iris-example classif.ksvm.tuned     0.9400000    0.05257937
## 2  iris-example classif.kknn.tuned     0.9400000    0.06234737
## 3 Sonar-example classif.ksvm.tuned     0.5634921    0.48571429
## 4 Sonar-example classif.kknn.tuned     0.8369408    0.16488095
```

The `print` method for the `BenchmarkResult()` shows the aggregated performances from the outer resampling loop.

As you might recall, `mlr` offers several accessor function to extract information from the benchmark result. These are listed on the help page of `BenchmarkResult()` and many examples are shown on the tutorial page about benchmark experiments.

The performance values in individual outer resampling runs can be obtained by `getBMRPerformances()`. Note that, since we used different outer resampling strategies for the two tasks, the number of rows per task differ.

```
getBMRPerformances(res, as.df = TRUE)
##         task.id         learner.id iter       acc        ber
## 1  iris-example classif.ksvm.tuned    1 0.9400000 0.05257937
## 2  iris-example classif.kknn.tuned    1 0.9400000 0.06234737
## 3 Sonar-example classif.ksvm.tuned    1 0.5555556 0.50000000
## 4 Sonar-example classif.ksvm.tuned    2 0.5714286 0.47142857
## 5 Sonar-example classif.kknn.tuned    1 0.7777778 0.22500000
## 6 Sonar-example classif.kknn.tuned    2 0.8961039 0.10476190
```

The results from the parameter tuning can be obtained through function `getBMRTuneResults()`.

```
getBMRTuneResults(res)
## $`iris-example`
## $`iris-example`$classif.ksvm.tuned
## $`iris-example`$classif.ksvm.tuned[[1]]
## Tune result:
## Op. pars: C=2; sigma=2
## mmce.test.mean=0.0882353
##
##
## $`iris-example`$classif.kknn.tuned
## $`iris-example`$classif.kknn.tuned[[1]]
## Tune result:
## Op. pars: k=3
## mmce.test.mean=0.0490196
##
##
##
## $`Sonar-example`
## $`Sonar-example`$classif.ksvm.tuned
## $`Sonar-example`$classif.ksvm.tuned[[1]]
```

```
## Tune result:
## Op. pars: C=2; sigma=0.5
## mmce.test.mean=0.3428571
##
## $`Sonar-example`$classif.ksvm.tuned[[2]]
## Tune result:
## Op. pars: C=1; sigma=0.5
## mmce.test.mean=0.3428571
##
##
## $`Sonar-example`$classif.kknn.tuned
## $`Sonar-example`$classif.kknn.tuned[[1]]
## Tune result:
## Op. pars: k=5
## mmce.test.mean=0.0857143
##
## $`Sonar-example`$classif.kknn.tuned[[2]]
## Tune result:
## Op. pars: k=4
## mmce.test.mean=0.0904762
```

As for several other accessor functions a clearer representation as `data.frame` can be achieved by setting `as.df = TRUE`.

```
getBMRTuneResults(res, as.df = TRUE)
##         task.id         learner.id iter  C sigma mmce.test.mean  k
## 1  iris-example classif.ksvm.tuned    1  2   2.0     0.08823529 NA
## 2  iris-example classif.kknn.tuned    1 NA    NA     0.04901961  3
## 3 Sonar-example classif.ksvm.tuned    1  2   0.5     0.34285714 NA
## 4 Sonar-example classif.ksvm.tuned    2  1   0.5     0.34285714 NA
## 5 Sonar-example classif.kknn.tuned    1 NA    NA     0.08571429  5
## 6 Sonar-example classif.kknn.tuned    2 NA    NA     0.09047619  4
```

It is also possible to extract the tuning results for individual tasks and learners and, as shown in earlier examples, inspect the optimization path (`ParamHelpers::OptPath()`).

```
tune.res = getBMRTuneResults(res, task.ids = "Sonar-example", learner.ids = "classif.ksvm.tuned",
  as.df = TRUE)
tune.res
##         task.id         learner.id iter C sigma mmce.test.mean
## 1 Sonar-example classif.ksvm.tuned    1 2   0.5      0.3428571
## 2 Sonar-example classif.ksvm.tuned    2 1   0.5      0.3428571
getNestedTuneResultsOptPathDf(res$results[["Sonar-example"]][["classif.ksvm.tuned"]])
```

3.8.3.2 Example 2: One task, two learners, feature selection

Let's see how we can do feature selection in a benchmark experiment:

```
### Feature selection in inner resampling loop
ctrl = makeFeatSelControlSequential(method = "sfs")
inner = makeResampleDesc("Subsample", iters = 2)
lrn = makeFeatSelWrapper("regr.lm", resampling = inner, control = ctrl, show.info = FALSE)

### Learners
lrns = list("regr.rpart", lrn)
```

```
### Outer resampling loop
outer = makeResampleDesc("Subsample", iters = 2)
res = benchmark(tasks = bh.task, learners = lrns, resampling = outer, show.info = FALSE)

res
##                  task.id      learner.id mse.test.mean
## 1 BostonHousing-example      regr.rpart      27.18233
## 2 BostonHousing-example regr.lm.featsel      34.24948
```

The selected features can be extracted by function `getBMRFeatSelResults()`. By default, a nested `list`, with the first level indicating the task and the second level indicating the learner, is returned. If only a single learner or, as in our case, a single task is considered, setting `drop = TRUE` simplifies the result to a flat `list`.

```
getBMRFeatSelResults(res)
## $`BostonHousing-example`
## $`BostonHousing-example`$regr.rpart
## NULL
##
## $`BostonHousing-example`$regr.lm.featsel
## $`BostonHousing-example`$regr.lm.featsel[[1]]
## FeatSel result:
## Features (11): crim, zn, chas, nox, rm, dis, rad, tax, ptratio, b, lstat
## mse.test.mean=21.2094120
##
## $`BostonHousing-example`$regr.lm.featsel[[2]]
## FeatSel result:
## Features (8): crim, zn, rm, dis, rad, tax, ptratio, lstat
## mse.test.mean=18.9483065
getBMRFeatSelResults(res, drop = TRUE)
## $regr.rpart
## NULL
##
## $regr.lm.featsel
## $regr.lm.featsel[[1]]
## FeatSel result:
## Features (11): crim, zn, chas, nox, rm, dis, rad, tax, ptratio, b, lstat
## mse.test.mean=21.2094120
##
## $regr.lm.featsel[[2]]
## FeatSel result:
## Features (8): crim, zn, rm, dis, rad, tax, ptratio, lstat
## mse.test.mean=18.9483065
```

You can access results for individual learners and tasks and inspect them further.

```
feats = getBMRFeatSelResults(res, learner.id = "regr.lm.featsel", drop = TRUE)

### Selected features in the first outer resampling iteration
feats[[1]]$x
##  [1] "crim"    "zn"      "chas"    "nox"     "rm"      "dis"     "rad"
##  [8] "tax"     "ptratio" "b"       "lstat"
### Resampled performance of the selected feature subset on the first inner training set
feats[[1]]$y
## mse.test.mean
##      21.20941
```

As for tuning, you can extract the optimization paths. The resulting `data.frames` contain, among others, binary columns for all features, indicating if they were included in the linear regression model, and the corresponding performances. `analyzeFeatSelResult()` gives a clearer overview.

```
opt.paths = lapply(feats, function(x) as.data.frame(x$opt.path))
head(opt.paths[[1]])
##   crim zn indus chas nox rm age dis rad tax ptratio b lstat mse.test.mean
## 1    0  0     0    0   0  0   0   0   0   0       0 0     0      83.27938
## 2    1  0     0    0   0  0   0   0   0   0       0 0     0      76.09974
## 3    0  1     0    0   0  0   0   0   0   0       0 0     0      72.71235
## 4    0  0     1    0   0  0   0   0   0   0       0 0     0      66.05616
## 5    0  0     0    1   0  0   0   0   0   0       0 0     0      79.34454
## 6    0  0     0    0   1  0   0   0   0   0       0 0     0      72.26475
##   dob eol error.message exec.time
## 1   1   2          <NA>     0.022
## 2   2   2          <NA>     0.034
## 3   2   2          <NA>     0.034
## 4   2   2          <NA>     0.034
## 5   2   2          <NA>     0.036
## 6   2   2          <NA>     0.034
analyzeFeatSelResult(feats[[1]])
## Features         : 11
## Performance      : mse.test.mean=21.2094120
## crim, zn, chas, nox, rm, dis, rad, tax, ptratio, b, lstat
##
## Path to optimum:
## - Features:    0  Init   :                       Perf = 83.279  Diff: NA  *
## - Features:    1  Add    : lstat                 Perf = 37.271  Diff: 46.008  *
## - Features:    2  Add    : rm                    Perf = 29.411  Diff: 7.8606  *
## - Features:    3  Add    : ptratio               Perf = 26.323  Diff: 3.0877  *
## - Features:    4  Add    : chas                  Perf = 24.989  Diff: 1.3339  *
## - Features:    5  Add    : b                     Perf = 24.327  Diff: 0.6619  *
## - Features:    6  Add    : dis                   Perf = 23.77  Diff: 0.55674  *
## - Features:    7  Add    : nox                   Perf = 22.501  Diff: 1.2694  *
## - Features:    8  Add    : crim                  Perf = 22.125  Diff: 0.37577  *
## - Features:    9  Add    : rad                   Perf = 21.699  Diff: 0.42614  *
## - Features:   10  Add    : zn                    Perf = 21.389  Diff: 0.31017  *
## - Features:   11  Add    : tax                   Perf = 21.209  Diff: 0.17953  *
##
## Stopped, because no improving feature was found.
```

3.8.3.3 Example 3: One task, two learners, feature filtering with tuning

Here is a minimal example for feature filtering with tuning of the feature subset size.

```
### Feature filtering with tuning in the inner resampling loop
lrn = makeFilterWrapper(learner = "regr.lm", fw.method = "chi.squared")
ps = makeParamSet(makeDiscreteParam("fw.abs", values = seq_len(getTaskNFeats(bh.task))))
ctrl = makeTuneControlGrid()
inner = makeResampleDesc("CV", iter = 2)
lrn = makeTuneWrapper(lrn, resampling = inner, par.set = ps, control = ctrl,
  show.info = FALSE)

### Learners
```

```
lrns = list("regr.rpart", lrn)

### Outer resampling loop
outer = makeResampleDesc("Subsample", iter = 3)
res = benchmark(tasks = bh.task, learners = lrns, resampling = outer, show.info = FALSE)

res
##                 task.id             learner.id mse.test.mean
## 1 BostonHousing-example             regr.rpart      18.65933
## 2 BostonHousing-example regr.lm.filtered.tuned      19.90791
### Performances on individual outer test data sets
getBMRPerformances(res, as.df = TRUE)
##                 task.id             learner.id iter      mse
## 1 BostonHousing-example             regr.rpart    1 19.18995
## 2 BostonHousing-example             regr.rpart    2 18.67907
## 3 BostonHousing-example             regr.rpart    3 18.10897
## 4 BostonHousing-example regr.lm.filtered.tuned    1 20.06960
## 5 BostonHousing-example regr.lm.filtered.tuned    2 19.16824
## 6 BostonHousing-example regr.lm.filtered.tuned    3 20.48590
```

3.9 Cost-Sensitive Classification

In *regular classification* the aim is to minimize the misclassification rate and thus all types of misclassification errors are deemed equally severe. A more general setting is *cost-sensitive classification* where the costs caused by different kinds of errors are not assumed to be equal and the objective is to minimize the expected costs.

In case of *class-dependent costs* the costs depend on the true and predicted class label. The costs $c(k, l)$ for predicting class k if the true label is l are usually organized into a $K \times K$ cost matrix where K is the number of classes. Naturally, it is assumed that the cost of predicting the correct class label y is minimal (that is $c(y, y) \leq c(k, y)$ for all $k = 1, \ldots, K$).

A further generalization of this scenario are *example-dependent misclassification costs* where each example (x, y) is coupled with an individual cost vector of length K. Its k-th component expresses the cost of assigning x to class k. A real-world example is fraud detection where the costs do not only depend on the true and predicted status fraud/non-fraud, but also on the amount of money involved in each case. Naturally, the cost of predicting the true class label y is assumed to be minimum. The true class labels are redundant information, as they can be easily inferred from the cost vectors. Moreover, given the cost vector, the expected costs do not depend on the true class label y. The classification problem is therefore completely defined by the feature values x and the corresponding cost vectors.

In the following we show ways to handle cost-sensitive classification problems in `mlr`. Some of the functionality is currently experimental, and there may be changes in the future.

3.9.0.1 Class-dependent misclassification costs

There are some classification methods that can accomodate misclassification costs directly. One example is `rpart::rpart()`.

Alternatively, we can use cost-insensitive methods and manipulate the predictions or the training data in order to take misclassification costs into account. `mlr` supports *thresholding* and *rebalancing*.

1. **Thresholding**: The thresholds used to turn posterior probabilities into class labels are chosen such that the costs are minimized. This requires a Learner (`makeLearner()`) that can predict posterior probabilities. During training the costs are not taken into account.

2. **Rebalancing**: The idea is to change the proportion of the classes in the training data set in order to account for costs during training, either by *weighting* or by *sampling*. Rebalancing does not require that the Learner (`makeLearner()`) can predict probabilities.

   i. For *weighting* we need a Learner (`makeLearner()`) that supports class weights or observation weights.

   ii. If the Learner (`makeLearner()`) cannot deal with weights the proportion of classes can be changed by *over-* and *undersampling*.

We start with binary classification problems and afterwards deal with multi-class problems.

3.9.0.2 Binary classification problems

The positive and negative classes are labeled 1 and -1, respectively, and we consider the following cost matrix where the rows indicate true classes and the columns predicted classes:

true/pred.	$+1$	-1
$+1$	$c(+1,+1)$	$c(-1,+1)$
-1	$c(+1,-1)$	$c(-1,-1)$

Often, the diagonal entries are zero or the cost matrix is rescaled to achieve zeros in the diagonal (see for example O'Brien et al, 2008).

A well-known cost-sensitive classification problem is posed by the German Credit data set (`caret::GermanCredit()`) (see also the UCI Machine Learning Repository). The corresponding cost matrix (though Elkan (2001) argues that this matrix is economically unreasonable) is given as:

true/pred.	Bad	Good
Bad	0	5
Good	1	0

As in the table above, the rows indicate true and the columns predicted classes.

In case of class-dependent costs it is sufficient to generate an ordinary `ClassifTask` (`Task()`). A `CostSensTask` (`Task()`) is only needed if the costs are example-dependent. In the **R** code below we create the `ClassifTask` (`Task()`), remove two constant features from the data set and generate the cost matrix. Per default, Bad is the positive class.

```
data(GermanCredit, package = "caret")
credit.task = makeClassifTask(data = GermanCredit, target = "Class")
credit.task = removeConstantFeatures(credit.task)
## Removing 2 columns: Purpose.Vacation,Personal.Female.Single
credit.task
## Supervised task: GermanCredit
## Type: classif
## Target: Class
## Observations: 1000
## Features:
##    numerics     factors     ordered functionals
##          59           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
```

```
## Classes: 2
##  Bad Good
##  300  700
## Positive class: Bad
costs = matrix(c(0, 1, 5, 0), 2)
colnames(costs) = rownames(costs) = getTaskClassLevels(credit.task)
costs
##      Bad Good
## Bad    0    5
## Good   1    0
```

3.9.0.2.1 1. Thresholding

We start by fitting a logistic regression model (`nnet::multinom()`) to the German Credit data set (`caret::GermanCredit()`) and predict posterior probabilities.

```
### Train and predict posterior probabilities
lrn = makeLearner("classif.multinom", predict.type = "prob", trace = FALSE)
mod = train(lrn, credit.task)
pred = predict(mod, task = credit.task)
pred
## Prediction: 1000 observations
## predict.type: prob
## threshold: Bad=0.50,Good=0.50
## time: 0.02
##   id truth   prob.Bad prob.Good response
## 1  1  Good 0.03525092 0.9647491     Good
## 2  2   Bad 0.63222363 0.3677764      Bad
## 3  3  Good 0.02807414 0.9719259     Good
## 4  4  Good 0.25182703 0.7481730     Good
## 5  5   Bad 0.75193275 0.2480673      Bad
## 6  6  Good 0.26230149 0.7376985     Good
## ... (#rows: 1000, #cols: 5)
```

The default thresholds for both classes are 0.5. But according to the cost matrix we should predict class Good only if we are very sure that Good is indeed the correct label. Therefore we should increase the threshold for class Good and decrease the threshold for class Bad.

i. Theoretical thresholding

The theoretical threshold for the *positive* class can be calculated from the cost matrix as

$$t^* = \frac{c(+1,-1) - c(-1,-1)}{c(+1,-1) - c(+1,+1) + c(-1,+1) - c(-1,-1)}.$$

For more details see Elkan (2001).

Below the theoretical threshold for the German Credit data set (`caret::GermanCredit()`) is calculated and used to predict class labels. Since the diagonal of the cost matrix is zero the formula given above simplifies accordingly.

```
### Calculate the theoretical threshold for the positive class
th = costs[2,1]/(costs[2,1] + costs[1,2])
th
## [1] 0.1666667
```

As you may recall you can change thresholds in `mlr` either before training by using the `predict.threshold` option of `makeLearner()` or after prediction by calling `setThreshold()` on the `Prediction()` object.

As we already have a prediction we use the `setThreshold()` function. It returns an altered `Prediction()` object with class predictions for the theoretical threshold.

```
### Predict class labels according to the theoretical threshold
pred.th = setThreshold(pred, th)
pred.th
## Prediction: 1000 observations
## predict.type: prob
## threshold: Bad=0.17,Good=0.83
## time: 0.02
##   id truth   prob.Bad prob.Good response
## 1  1  Good 0.03525092 0.9647491     Good
## 2  2   Bad 0.63222363 0.3677764      Bad
## 3  3  Good 0.02807414 0.9719259     Good
## 4  4  Good 0.25182703 0.7481730      Bad
## 5  5   Bad 0.75193275 0.2480673      Bad
## 6  6  Good 0.26230149 0.7376985      Bad
## ... (#rows: 1000, #cols: 5)
```

In order to calculate the average costs over the entire data set we first need to create a new performance Measure (`makeMeasure()`). This can be done through function `makeCostMeasure()`. It is expected that the rows of the cost matrix indicate true and the columns predicted class labels.

```
credit.costs = makeCostMeasure(id = "credit.costs", name = "Credit costs", costs = costs,
  best = 0, worst = 5)
credit.costs
## Name: Credit costs
## Performance measure: credit.costs
## Properties: classif,classif.multi,req.pred,req.truth,predtype.response,predtype.prob
## Minimize: TRUE
## Best: 0; Worst: 5
## Aggregated by: test.mean
## Arguments: <unnamed>=<matrix>, <unnamed>=<function>
## Note:
```

Then the average costs can be computed by function `performance()`. Below we compare the average costs and the error rate (mmce) of the learning algorithm with both default thresholds 0.5 and theoretical thresholds.

```
### Performance with default thresholds 0.5
performance(pred, measures = list(credit.costs, mmce))
## credit.costs         mmce
##        0.774        0.214
### Performance with theoretical thresholds
performance(pred.th, measures = list(credit.costs, mmce))
## credit.costs         mmce
##        0.478        0.346
```

These performance values may be overly optimistic as we used the same data set for training and prediction, and resampling strategies should be preferred. In the **R** code below we make use of the `predict.threshold` argument of `makeLearner()` to set the threshold before doing a 3-fold cross-validation on the `credit.task()`. Note that we create a `ResampleInstance` (`makeResampleInstance()`) (`rin`) that is used throughout the next several code chunks to get comparable performance values.

```
### Cross-validated performance with theoretical thresholds
rin = makeResampleInstance("CV", iters = 3, task = credit.task)
lrn = makeLearner("classif.multinom", predict.type = "prob", predict.threshold = th, trace = FALSE)
r = resample(lrn, credit.task, resampling = rin, measures = list(credit.costs, mmce), show.info = FALSE)
```

```
r
## Resample Result
## Task: GermanCredit
## Learner: classif.multinom
## Aggr perf: credit.costs.test.mean=0.5919962,mmce.test.mean=0.3680477
## Runtime: 0.224672
```

If we are also interested in the cross-validated performance for the default threshold values we can call `setThreshold()` on the resample prediction (`ResamplePrediction()`) `r$pred`.

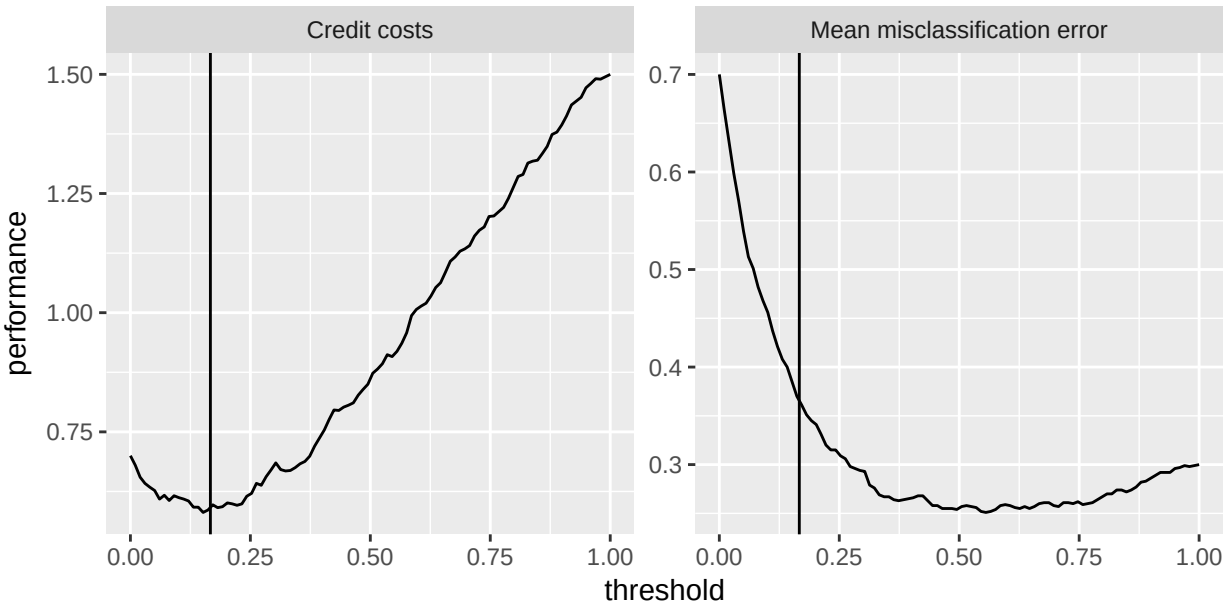
```
### Cross-validated performance with default thresholds
performance(setThreshold(r$pred, 0.5), measures = list(credit.costs, mmce))
## credit.costs         mmce
##    0.8589428    0.2549855
```

Theoretical thresholding is only reliable if the predicted posterior probabilities are correct. If there is bias the thresholds have to be shifted accordingly.

Useful in this regard is function `plotThreshVsPerf()` that you can use to plot the average costs as well as any other performance measure versus possible threshold values for the positive class in $[0, 1]$. The underlying data is generated by `generateThreshVsPerfData()`.

The following plots show the cross-validated costs and error rate (mmce). The theoretical threshold `th` calculated above is indicated by the vertical line. As you can see from the left-hand plot the theoretical threshold seems a bit large.

```
d = generateThreshVsPerfData(r, measures = list(credit.costs, mmce))
plotThreshVsPerf(d, mark.th = th)
```



ii. Empirical thresholding

The idea of *empirical thresholding* (see Sheng and Ling, 2006) is to select cost-optimal threshold values for a given learning method based on the training data. In contrast to *theoretical thresholding* it suffices if the estimated posterior probabilities are order-correct.

In order to determine optimal threshold values you can use `mlr`'s function `tuneThreshold()`. As tuning the threshold on the complete training data set can lead to overfitting, you should use resampling strategies. Below we perform 3-fold cross-validation and use `tuneThreshold()` to calculate threshold values with lowest

average costs over the 3 test data sets.

```
lrn = makeLearner("classif.multinom", predict.type = "prob", trace = FALSE)

### 3-fold cross-validation
r = resample(lrn, credit.task, resampling = rin, measures = list(credit.costs, mmce), show.info = FALSE)
r
## Resample Result
## Task: GermanCredit
## Learner: classif.multinom
## Aggr perf: credit.costs.test.mean=0.8589428,mmce.test.mean=0.2549855
## Runtime: 0.412458
### Tune the threshold based on the predicted probabilities on the 3 test data sets
tune.res = tuneThreshold(pred = r$pred, measure = credit.costs)
tune.res
## $th
## [1] 0.1596003
##
## $perf
## credit.costs
##    0.5769722
```

`tuneThreshold()` returns the optimal threshold value for the positive class and the corresponding performance. As expected the tuned threshold is smaller than the theoretical threshold.

3.9.0.2.2 2. Rebalancing

In order to minimize the average costs, observations from the less costly class should be given higher importance during training. This can be achieved by *weighting* the classes, provided that the learner under consideration has a 'class weights' or an 'observation weights' argument. To find out which learning methods support either type of weights have a look at the list of integrated learners in the Appendix or use `listLearners()`.

```
### Learners that accept observation weights
listLearners("classif", properties = "weights")[c("class", "package")]
## Warning in listLearners.character("classif", properties = "weights"): The following learners could no
## classif.mxff,regr.mxff
## Check ?learners to see which packages you need or install mlr with all suggestions.
##                class      package
## 1   classif.binomial        stats
## 2 classif.blackboost mboost,party
## 3        classif.C50          C50
## 4    classif.cforest        party
## 5      classif.ctree        party
## 6   classif.cvglmnet       glmnet
## ... (#rows: 25, #cols: 2)
### Learners that can deal with class weights
listLearners("classif", properties = "class.weights")[c("class", "package")]
## Warning in listLearners.character("classif", properties = "class.weights"): The following learners co
## classif.mxff,regr.mxff
## Check ?learners to see which packages you need or install mlr with all suggestions.
##                        class   package
## 1              classif.ksvm   kernlab
## 2  classif.LiblineaRL1L2SVC LiblineaR
## 3 classif.LiblineaRL1LogReg LiblineaR
## 4  classif.LiblineaRL2L1SVC LiblineaR
```

```
## 5 classif.LiblineaRL2LogReg LiblineaR
## 6    classif.LiblineaRL2SVC LiblineaR
## ... (#rows: 9, #cols: 2)
```

Alternatively, *over- and undersampling* techniques can be used.

i. Weighting

Just as *theoretical thresholds*, *theoretical weights* can be calculated from the cost matrix. If t indicates the target threshold and t_0 the original threshold for the positive class the proportion of observations in the positive class has to be multiplied by

$$\frac{1-t}{t}\frac{t_0}{1-t_0}.$$

Alternatively, the proportion of observations in the negative class can be multiplied by the inverse. A proof is given by Elkan (2001).

In most cases, the original threshold is $t_0 = 0.5$ and thus the second factor vanishes. If additionally the target threshold t equals the theoretical threshold t^* the proportion of observations in the positive class has to be multiplied by

$$\frac{1-t^*}{t^*} = \frac{c(-1,+1) - c(+1,+1)}{c(+1,-1) - c(-1,-1)}.$$

For the credit example (`caret:GermanCredit()`) the theoretical threshold corresponds to a weight of 5 for the positive class.

```
### Weight for positive class corresponding to theoretical treshold
w = (1 - th)/th
w
## [1] 5
```

A unified and convenient way to assign class weights to a Learner (`makeLearner()`) (and tune them) is provided by function `makeWeightedClassesWrapper()`. The class weights are specified using argument `wcw.weight`. For learners that support observation weights a suitable weight vector is then generated internally during training or resampling. If the learner can deal with class weights, the weights are basically passed on to the appropriate learner parameter. The advantage of using the wrapper in this case is the unified way to specify the class weights.

Below is an example using learner `"classif.multinom"` (`nnet::multinom()`) from package `nnet`) which accepts observation weights. For binary classification problems it is sufficient to specify the weight `w` for the positive class. The negative class then automatically receives weight 1.

```
### Weighted learner
lrn = makeLearner("classif.multinom", trace = FALSE)
lrn = makeWeightedClassesWrapper(lrn, wcw.weight = w)
lrn
## Learner weightedclasses.classif.multinom from package nnet
## Type: classif
## Name: ; Short name:
## Class: WeightedClassesWrapper
## Properties: twoclass,multiclass,numerics,factors,prob
## Predict-Type: response
## Hyperparameters: trace=FALSE,wcw.weight=5
r = resample(lrn, credit.task, rin, measures = list(credit.costs, mmce), show.info = FALSE)
r
## Resample Result
## Task: GermanCredit
## Learner: weightedclasses.classif.multinom
```

```
## Aggr perf: credit.costs.test.mean=0.5959492,mmce.test.mean=0.3640287
## Runtime: 0.308758
```

For classification methods like `"classif.ksvm"` (the support vector machine `kernlab::ksvm()` in package `kernlab`) that support class weights you can pass them directly.

```
lrn = makeLearner("classif.ksvm", class.weights = c(Bad = w, Good = 1))
```

Or, more conveniently, you can again use `makeWeightedClassesWrapper()`.

```
lrn = makeWeightedClassesWrapper("classif.ksvm", wcw.weight = w)
r = resample(lrn, credit.task, rin, measures = list(credit.costs, mmce), show.info = FALSE)
r
## Resample Result
## Task: GermanCredit
## Learner: weightedclasses.classif.ksvm
## Aggr perf: credit.costs.test.mean=0.6739524,mmce.test.mean=0.3420157
## Runtime: 0.458599
```

Just like the theoretical threshold, the theoretical weights may not always be suitable, therefore you can tune the weight for the positive class as shown in the following example. Calculating the theoretical weight beforehand may help to narrow down the search interval.

```
lrn = makeLearner("classif.multinom", trace = FALSE)
lrn = makeWeightedClassesWrapper(lrn)
ps = makeParamSet(makeDiscreteParam("wcw.weight", seq(4, 12, 0.5)))
ctrl = makeTuneControlGrid()
tune.res = tuneParams(lrn, credit.task, resampling = rin, par.set = ps,
  measures = list(credit.costs, mmce), control = ctrl, show.info = FALSE)
tune.res
## Tune result:
## Op. pars: wcw.weight=11
## credit.costs.test.mean=0.5679542,mmce.test.mean=0.4360498
as.data.frame(tune.res$opt.path)[1:3]
##    wcw.weight credit.costs.test.mean mmce.test.mean
## 1           4              0.6159453      0.3480247
## 2         4.5              0.5799482      0.3480277
## 3           5              0.5959492      0.3640287
## 4         5.5              0.6019493      0.3780247
## 5           6              0.5949542      0.3830297
## 6         6.5              0.5859572      0.3900367
## 7           7              0.5869582      0.3950417
## 8         7.5              0.5759502      0.4000378
## 9           8              0.5809492      0.4090408
## 10        8.5              0.5909532      0.4190448
## 11          9              0.5779492      0.4220448
## 12        9.5              0.5819502      0.4260458
## 13         10              0.5849502      0.4290458
## 14       10.5              0.5689642      0.4290518
## 15         11              0.5679542      0.4360498
## 16       11.5              0.5729532      0.4410488
## 17         12              0.5709482      0.4430478
```

ii. Over- and undersampling

If the Learner (`makeLearner()`) supports neither observation nor class weights the proportions of the classes in the training data can be changed by over- or undersampling.

In the GermanCredit data set (`caret::GermanCredit()`) the positive class Bad should receive a theoretical weight of `w = (1 - th)/th = 5`. This can be achieved by oversampling class Bad with a `rate` of 5 or by undersampling class Good with a `rate` of 1/5 (using functions `oversample()` or undersample (`undersample()`).

```
credit.task.over = oversample(credit.task, rate = w, cl = "Bad")
lrn = makeLearner("classif.multinom", trace = FALSE)
mod = train(lrn, credit.task.over)
pred = predict(mod, task = credit.task)
performance(pred, measures = list(credit.costs, mmce))
## credit.costs         mmce
##        0.457        0.325
```

Note that in the above example the learner was trained on the oversampled task `credit.task.over`. In order to get the training performance on the original task predictions were calculated for `credit.task`.

We usually prefer resampled performance values, but simply calling `resample()` on the oversampled task does not work since predictions have to be based on the original task. The solution is to create a wrapped Learner (`makeLearner()`) via function `makeUndersampleWrapper()`. Internally, `oversample()` is called before training, but predictions are done on the original data.

```
lrn = makeLearner("classif.multinom", trace = FALSE)
lrn = makeOversampleWrapper(lrn, osw.rate = w, osw.cl = "Bad")
lrn
## Learner classif.multinom.oversampled from package mlr,nnet
## Type: classif
## Name: ; Short name:
## Class: OversampleWrapper
## Properties: numerics,factors,weights,prob,twoclass,multiclass
## Predict-Type: response
## Hyperparameters: trace=FALSE,osw.rate=5,osw.cl=Bad
r = resample(lrn, credit.task, rin, measures = list(credit.costs, mmce), show.info = FALSE)
r
## Resample Result
## Task: GermanCredit
## Learner: classif.multinom.oversampled
## Aggr perf: credit.costs.test.mean=0.6019253,mmce.test.mean=0.3580287
## Runtime: 0.542073
```

Of course, we can also tune the oversampling rate. For this purpose we again have to create an OversampleWrapper (`makeUndersampleWrapper()`). Optimal values for parameter `osw.rate` can be obtained using function `tuneParams()`.

```
lrn = makeLearner("classif.multinom", trace = FALSE)
lrn = makeOversampleWrapper(lrn, osw.cl = "Bad")
ps = makeParamSet(makeDiscreteParam("osw.rate", seq(3, 7, 0.25)))
ctrl = makeTuneControlGrid()
tune.res = tuneParams(lrn, credit.task, rin, par.set = ps, measures = list(credit.costs, mmce),
  control = ctrl, show.info = FALSE)
tune.res
## Tune result:
## Op. pars: osw.rate=5.75
## credit.costs.test.mean=0.5829512,mmce.test.mean=0.3710267
```

3.9.0.3 Multi-class problems

We consider the waveform `mlbench::mlbench.waveform()` data set from package `mlbench::mlbench()` and add an artificial cost matrix:

true/pred.	1	2	3
1	0	30	80
2	5	0	4
3	10	8	0

We start by creating the `Task()`, the cost matrix and the corresponding performance measure.

```
### Task
df = mlbench::mlbench.waveform(500)
wf.task = makeClassifTask(id = "waveform", data = as.data.frame(df), target = "classes")

### Cost matrix
costs = matrix(c(0, 5, 10, 30, 0, 8, 80, 4, 0), 3)
colnames(costs) = rownames(costs) = getTaskClassLevels(wf.task)

### Performance measure
wf.costs = makeCostMeasure(id = "wf.costs", name = "Waveform costs", costs = costs,
  best = 0, worst = 10)
```

In the multi-class case, both, *thresholding* and *rebalancing* correspond to cost matrices of a certain structure where $c(k, l) = c(l)$ for k, $l = 1, \ldots, K$, $k \neq l$. This condition means that the cost of misclassifying an observation is independent of the predicted class label (see Domingos, 1999). Given a cost matrix of this type, theoretical thresholds and weights can be derived in a similar manner as in the binary case. Obviously, the cost matrix given above does not have this special structure.

3.9.0.3.1 1. Thresholding

Given a vector of positive threshold values as long as the number of classes K, the predicted probabilities for all classes are adjusted by dividing them by the corresponding threshold value. Then the class with the highest adjusted probability is predicted. This way, as in the binary case, classes with a low threshold are preferred to classes with a larger threshold.

Again this can be done by function `setThreshold()` as shown in the following example (or alternatively by the `predict.threshold` option of `makeLearner()`). Note that the threshold vector needs to have names that correspond to the class labels.

```
lrn = makeLearner("classif.rpart", predict.type = "prob")
rin = makeResampleInstance("CV", iters = 3, task = wf.task)
r = resample(lrn, wf.task, rin, measures = list(wf.costs, mmce), show.info = FALSE)
r
## Resample Result
## Task: waveform
## Learner: classif.rpart
## Aggr perf: wf.costs.test.mean=6.9600678,mmce.test.mean=0.2739822
## Runtime: 0.0676339
### Calculate thresholds as 1/(average costs of true classes)
th = 2/rowSums(costs)
names(th) = getTaskClassLevels(wf.task)
th
##          1          2          3
## 0.01818182 0.22222222 0.11111111
pred.th = setThreshold(r$pred, threshold = th)
```

```
performance(pred.th, measures = list(wf.costs, mmce))
##  wf.costs      mmce
## 5.1930837 0.3059904
```

The threshold vector `th` in the above example is chosen according to the average costs of the true classes 55, 4.5 and 9. More exactly, `th` corresponds to an artificial cost matrix of the structure mentioned above with off-diagonal elements $c(2,1) = c(3,1) = 55$, $c(1,2) = c(3,2) = 4.5$ and $c(1,3) = c(2,3) = 9$. This threshold vector may be not optimal but leads to smaller total costs on the data set than the default.

ii. Empirical thresholding

As in the binary case it is possible to tune the threshold vector using function `tuneThreshold()`. Since the scaling of the threshold vector does not change the predicted class labels `tuneThreshold()` returns threshold values that lie in [0,1] and sum to unity.

```
tune.res = tuneThreshold(pred = r$pred, measure = wf.costs)
tune.res
## $th
##          1          2          3
## 0.03321301 0.33816618 0.62862081
##
## $perf
## [1] 4.255333
```

For comparison we show the standardized version of the theoretically motivated threshold vector chosen above.

```
th/sum(th)
##          1          2          3
## 0.05172414 0.63218391 0.31609195
```

3.9.0.3.2 2. Rebalancing

i. Weighting

In the multi-class case you have to pass a vector of weights as long as the number of classes K to function `makeWeightedClassesWrapper()`. The weight vector can be tuned using function `tuneParams()`.

```
lrn = makeLearner("classif.multinom", trace = FALSE)
lrn = makeWeightedClassesWrapper(lrn)

ps = makeParamSet(makeNumericVectorParam("wcw.weight", len = 3, lower = 0, upper = 1))
ctrl = makeTuneControlRandom()

tune.res = tuneParams(lrn, wf.task, resampling = rin, par.set = ps,
  measures = list(wf.costs, mmce), control = ctrl, show.info = FALSE)
tune.res
## Tune result:
## Op. pars: wcw.weight=0.426,0.215,...
## wf.costs.test.mean=3.3868167,mmce.test.mean=0.1999735
```

3.9.1 Example-dependent misclassification costs

In case of example-dependent costs we have to create a special `Task()` via function `makeCostSensTask()`. For this purpose the feature values x and an $n \times K$ `cost` matrix that contains the cost vectors for all n examples in the data set are required.

We use the iris (`datasets::iris()`) data and generate an artificial cost matrix (see Beygelzimer et al., 2005).

```
df = iris
cost = matrix(runif(150 * 3, 0, 2000), 150) * (1 - diag(3))[df$Species,] + runif(150, 0, 10)
colnames(cost) = levels(iris$Species)
rownames(cost) = rownames(iris)
df$Species = NULL

costsens.task = makeCostSensTask(id = "iris", data = df, cost = cost)
costsens.task
## Supervised task: iris
## Type: costsens
## Observations: 150
## Features:
##    numerics     factors     ordered functionals
##           4           0           0           0
## Missings: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
## Classes: 3
## setosa, versicolor, virginica
```

`mlr` provides several wrappers to turn regular classification or regression methods into Learner (`makeLearner()`)s that can deal with example-dependent costs.

- `makeCostSensClassifWrapper()` (wraps a classification Learner (`makeLearner()`)): This is a naive approach where the costs are coerced into class labels by choosing the class label with minimum cost for each example. Then a regular classification method is used.
- `makeCostSensRegrWrapper()` (wraps a regression Learner (`makeLearner()`)): An individual regression model is fitted for the costs of each class. In the prediction step first the costs are predicted for all classes and then the class with the lowest predicted costs is selected.
- `makeCostSensWeightedPairsWrapper()` (wraps a classification Learner (`makeLearner()`)): This is also known as *cost-sensitive one-vs-one* (CS-OVO) and the most sophisticated of the currently supported methods. For each pair of classes, a binary classifier is fitted. For each observation the class label is defined as the element of the pair with minimal costs. During fitting, the observations are weighted with the absolute difference in costs. Prediction is performed by simple voting.

In the following example we use the third method. We create the wrapped Learner (`makeLearner()`) and train it on the `CostSensTask(Task())` defined above.

```
lrn = makeLearner("classif.multinom", trace = FALSE)
lrn = makeCostSensWeightedPairsWrapper(lrn)
lrn
## Learner costsens.classif.multinom from package nnet
## Type: costsens
## Name: ; Short name:
## Class: CostSensWeightedPairsWrapper
## Properties: twoclass,multiclass,numerics,factors
## Predict-Type: response
## Hyperparameters: trace=FALSE
mod = train(lrn, costsens.task)
mod
## Model for learner.id=costsens.classif.multinom; learner.class=CostSensWeightedPairsWrapper
## Trained on: task.id = iris; obs = 150; features = 4
## Hyperparameters: trace=FALSE
```

The models corresponding to the individual pairs can be accessed by function `getLearnerModel()`.

```
getLearnerModel(mod)
## [[1]]
## Model for learner.id=classif.multinom; learner.class=classif.multinom
## Trained on: task.id = feats; obs = 150; features = 4
## Hyperparameters: trace=FALSE
##
## [[2]]
## Model for learner.id=classif.multinom; learner.class=classif.multinom
## Trained on: task.id = feats; obs = 150; features = 4
## Hyperparameters: trace=FALSE
##
## [[3]]
## Model for learner.id=classif.multinom; learner.class=classif.multinom
## Trained on: task.id = feats; obs = 150; features = 4
## Hyperparameters: trace=FALSE
```

`mlr` provides some performance measures for example-specific cost-sensitive classification. In the following example we calculate the mean costs of the predicted class labels (meancosts) and the misclassification penalty (mcp). The latter measure is the average difference between the costs caused by the predicted class labels, i.e., meancosts, and the costs resulting from choosing the class with lowest cost for each observation. In order to compute these measures the costs for the test observations are required and therefore the `Task()` has to be passed to `performance()`.

```
pred = predict(mod, task = costsens.task)
pred
## Prediction: 150 observations
## predict.type: response
## threshold:
## time: 0.19
##   id response
## 1  1   setosa
## 2  2   setosa
## 3  3   setosa
## 4  4   setosa
## 5  5   setosa
## 6  6   setosa
## ... (#rows: 150, #cols: 2)
performance(pred, measures = list(meancosts, mcp), task = costsens.task)
## meancosts       mcp
##  110.2515  105.3210
```

3.10 Imbalanced Classification Problems

In case of *binary classification* strongly imbalanced classes often lead to unsatisfactory results regarding the prediction of new observations, especially for the small class. In this context *imbalanced classes* simply means that the number of observations of one class (usu. positive or majority class) by far exceeds the number of observations of the other class (usu. negative or minority class). This setting can be observed fairly often in practice and in various disciplines like credit scoring, fraud detection, medical diagnostics or churn management.

Most classification methods work best when the number of observations per class are roughly equal. The problem with *imbalanced classes* is that because of the dominance of the majority class classifiers tend to ignore cases of the minority class as noise and therefore predict the majority class far more often. In order

to lay more weight on the cases of the minority class, there are numerous correction methods which tackle the *imbalanced classification problem*. These methods can generally be divided into *cost- and sampling-based approaches*. Below all methods supported by `mlr` are introduced.

3.10.1 Sampling-based approaches

The basic idea of *sampling methods* is to simply adjust the proportion of the classes in order to increase the weight of the minority class observations within the model.

The *sampling-based approaches* can be divided further into three different categories:

1. **Undersampling methods**: Elimination of randomly chosen cases of the majority class to decrease their effect on the classifier. All cases of the minority class are kept.
2. **Oversampling methods**: Generation of additional cases (copies, artificial observations) of the minority class to increase their effect on the classifier. All cases of the majority class are kept.
3. **Hybrid methods**: Mixture of under- and oversampling strategies.

All these methods directly access the underlying data and "rearrange" it. In this way the sampling is done as part of the *preprocesssing* and can therefore be combined with every appropriate classifier.

`mlr` currently supports the first two approaches.

3.10.1.1 (Simple) over- and undersampling

As mentioned above *undersampling* always refers to the majority class, while *oversampling* affects the minority class. By the use of *undersampling*, randomly chosen observations of the majority class are eliminated. Through (simple) *oversampling* all observations of the minority class are considered at least once when fitting the model. In addition, exact copies of minority class cases are created by random sampling with repetitions.

First, let's take a look at the effect for a classification task. Based on a simulated `ClassifTask` (`Task()`) with imbalanced classes two new tasks (`task.over`, `task.under`) are created via `mlr` functions `oversample()` and `undersample()`, respectively.

```
data.imbal.train = rbind(
  data.frame(x = rnorm(100, mean = 1), class = "A"),
  data.frame(x = rnorm(5000, mean = 2), class = "B")
)
task = makeClassifTask(data = data.imbal.train, target = "class")
task.over = oversample(task, rate = 8)
task.under = undersample(task, rate = 1/8)

table(getTaskTargets(task))
##
##    A    B
##  100 5000
table(getTaskTargets(task.over))
##
##    A    B
##  800 5000
table(getTaskTargets(task.under))
##
##   A   B
## 100 625
```

Please note that the *undersampling rate* has to be between 0 and 1, where 1 means no undersampling and 0.5 implies a reduction of the majority class size to 50 percent. Correspondingly, the *oversampling rate* must be greater or equal to 1, where 1 means no oversampling and 2 would result in doubling the minority class size.

As a result the performance should improve if the model is applied to new data.

```
lrn = makeLearner("classif.rpart", predict.type = "prob")
mod = train(lrn, task)
mod.over = train(lrn, task.over)
mod.under = train(lrn, task.under)
data.imbal.test = rbind(
  data.frame(x = rnorm(10, mean = 1), class = "A"),
  data.frame(x = rnorm(500, mean = 2), class = "B")
)

performance(predict(mod, newdata = data.imbal.test), measures = list(mmce, ber, auc))
##       mmce        ber        auc
## 0.01960784 0.50000000 0.50000000
performance(predict(mod.over, newdata = data.imbal.test), measures = list(mmce, ber, auc))
##      mmce       ber       auc
## 0.0254902 0.4540000 0.7318000
performance(predict(mod.under, newdata = data.imbal.test), measures = list(mmce, ber, auc))
##       mmce        ber        auc
## 0.06470588 0.52300000 0.63370000
```

In this case the *performance measure* has to be considered very carefully. As the *misclassification rate* (mmce) evaluates the overall accuracy of the predictions, the *balanced error rate* (ber) and *area under the ROC Curve* (auc) might be more suitable here, as the misclassifications within each class are separately taken into account.

3.10.1.2 Over- and undersampling wrappers

Alternatively, `mlr` also offers the integration of over- and undersampling via a wrapper approach. This way over- and undersampling can be applied to already existing learners to extend their functionality.

The example given above is repeated once again, but this time with extended learners instead of modified tasks (see `makeOversampleWrapper()` and `makeUndersampleWrapper()`). Just like before the *undersampling rate* has to be between 0 and 1, while the *oversampling rate* has a lower boundary of 1.

```
lrn.over = makeOversampleWrapper(lrn, osw.rate = 8)
lrn.under = makeUndersampleWrapper(lrn, usw.rate = 1/8)
mod = train(lrn, task)
mod.over = train(lrn.over, task)
mod.under = train(lrn.under, task)

performance(predict(mod, newdata = data.imbal.test), measures = list(mmce, ber, auc))
##       mmce        ber        auc
## 0.01960784 0.50000000 0.50000000
performance(predict(mod.over, newdata = data.imbal.test), measures = list(mmce, ber, auc))
##       mmce        ber        auc
## 0.02745098 0.50400000 0.72770000
performance(predict(mod.under, newdata = data.imbal.test), measures = list(mmce, ber, auc))
##      mmce       ber       auc
## 0.0372549 0.5090000 0.6998000
```

3.10.1.3 Extensions to oversampling

Two extensions to (simple) oversampling are available in `mlr`.

3.10.1.3.1 1. SMOTE (Synthetic Minority Oversampling Technique)

As the duplicating of the minority class observations can lead to overfitting, within *SMOTE* the "new cases" are constructed in a different way. For each new observation, one randomly chosen minority class observation as well as one of its *randomly chosen next neighbours* are interpolated, so that finally a new *artificial observation* of the minority class is created. The `smote()` function in `mlr` handles numeric as well as factor features, as the gower distance is used for nearest neighbour calculation. The factor level of the new artificial case is sampled from the given levels of the two input observations.

Analogous to oversampling, *SMOTE preprocessing* is possible via modification of the task.

```
task.smote = smote(task, rate = 8, nn = 5)
table(getTaskTargets(task))
##
##    A    B
##  100 5000
table(getTaskTargets(task.smote))
##
##    A    B
##  800 5000
```

Alternatively, a new wrapped learner can be created via `makeSMOTEWrapper()`.

```
lrn.smote = makeSMOTEWrapper(lrn, sw.rate = 8, sw.nn = 5)
mod.smote = train(lrn.smote, task)
performance(predict(mod.smote, newdata = data.imbal.test), measures = list(mmce, ber, auc))
##       mmce        ber        auc
## 0.03921569 0.51000000 0.72130000
```

By default the number of nearest neighbours considered within the algorithm is set to 5.

3.10.1.3.2 2. Overbagging

Another extension of oversampling consists in the combination of sampling with the bagging approach. For each iteration of the bagging process, minority class observations are oversampled with a given rate in `obw.rate`. The majority class cases can either all be taken into account for each iteration (`obw.maxcl = "all"`) or bootstrapped with replacement to increase variability between training data sets during iterations (`obw.maxcl = "boot"`).

The construction of the **Overbagging Wrapper** works similar to `makeBaggingWrapper()`. First an existing `mlr` learner has to be passed to `makeOverBaggingWrapper()`. The number of iterations or fitted models can be set via `obw.iters`.

```
lrn = makeLearner("classif.rpart", predict.type = "response")
obw.lrn = makeOverBaggingWrapper(lrn, obw.rate = 8, obw.iters = 3)
```

For *binary classification* the prediction is based on majority voting to create a discrete label. Corresponding probabilities are predicted by considering the proportions of all the predicted labels. Please note that the benefit of the sampling process is *highly dependent* on the specific learner as shown in the following example.

First, let's take a look at the tree learner with and without overbagging:

```
lrn = setPredictType(lrn, "prob")
rdesc = makeResampleDesc("CV", iters = 5)
r1 = resample(learner = lrn, task = task, resampling = rdesc, show.info = FALSE,
  measures = list(mmce, ber, auc))
```

```
r1$aggr
## mmce.test.mean  ber.test.mean  auc.test.mean
##     0.01960784     0.50000000     0.50000000
obw.lrn = setPredictType(obw.lrn, "prob")
r2 = resample(learner = obw.lrn, task = task, resampling = rdesc, show.info = FALSE,
  measures = list(mmce, ber, auc))
r2$aggr
## mmce.test.mean  ber.test.mean  auc.test.mean
##     0.03431373     0.45843465     0.55686887
```

Now let's consider a *random forest* as initial learner:

```
lrn = makeLearner("classif.randomForest")
obw.lrn = makeOverBaggingWrapper(lrn, obw.rate = 8, obw.iters = 3)

lrn = setPredictType(lrn, "prob")
r1 = resample(learner = lrn, task = task, resampling = rdesc, show.info = FALSE,
  measures = list(mmce, ber, auc))
r1$aggr
## mmce.test.mean  ber.test.mean  auc.test.mean
##     0.03470588     0.45728728     0.63109296
obw.lrn = setPredictType(obw.lrn, "prob")
r2 = resample(learner = obw.lrn, task = task, resampling = rdesc, show.info = FALSE,
  measures = list(mmce, ber, auc))
r2$aggr
## mmce.test.mean  ber.test.mean  auc.test.mean
##     0.03803922     0.41623270     0.59567669
```

While *overbagging* slighty improves the performance of the *decision tree*, the auc decreases in the second example when additional overbagging is applied. As the *random forest* itself is already a strong learner (and a bagged one as well), a further bagging step isn't very helpful here and usually won't improve the model.

3.10.2 Cost-based approaches

In contrast to sampling, *cost-based approaches* usually require particular learners, which can deal with different *class-dependent costs* Cost-Sensitive Classification.

3.10.2.1 Weighted classes wrapper

Another approach independent of the underlying classifier is to assign the costs as *class weights*, so that each observation receives a weight, depending on the class it belongs to. Similar to the sampling-based approaches, the effect of the minority class observations is thereby increased simply by a higher weight of these instances and vice versa for majority class observations.

In this way every learner which supports weights can be extended through the wrapper approach. If the learner does not have a direct parameter for class weights, but supports observation weights, the weights depending on the class are internally set in the wrapper.

```
lrn = makeLearner("classif.logreg")
wcw.lrn = makeWeightedClassesWrapper(lrn, wcw.weight = 0.01)
```

For binary classification, the single number passed to the classifier corresponds to the weight of the positive / majority class, while the negative / minority class receives a weight of 1. So actually, no real costs are used within this approach, but the cost ratio is taken into account.

If the underlying learner already has a parameter for class weighting (e.g., `class.weights` in `"classif.ksvm"`), the `wcw.weight` is basically passed to the specific class weighting parameter.

```
lrn = makeLearner("classif.ksvm")
wcw.lrn = makeWeightedClassesWrapper(lrn, wcw.weight = 0.01)
```

3.11 ROC Analysis and Performance Curves

For binary scoring classifiers a *threshold* (or *cutoff*) value controls how predicted posterior probabilities are converted into class labels. ROC curves and other performance plots serve to visualize and analyse the relationship between one or two performance measures and the threshold.

This page is mainly devoted to *receiver operating characteristic* (ROC) curves that plot the *true positive rate* (sensitivity) on the vertical axis against the *false positive rate* (1 - specificity, fall-out) on the horizontal axis for all possible threshold values. Creating other performance plots like *lift charts* or *precision/recall graphs* works analogously and is shown briefly.

In addition to performance visualization ROC curves are helpful in

- determining an optimal decision threshold for given class prior probabilities and misclassification costs (for alternatives see also the pages about cost-sensitive classification and imbalanced classification problems in this tutorial),
- identifying regions where one classifier outperforms another and building suitable multi-classifier systems,
- obtaining calibrated estimates of the posterior probabilities.

For more information see the tutorials and introductory papers by Fawcett (2004), Fawcett (2006) as well as Flach (ICML 2004).

In many applications as, e.g., diagnostic tests or spam detection, there is uncertainty about the class priors or the misclassification costs at the time of prediction, for example because it's hard to quantify the costs or because costs and class priors vary over time. Under these circumstances the classifier is expected to work well for a whole range of decision thresholds and the area under the ROC curve (AUC) provides a scalar performance measure for comparing and selecting classifiers. `mlr` provides the AUC for binary classification (auc) and also several generalizations of the AUC to the multi-class case (e.g., multiclass.au1p, multiclass.au1u based on Ferri et al. (2009)).

`mlr` offers three ways to plot ROC and other performance curves.

1. Function `plotROCCurves()` can, based on the output of `generateThreshVsPerfData()`, plot performance curves for any pair of performance measures available in `mlr`.
2. `mlr` offers an interface to package `ROCR` through function `asROCRPrediction()`.
3. `mlr`'s function `plotViperCharts()` provides an interface to ViperCharts.

With `mlr` version 2.8 functions `generateROCRCurvesData`, `plotROCRCurves`, and `plotROCRCurvesGGVIS` were deprecated.

Below are some examples that demonstrate the three possible ways. Note that you can only use learners that are capable of predicting probabilities. Have a look at the learner table in the Appendix or run `listLearners("classif", properties = c("twoclass", "prob"))` to get a list of all learners that support this.

3.11.1 Performance plots with plotROCCurves

As you might recall `generateThreshVsPerfData()` calculates one or several performance measures for a sequence of decision thresholds from 0 to 1. It provides S3 methods for objects of class `Prediction()`, `ResampleResult()` and `BenchmarkResult()` (resulting from `predict` (`predict.WrappedModel()`),

`resample()` or `benchmark()`). `plotROCCurves()` plots the result of `generateThreshVsPerfData()` using ggplot2.

3.11.1.1 Example 1: Single predictions

We consider the `Sonar` (`mlbench::Sonar()`) data set from package `mlbench`, which poses a binary classification problem (`sonar.task()`) and apply linear discriminant analysis (`MASS::lda()`).

```
n = getTaskSize(sonar.task)
train.set = sample(n, size = round(2/3 * n))
test.set = setdiff(seq_len(n), train.set)

lrn1 = makeLearner("classif.lda", predict.type = "prob")
mod1 = train(lrn1, sonar.task, subset = train.set)
pred1 = predict(mod1, task = sonar.task, subset = test.set)
```

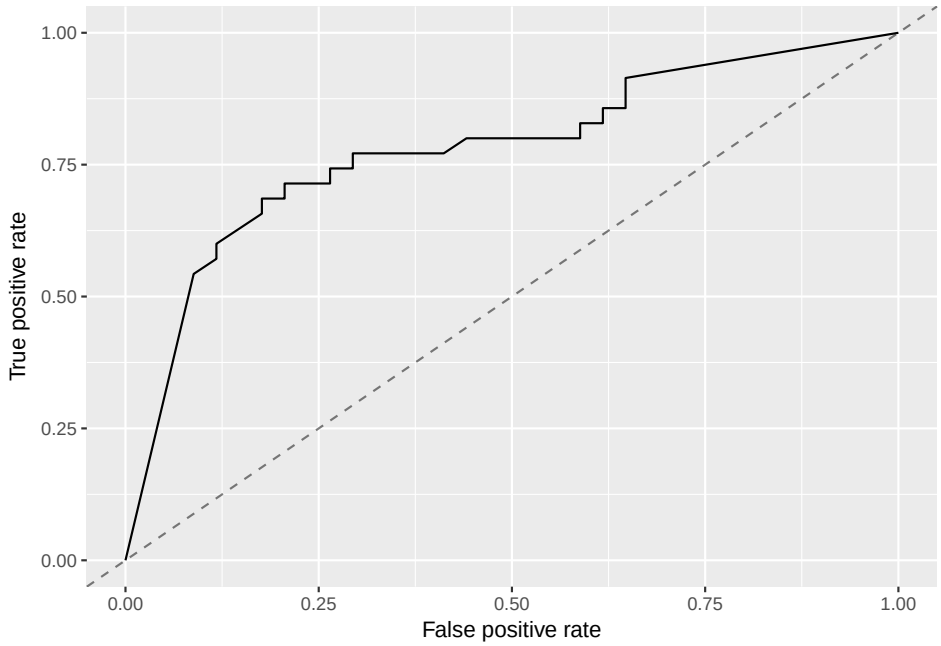
Since we want to plot ROC curves we calculate the false and true positive rates (fpr and tpr). Additionally, we also compute error rates (mmce).

```
df = generateThreshVsPerfData(pred1, measures = list(fpr, tpr, mmce))
```

`generateThreshVsPerfData()` returns an object of class `ThreshVsPerfData` (`generateThreshVsPerfData()`) which contains the performance values in the `$data` element.

Per default, `plotROCCurves()` plots the performance values of the first two measures passed to `generateThreshVsPerfData()`. The first is shown on the x-axis, the second on the y-axis. Moreover, a diagonal line that represents the performance of a random classifier is added. You can remove the diagonal by setting `diagonal = FALSE`.

```
plotROCCurves(df)
```

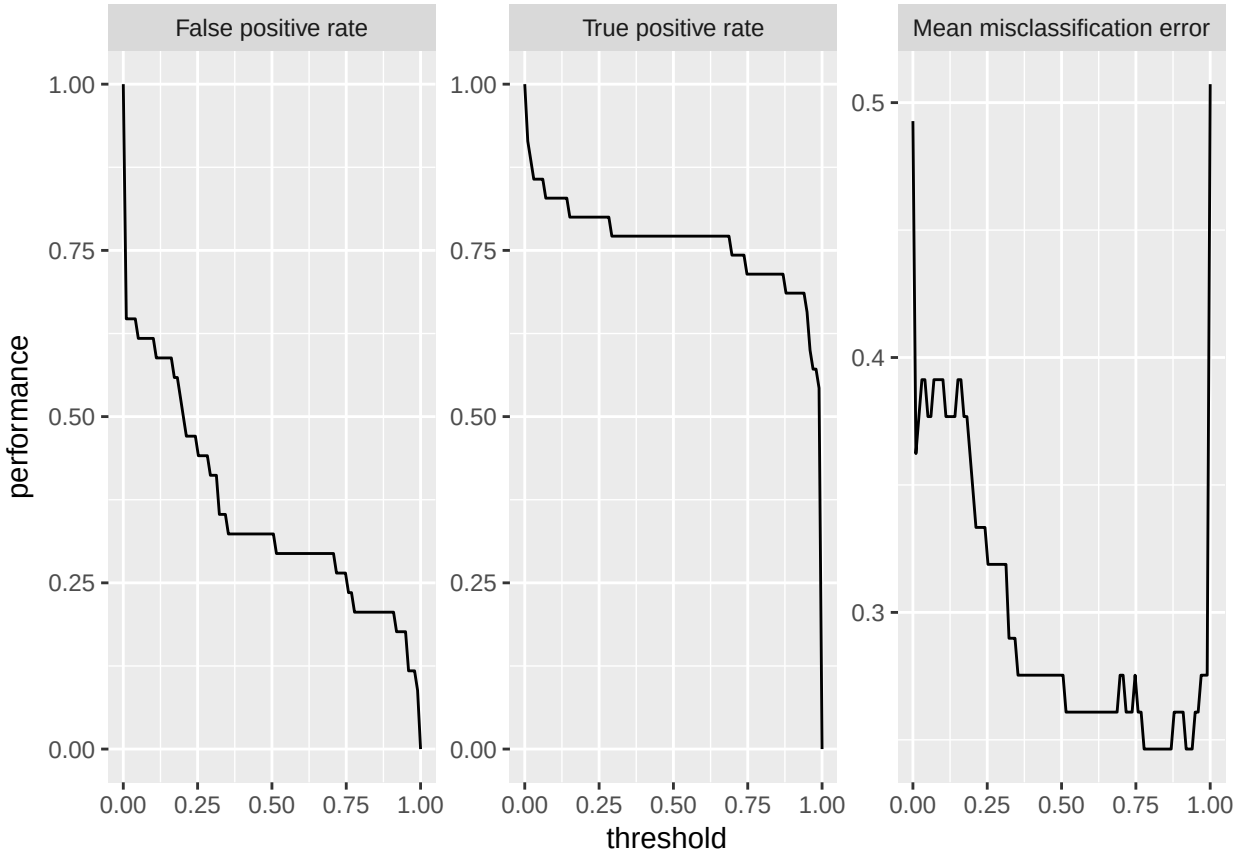


The corresponding area under curve (auc) can be calculated as usual by calling `performance()`.

```
performance(pred1, auc)
##       auc
## 0.7789916
```

`plotROCCurves()` always requires a pair of performance measures that are plotted against each other. If you want to plot individual measures versus the decision threshold you can use function `plotThreshVsPerf()`.

```
plotThreshVsPerf(df)
```

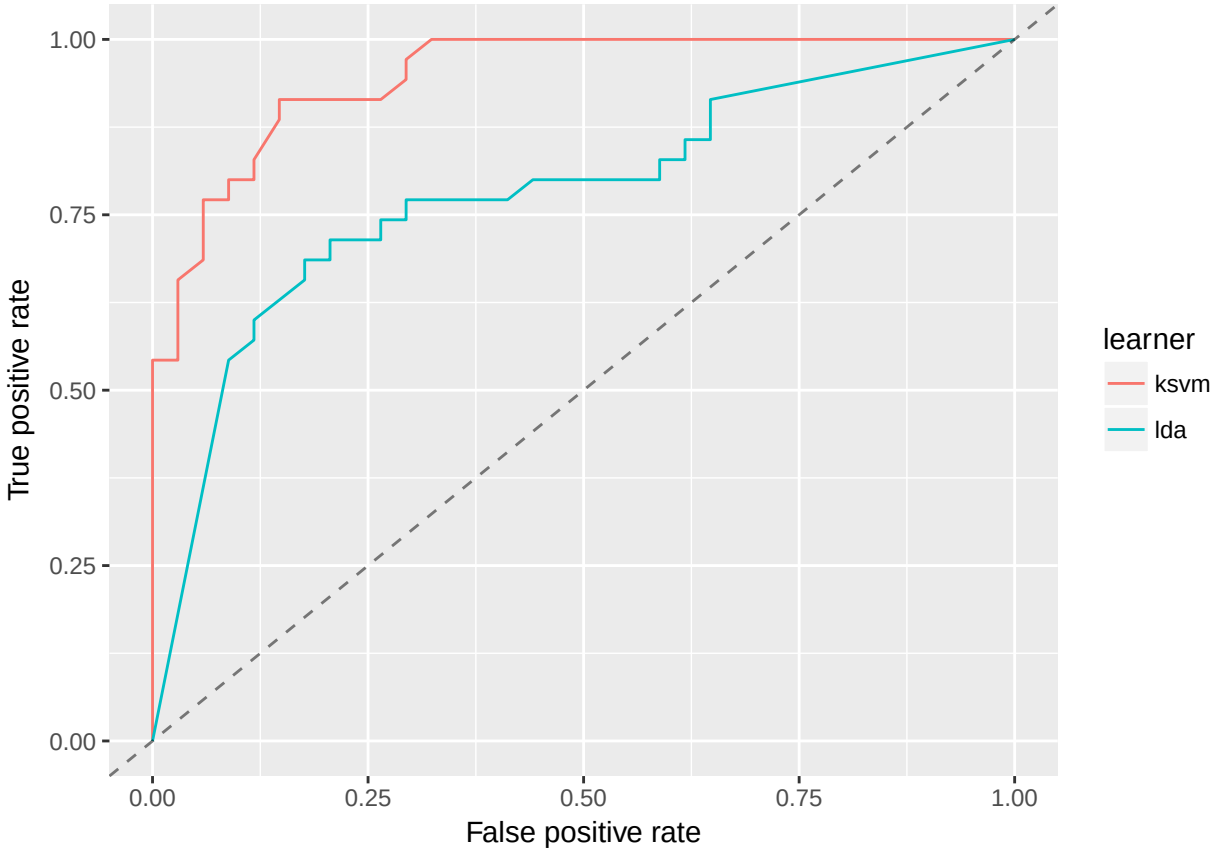


Additional to linear discriminant analysis (`MASS::lda()`) we try a support vector machine with RBF kernel (`kernlab::ksvm()`).

```
lrn2 = makeLearner("classif.ksvm", predict.type = "prob")
mod2 = train(lrn2, sonar.task, subset = train.set)
pred2 = predict(mod2, task = sonar.task, subset = test.set)
```

In order to compare the performance of the two learners you might want to display the two corresponding ROC curves in one plot. For this purpose just pass a named `list` of `Prediction()`s to `generateThreshVsPerfData()`.

```
df = generateThreshVsPerfData(list(lda = pred1, ksvm = pred2), measures = list(fpr, tpr))
plotROCCurves(df)
```

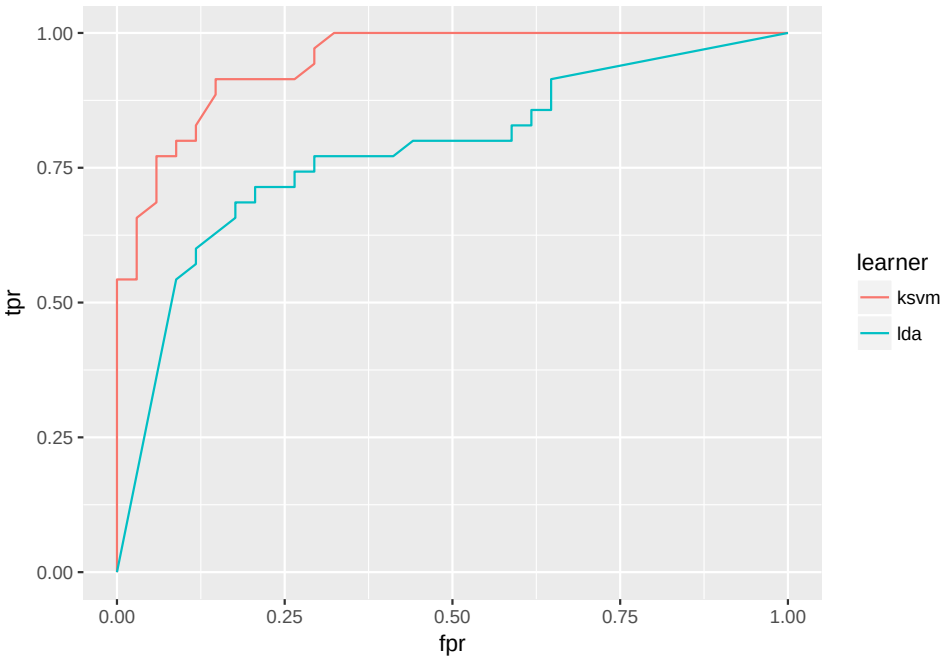


It's clear from the plot above that `kernlab::ksvm()` has a slightly higher AUC than lda (`MASS::lda()`).

```
performance(pred2, auc)
##       auc
## 0.9478992
```

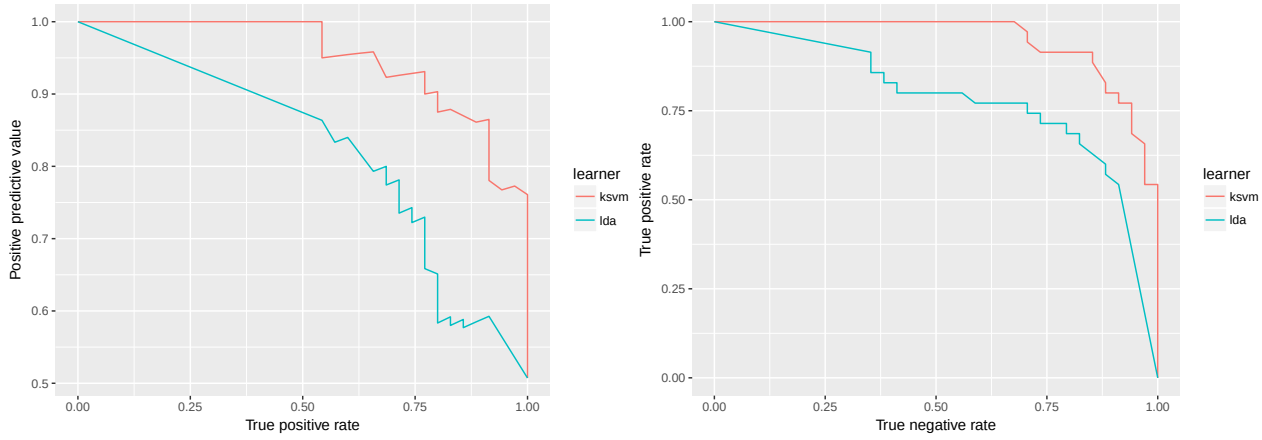
Based on the `$data` member of `df` you can easily generate custom plots. Below the curves for the two learners are superposed.

```
qplot(x = fpr, y = tpr, color = learner, data = df$data, geom = "path")
```



It is easily possible to generate other performance plots by passing the appropriate performance measures to `generateThreshVsPerfData()` and `plotROCCurves()`. Below, we generate a *precision/recall graph* (precision = positive predictive value = ppv, recall = tpr) and a *sensitivity/specificity plot* (sensitivity = tpr, specificity = tnr).

```
df = generateThreshVsPerfData(list(lda = pred1, ksvm = pred2), measures = list(ppv, tpr, tnr))

### Precision/recall graph
plotROCCurves(df, measures = list(tpr, ppv), diagonal = FALSE)

### Sensitivity/specificity plot
plotROCCurves(df, measures = list(tnr, tpr), diagonal = FALSE)
```



3.11.1.2 Example 2: Benchmark experiment

The analysis in the example above can be improved a little. Instead of writing individual code for training/prediction of each learner, which can become tedious very quickly, we can use function `benchmark()` (see also Benchmark Experiments) and, ideally, the support vector machine should have been tuned.

We again consider the `Sonar` (`mlbench::Sonar()`) data set and apply `MASS::lda()` as well as `kernlab::ksvm()`. We first generate a tuning wrapper (`makeTuneWrapper()`) for `kernlab::ksvm()`. The cost parameter is tuned on a (for demonstration purposes small) parameter grid. We assume that we are interested in a good performance over the complete threshold range and therefore tune with regard to the auc. The error rate (mmce) for a threshold value of 0.5 is reported as well.

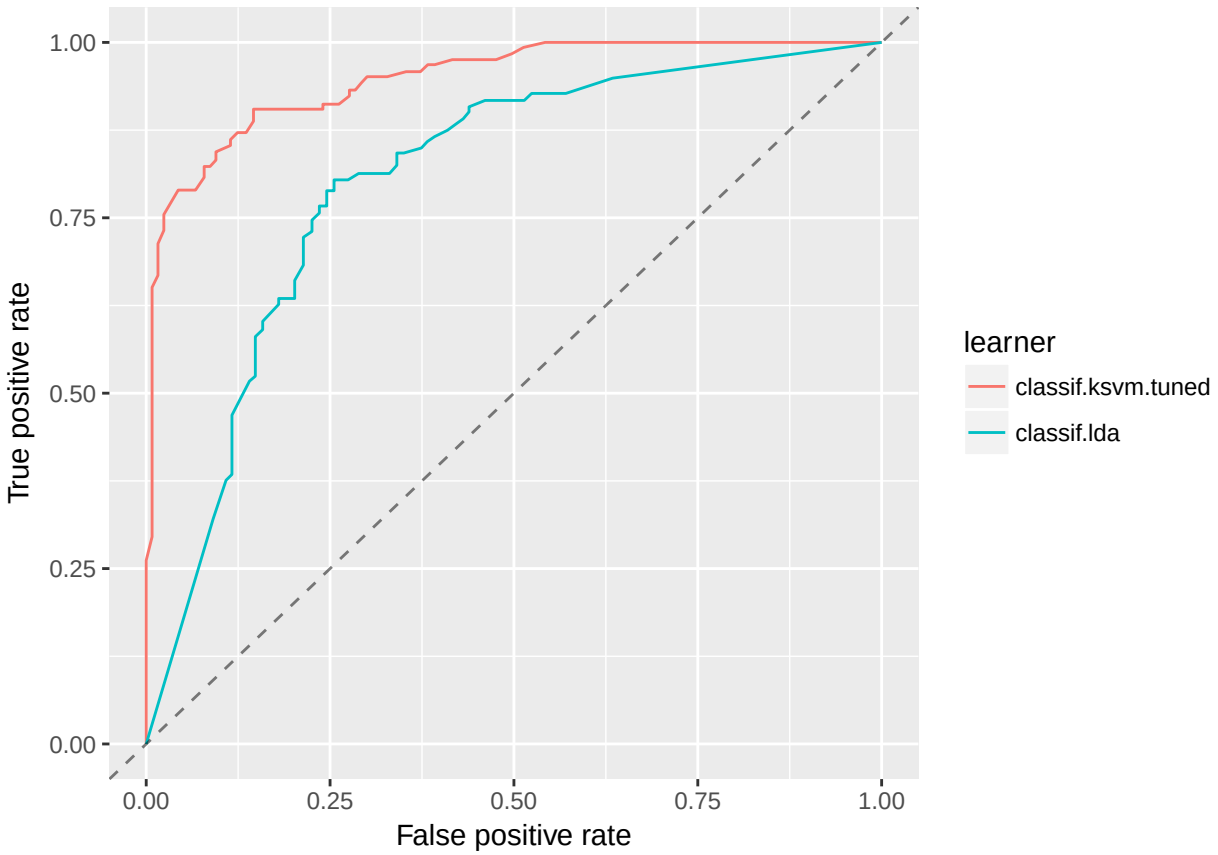
```
### Tune wrapper for ksvm
rdesc.inner = makeResampleDesc("Holdout")
ms = list(auc, mmce)
ps = makeParamSet(
  makeDiscreteParam("C", 2^(-1:1))
)
ctrl = makeTuneControlGrid()
lrn2 = makeTuneWrapper(lrn2, rdesc.inner, ms, ps, ctrl, show.info = FALSE)
```

Below the actual benchmark experiment is conducted. As resampling strategy we use 5-fold cross-validation and again calculate the auc as well as the error rate (for a threshold/cutoff value of 0.5).

```
### Benchmark experiment
lrns = list(lrn1, lrn2)
rdesc.outer = makeResampleDesc("CV", iters = 5)

bmr = benchmark(lrns, tasks = sonar.task, resampling = rdesc.outer, measures = ms, show.info = FALSE)
bmr
##         task.id         learner.id auc.test.mean mmce.test.mean
## 1 Sonar-example        classif.lda     0.8130728      0.2354239
## 2 Sonar-example classif.ksvm.tuned     0.9538634      0.1298490
```

Calling `generateThreshVsPerfData()` and `plotROCCurves()` on the benchmark result (`BenchmarkResult()`) produces a plot with ROC curves for all learners in the experiment.

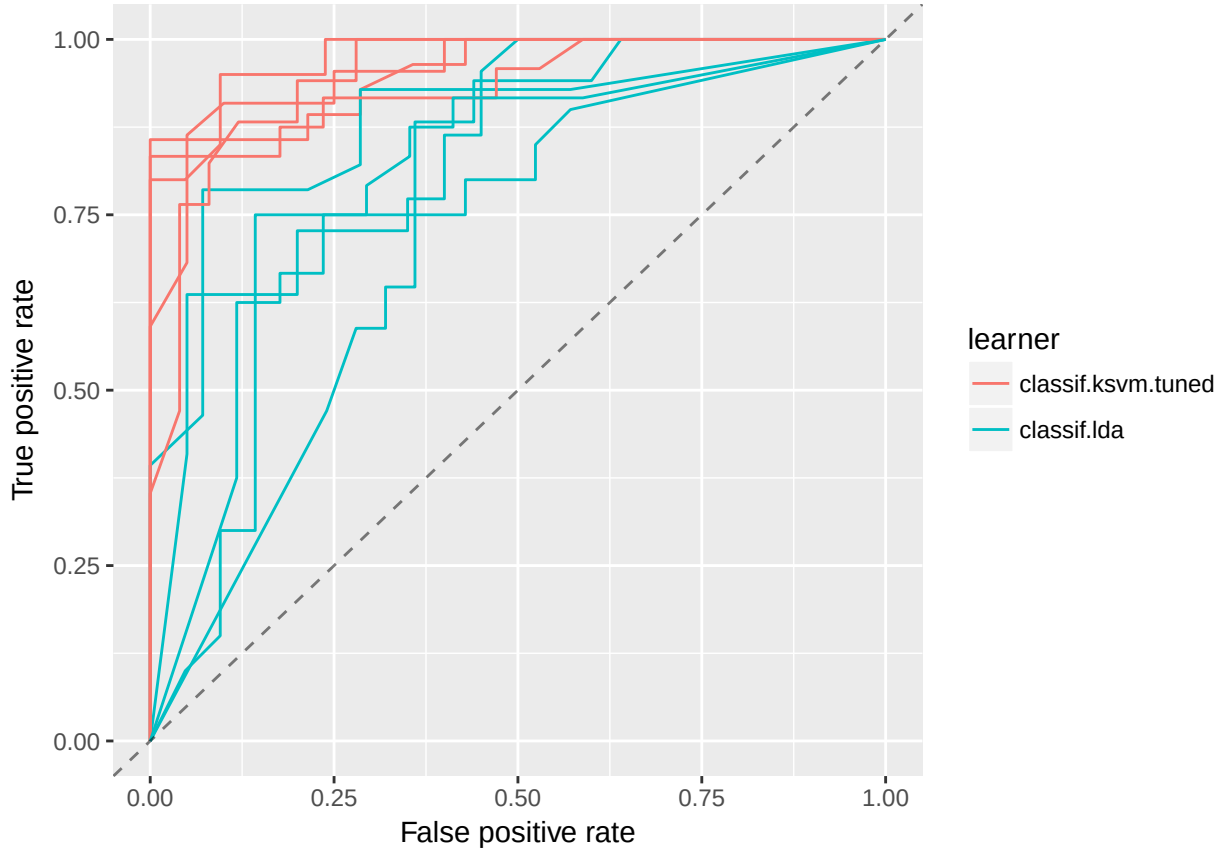
```
df = generateThreshVsPerfData(bmr, measures = list(fpr, tpr, mmce))
plotROCCurves(df)
```



Per default, `generateThreshVsPerfData()` calculates aggregated performances according to the chosen resampling strategy (5-fold cross-validation) and aggregation scheme (`test.mean` (`aggregations()`)) for each threshold in the sequence. This way we get *threshold-averaged* ROC curves.

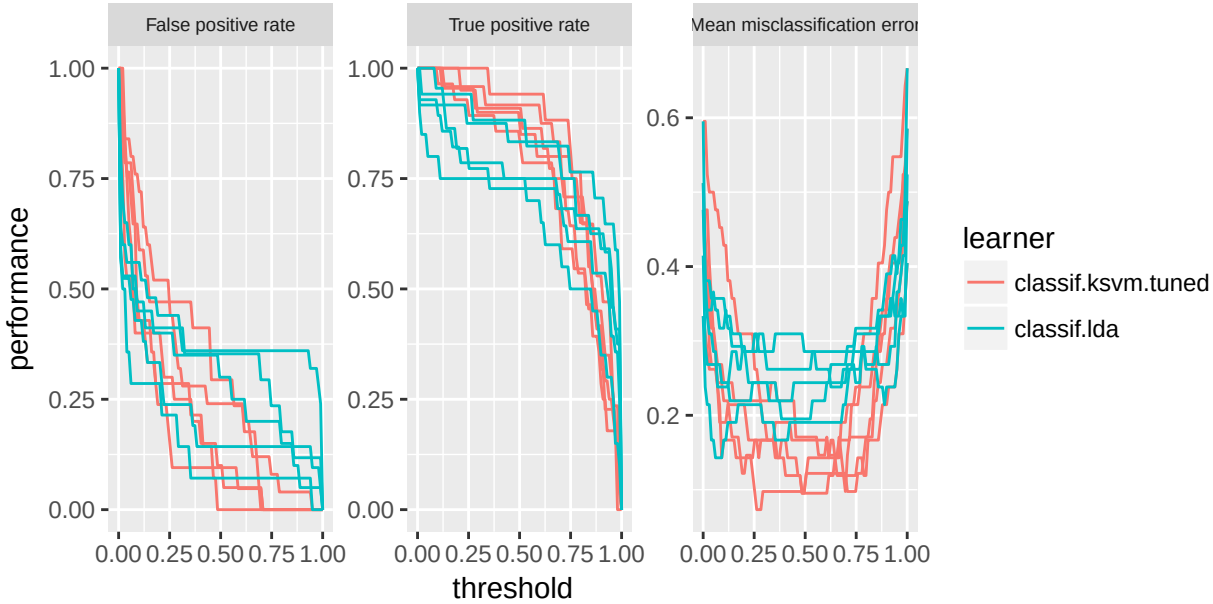
If you want to plot the individual ROC curves for each resample iteration set `aggregate = FALSE`.

```
df = generateThreshVsPerfData(bmr, measures = list(fpr, tpr, mmce), aggregate = FALSE)
plotROCCurves(df)
```



The same applies for `plotThreshVsPerf()`.

```
plotThreshVsPerf(df) +
  theme(strip.text.x = element_text(size = 7))
```

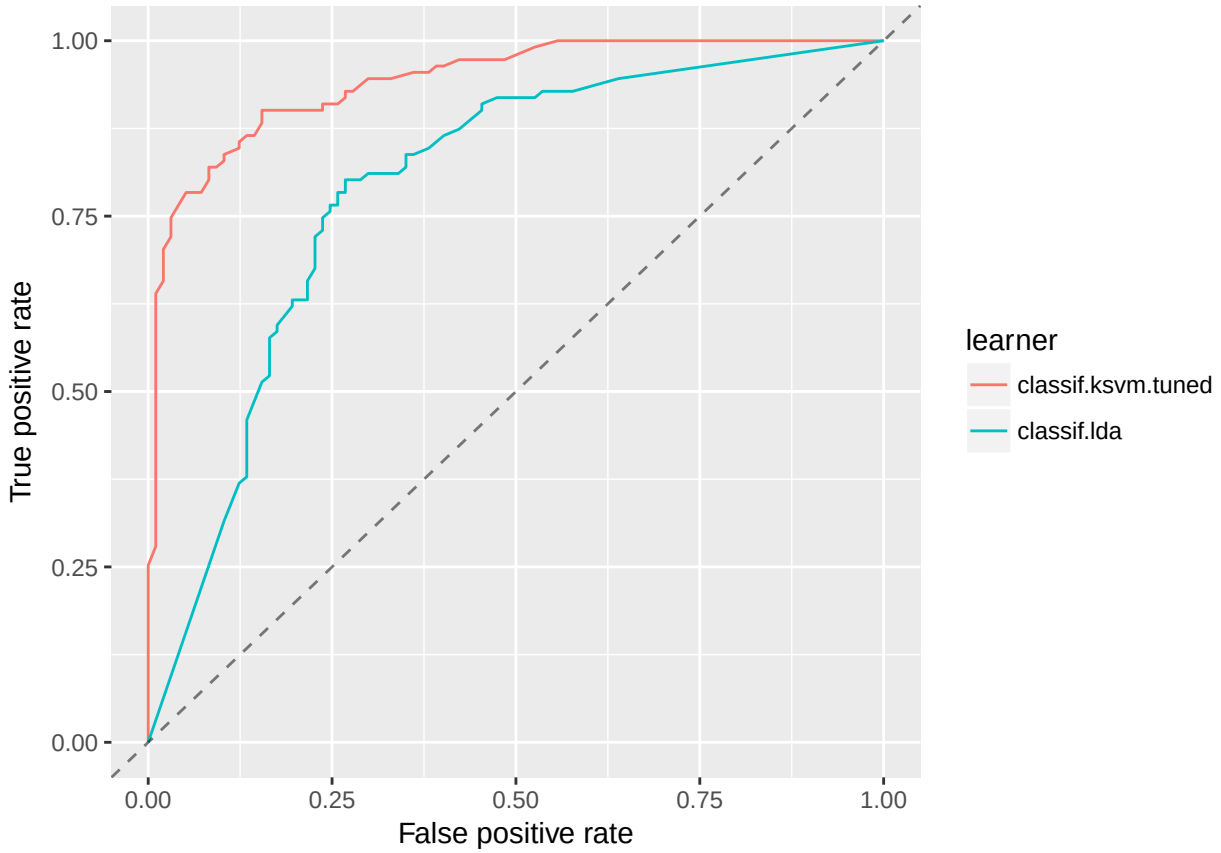


An alternative to averaging is to just merge the 5 test folds and draw a single ROC curve. Merging can be achieved by manually changing the class attribute of the prediction objects from `ResamplePrediction()` to `Prediction()`.

Below, the predictions are extracted from the `BenchmarkResult()` via function `getBMRPredictions()`, the class is changed and the ROC curves are created.

Averaging methods are normally preferred (cp. Fawcett, 2006), as they permit to assess the variability, which is needed to properly compare classifier performance.

```
### Extract predictions
preds = getBMRPredictions(bmr, drop = TRUE)

### Change the class attribute
preds2 = lapply(preds, function(x) {class(x) = "Prediction"; return(x)})

### Draw ROC curves
df = generateThreshVsPerfData(preds2, measures = list(fpr, tpr, mmce))
plotROCCurves(df)
```



Again, you can easily create other standard evaluation plots by passing the appropriate performance measures to `generateThreshVsPerfData()` and `plotROCCurves()`.

3.11.2 Performance plots with asROCRPrediction

Drawing performance plots with package `ROCR` works through three basic commands:

1. `ROCR::prediction()`: Create a `ROCR` prediction object.
2. `ROCR::performance()`: Calculate one or more performance measures for the given prediction object.
3. `ROCR::plot()`: Generate the performance plot.

`mlr`'s function `asROCRPrediction()` converts an `mlr Prediction()` object to a `ROCR` prediction

(ROCR::prediction-class()) object, so you can easily generate performance plots by doing steps 2. and 3. yourself. ROCR's plot (ROCR::plot-methods()) method has some nice features which are not (yet) available in plotROCCurves(), for example plotting the convex hull of the ROC curves. Some examples are shown below.

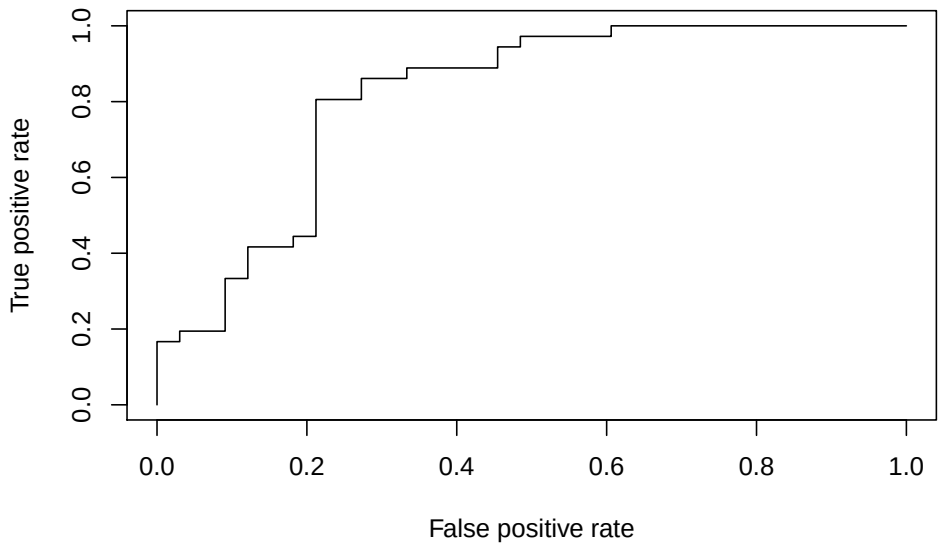
3.11.2.1 Example 1: Single predictions (continued)

We go back to out first example where we trained and predicted MASS::lda() on the sonar classification task (sonar.task()).

```
n = getTaskSize(sonar.task)
train.set = sample(n, size = round(2/3 * n))
test.set = setdiff(seq_len(n), train.set)

### Train and predict linear discriminant analysis
lrn1 = makeLearner("classif.lda", predict.type = "prob")
mod1 = train(lrn1, sonar.task, subset = train.set)
pred1 = predict(mod1, task = sonar.task, subset = test.set)
```

Below we use asROCRPrediction() to convert the lda prediction, let ROCR calculate the true and false positive rate and plot the ROC curve.

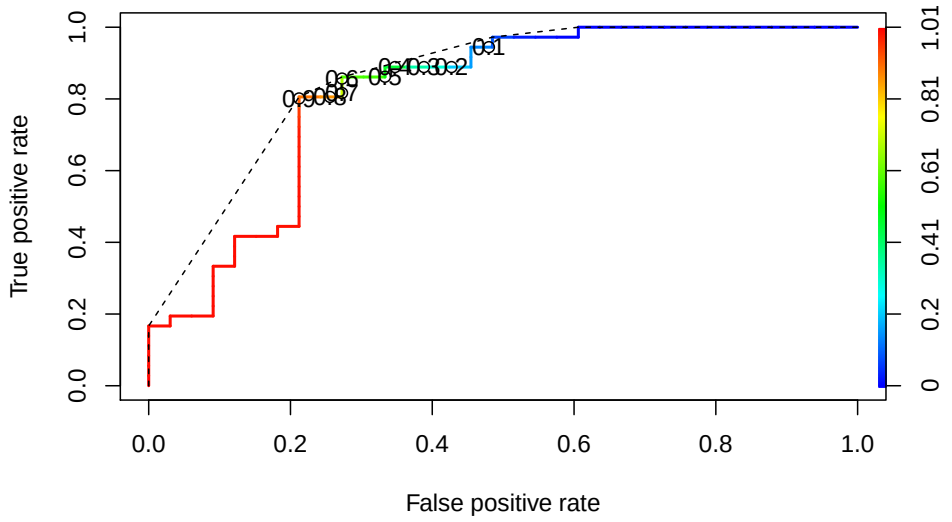
```
### Convert prediction
ROCRpred1 = asROCRPrediction(pred1)

### Calculate true and false positive rate
ROCRperf1 = ROCR::performance(ROCRpred1, "tpr", "fpr")

### Draw ROC curve
ROCR::plot(ROCRperf1)
```



Below is the same ROC curve, but we make use of some more graphical parameters: The ROC curve is color-coded by the threshold and selected threshold values are printed on the curve. Additionally, the convex hull (black broken line) of the ROC curve is drawn.

```
### Draw ROC curve
ROCR::plot(ROCRperf1, colorize = TRUE, print.cutoffs.at = seq(0.1, 0.9, 0.1), lwd = 2)
```

```
### Draw convex hull of ROC curve
ch = ROCR::performance(ROCRpred1, "rch")
ROCR::plot(ch, add = TRUE, lty = 2)
```



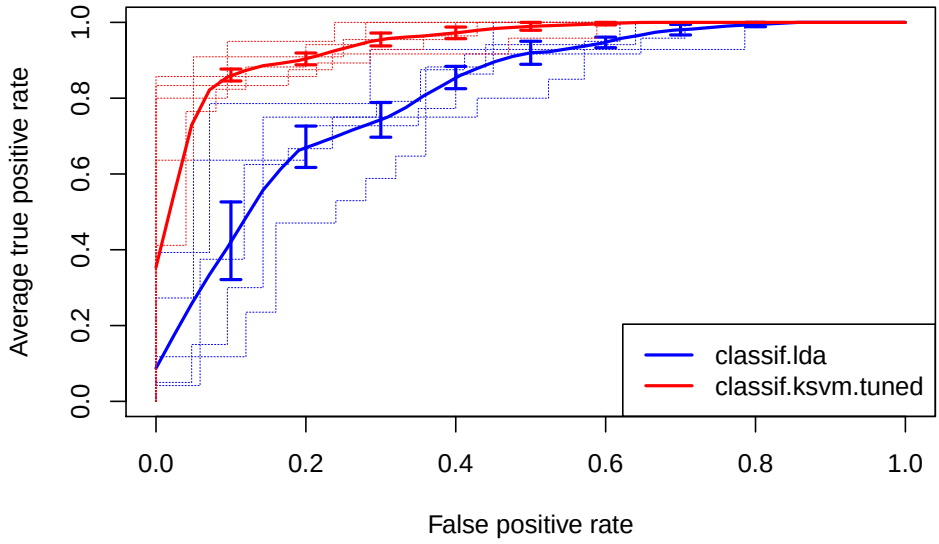
3.11.2.2 Example 2: Benchmark experiments (continued)

We again consider the benchmark experiment conducted earlier. We first extract the predictions by `getBMRPredictions()` and then convert them via function `asROCRPrediction()`.

```
### Extract predictions
preds = getBMRPredictions(bmr, drop = TRUE)

### Convert predictions
ROCRpreds = lapply(preds, asROCRPrediction)

### Calculate true and false positive rate
ROCRperfs = lapply(ROCRpreds, function(x) ROCR::performance(x, "tpr", "fpr"))
```

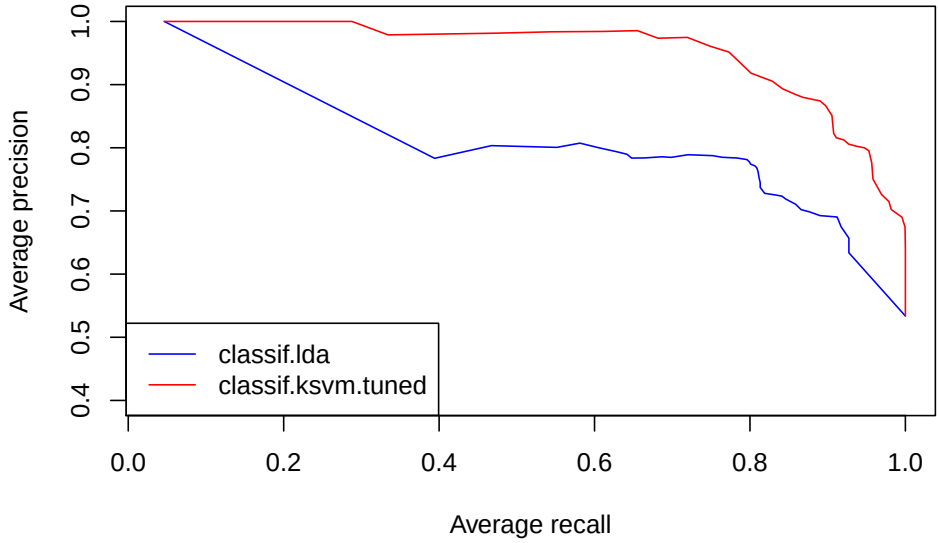
We draw the vertically averaged ROC curves (solid lines) as well as the ROC curves for the individual resampling iterations (broken lines). Moreover, standard error bars are plotted for selected true positive rates (0.1, 0.2, ..., 0.9). See `ROCR`'s plot (`ROCR::plot-methods()`) function for details.

```
### lda average ROC curve
plot(ROCRperfs[[1]], col = "blue", avg = "vertical", spread.estimate = "stderror",
  show.spread.at = seq(0.1, 0.8, 0.1), plotCI.col = "blue", plotCI.lwd = 2, lwd = 2)
### lda individual ROC curves
plot(ROCRperfs[[1]], col = "blue", lty = 2, lwd = 0.25, add = TRUE)

### ksvm average ROC curve
plot(ROCRperfs[[2]], col = "red", avg = "vertical", spread.estimate = "stderror",
  show.spread.at = seq(0.1, 0.6, 0.1), plotCI.col = "red", plotCI.lwd = 2, lwd = 2, add = TRUE)
### ksvm individual ROC curves
plot(ROCRperfs[[2]], col = "red", lty = 2, lwd = 0.25, add = TRUE)

legend("bottomright", legend = getBMRLearnerIds(bmr), lty = 1, lwd = 2, col = c("blue", "red"))
```



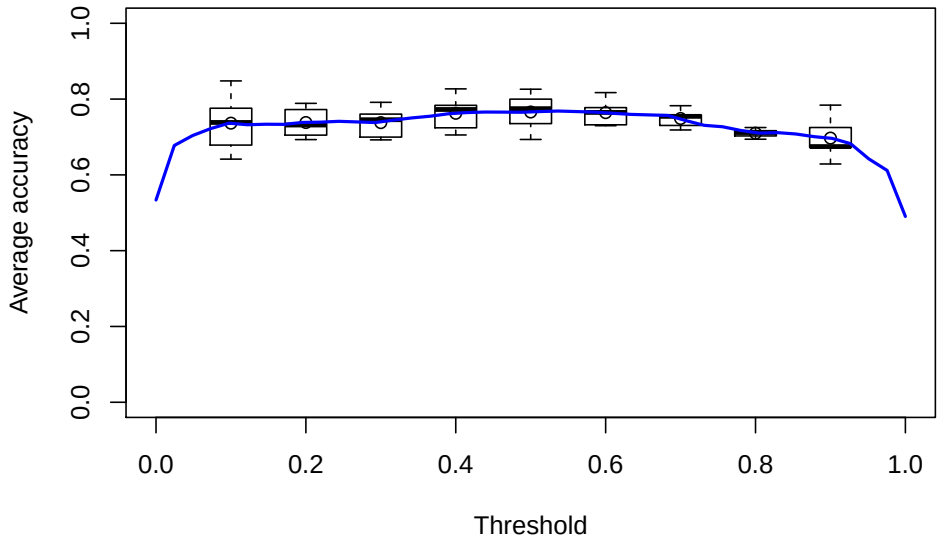
In order to create other evaluation plots like *precision/recall graphs* you just have to change the performance measures when calling `ROCR::performance()`. (Note that you have to use the measures provided by `ROCR` listed in `ROCR::performance()` and not `mlr`'s performance measures.)

```
### Extract and convert predictions
preds = getBMRPredictions(bmr, drop = TRUE)
ROCRpreds = lapply(preds, asROCRPrediction)

### Calculate precision and recall
ROCRperfs = lapply(ROCRpreds, function(x) ROCR::performance(x, "prec", "rec"))

### Draw performance plot
plot(ROCRperfs[[1]], col = "blue", avg = "threshold")
plot(ROCRperfs[[2]], col = "red", avg = "threshold", add = TRUE)
legend("bottomleft", legend = getBMRLearnerIds(bmr), lty = 1, col = c("blue", "red"))
```



If you want to plot a performance measure versus the threshold, specify only one measure when calling `ROCR::performance()`. Below the average accuracy over the 5 cross-validation iterations is plotted against the threshold. Moreover, boxplots for certain threshold values (0.1, 0.2, ..., 0.9) are drawn.

```
### Extract and convert predictions
preds = getBMRPredictions(bmr, drop = TRUE)
ROCRpreds = lapply(preds, asROCRPrediction)

### Calculate accuracy
ROCRperfs = lapply(ROCRpreds, function(x) ROCR::performance(x, "acc"))

### Plot accuracy versus threshold
plot(ROCRperfs[[1]], avg = "vertical", spread.estimate = "boxplot", lwd = 2, col = "blue",
  show.spread.at = seq(0.1, 0.9, 0.1), ylim = c(0,1), xlab = "Threshold")
```



3.11.3 Viper charts

`mlr` also supports ViperCharts for plotting ROC and other performance curves. Like `generateThreshVsPerfData()` it has S3 methods for objects of class `Prediction()`, `ResampleResult()` and `BenchmarkResult()`. Below plots for the benchmark experiment (Example 2) are generated.

```
z = plotViperCharts(bmr, chart = "rocc", browse = FALSE)
```

You can see the plot created this way here. Note that besides ROC curves you get several other plots like lift charts or cost curves. For details, see `plotViperCharts()`.

3.12 Multilabel Classification

Multilabel classification is a classification problem where multiple target labels can be assigned to each observation instead of only one like in multiclass classification.

Two different approaches exist for multilabel classification. *Problem transformation methods* try to transform the multilabel classification into binary or multiclass classification problems. *Algorithm adaptation methods* adapt multiclass algorithms so they can be applied directly to the problem.

3.12.1 Creating a task

The first thing you have to do for multilabel classification in `mlr` is to get your data in the right format. You need a `data.frame` which consists of the features and a logical vector for each label which indicates if

the label is present in the observation or not. After that you can create a `MultilabelTask` (`Task()`) like a normal `ClassifTask` (`Task()`). Instead of one target name you have to specify a vector of targets which correspond to the names of logical variables in the `data.frame`. In the following example we get the yeast data frame from the already existing `yeast.task()`, extract the 14 label names and create the task again.

```
yeast = getTaskData(yeast.task)
labels = colnames(yeast)[1:14]
yeast.task = makeMultilabelTask(id = "multi", data = yeast, target = labels)
yeast.task
## Supervised task: multi
## Type: multilabel
## Target: label1,label2,label3,label4,label5,label6,label7,label8,label9,label10,label11,label12,label1
## Observations: 2417
## Features:
##    numerics     factors     ordered functionals
##         103           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
## Classes: 14
##  label1  label2  label3  label4  label5  label6  label7  label8  label9
##     762    1038     983     862     722     597     428     480     178
## label10 label11 label12 label13 label14
##     253     289    1816    1799      34
```

3.12.2 Constructing a learner

Multilabel classification in `mlr` can currently be done in two ways:

- Algorithm adaptation methods: Treat the whole problem with a specific algorithm.
- Problem transformation methods: Transform the problem, so that simple binary classification algorithms can be applied.

3.12.2.1 Algorithm adaptation methods

Currently the available algorithm adaptation methods in **R** are the multivariate random forest in the [%randomForestSRC] package and the random ferns multilabel algorithm in the [%rFerns] package. You can create the learner for these algorithms like in multiclass classification problems.

```
lrn.rfsrc = makeLearner("multilabel.randomForestSRC")
lrn.rFerns = makeLearner("multilabel.rFerns")
lrn.rFerns
## Learner multilabel.rFerns from package rFerns
## Type: multilabel
## Name: Random ferns; Short name: rFerns
## Class: multilabel.rFerns
## Properties: numerics,factors,ordered
## Predict-Type: response
## Hyperparameters:
```

3.12.2.2 Problem transformation methods

For generating a wrapped multilabel learner first create a binary (or multiclass) classification learner with `makeLearner()`. Afterwards apply a function like `makeMultilabelBinaryRelevanceWrapper()`, `makeMultilabelClassifierChainsWrapper()`, `makeMultilabelNestedStackingWrapper()`, `makeMultilabelDBRWrapper()` or `makeMultilabelStackingWrapper()` on the learner to convert it to a learner that uses the respective problem transformation method.

You can also generate a binary relevance learner directly, as you can see in the example.

```
lrn.br = makeLearner("classif.rpart", predict.type = "prob")
lrn.br = makeMultilabelBinaryRelevanceWrapper(lrn.br)
lrn.br
## Learner multilabel.binaryRelevance.classif.rpart from package rpart
## Type: multilabel
## Name: ; Short name:
## Class: MultilabelBinaryRelevanceWrapper
## Properties: numerics,factors,ordered,missings,weights,prob,twoclass,multiclass
## Predict-Type: prob
## Hyperparameters: xval=0
lrn.br2 = makeMultilabelBinaryRelevanceWrapper("classif.rpart")
lrn.br2
## Learner multilabel.binaryRelevance.classif.rpart from package rpart
## Type: multilabel
## Name: ; Short name:
## Class: MultilabelBinaryRelevanceWrapper
## Properties: numerics,factors,ordered,missings,weights,prob,twoclass,multiclass
## Predict-Type: response
## Hyperparameters: xval=0
```

The different methods are shortly described in the following.

3.12.2.2.1 Binary relevance

This problem transformation method converts the multilabel problem to binary classification problems for each label and applies a simple binary classificator on these. In `mlr` this can be done by converting your binary learner to a wrapped binary relevance multilabel learner.

3.12.2.2.2 Classifier chains

Trains consecutively the labels with the input data. The input data in each step is augmented by the already trained labels (with the real observed values). Therefore an order of the labels has to be specified. At prediction time the labels are predicted in the same order as while training. The required labels in the input data are given by the previous done prediction of the respective label.

3.12.2.2.3 Nested stacking

Same as classifier chains, but the labels in the input data are not the real ones, but estimations of the labels obtained by the already trained learners.

3.12.2.2.4 Dependent binary relevance

Each label is trained with the real observed values of all other labels. In prediction phase for a label the other necessary labels are obtained in a previous step by a base learner like the binary relevance method.

3.12.2.2.5 Stacking

Same as the dependent binary relevance method, but in the training phase the labels used as input for each label are obtained by the binary relevance method.

3.12.3 Train

You can `train()` a model as usual with a multilabel learner and a multilabel task as input. You can also pass `subset` and `weights` arguments if the learner supports this.

```
mod = train(lrn.br, yeast.task)
mod = train(lrn.br, yeast.task, subset = 1:1500, weights = rep(1/1500, 1500))
mod
## Model for learner.id=multilabel.binaryRelevance.classif.rpart; learner.class=MultilabelBinaryRelevan
## Trained on: task.id = multi; obs = 1500; features = 103
## Hyperparameters: xval=0
mod2 = train(lrn.rfsrc, yeast.task, subset = 1:100)
mod2
## Model for learner.id=multilabel.randomForestSRC; learner.class=multilabel.randomForestSRC
## Trained on: task.id = multi; obs = 100; features = 103
## Hyperparameters: na.action=na.impute
```

3.12.4 Predict

Prediction can be done as usual in `mlr` with `predict` (`predict.WrappedModel()`) and by passing a trained model and either the task to the `task` argument or some new data to the `newdata` argument. As always you can specify a `subset` of the data which should be predicted.

```
pred = predict(mod, task = yeast.task, subset = 1:10)
pred = predict(mod, newdata = yeast[1501:1600,])
names(as.data.frame(pred))
##  [1] "truth.label1"     "truth.label2"     "truth.label3"
##  [4] "truth.label4"     "truth.label5"     "truth.label6"
##  [7] "truth.label7"     "truth.label8"     "truth.label9"
## [10] "truth.label10"    "truth.label11"    "truth.label12"
## [13] "truth.label13"    "truth.label14"    "prob.label1"
## [16] "prob.label2"      "prob.label3"      "prob.label4"
## [19] "prob.label5"      "prob.label6"      "prob.label7"
## [22] "prob.label8"      "prob.label9"      "prob.label10"
## [25] "prob.label11"     "prob.label12"     "prob.label13"
## [28] "prob.label14"     "response.label1"  "response.label2"
## [31] "response.label3"  "response.label4"  "response.label5"
## [34] "response.label6"  "response.label7"  "response.label8"
## [37] "response.label9"  "response.label10" "response.label11"
## [40] "response.label12" "response.label13" "response.label14"
pred2 = predict(mod2, task = yeast.task)
names(as.data.frame(pred2))
##  [1] "id"               "truth.label1"     "truth.label2"
##  [4] "truth.label3"     "truth.label4"     "truth.label5"
##  [7] "truth.label6"     "truth.label7"     "truth.label8"
## [10] "truth.label9"     "truth.label10"    "truth.label11"
## [13] "truth.label12"    "truth.label13"    "truth.label14"
## [16] "response.label1"  "response.label2"  "response.label3"
## [19] "response.label4"  "response.label5"  "response.label6"
```

```
## [22] "response.label7"  "response.label8"  "response.label9"
## [25] "response.label10" "response.label11" "response.label12"
## [28] "response.label13" "response.label14"
```

Depending on the chosen `predict.type` of the learner you get true and predicted values and possibly probabilities for each class label. These can be extracted by the usual accessor functions `getPredictionTruth()`, `getPredictionResponse()` and `getPredictionProbabilities()`.

3.12.5 Performance

The performance of your prediction can be assessed via function `performance()`. You can specify via the `measures` argument which measure(s) to calculate. The default measure for multilabel classification is the Hamming loss multilabel.hamloss. All available measures for multilabel classification can be shown by `listMeasures()` and found in the table of performance measures and the `?measures()` documentation page.

```
performance(pred)
## multilabel.hamloss
##          0.2257143
performance(pred2, measures = list(multilabel.subset01, multilabel.hamloss, multilabel.acc,
  multilabel.f1, timepredict))
## multilabel.subset01  multilabel.hamloss      multilabel.acc
##           0.8638808           0.2036172           0.4670494
##       multilabel.f1         timepredict
##           0.5768957           2.3520000
listMeasures("multilabel")
##  [1] "featperc"            "multilabel.tpr"      "multilabel.hamloss"
##  [4] "multilabel.subset01" "timeboth"            "timetrain"
##  [7] "timepredict"         "multilabel.ppv"      "multilabel.f1"
## [10] "multilabel.acc"
```

3.12.6 Resampling

For evaluating the overall performance of the learning algorithm you can do some resampling. As usual you have to define a resampling strategy, either via `makeResampleDesc()` or `makeResampleInstance()`. After that you can run the `resample()` function. Below the default measure Hamming loss is calculated.

```
rdesc = makeResampleDesc(method = "CV", stratify = FALSE, iters = 3)
r = resample(learner = lrn.br, task = yeast.task, resampling = rdesc, show.info = FALSE)
r
## Resample Result
## Task: multi
## Learner: multilabel.binaryRelevance.classif.rpart
## Aggr perf: multilabel.hamloss.test.mean=0.2203772
## Runtime: 6.65265
r = resample(learner = lrn.rFerns, task = yeast.task, resampling = rdesc, show.info = FALSE)
r
## Resample Result
## Task: multi
## Learner: multilabel.rFerns
## Aggr perf: multilabel.hamloss.test.mean=0.4743143
## Runtime: 0.875148
```

3.12.7 Binary performance

If you want to calculate a binary performance measure like, e.g., the accuracy, the mmce or the auc for each label, you can use function `getMultilabelBinaryPerformances()`. You can apply this function to any multilabel prediction, e.g., also on the resample multilabel prediction. For calculating the auc you need predicted probabilities.

```
getMultilabelBinaryPerformances(pred, measures = list(acc, mmce, auc))
##         acc.test.mean mmce.test.mean auc.test.mean
## label1           0.75           0.25     0.6321925
## label2           0.64           0.36     0.6547917
## label3           0.68           0.32     0.7118227
## label4           0.69           0.31     0.6764835
## label5           0.73           0.27     0.6676923
## label6           0.70           0.30     0.6417739
## label7           0.81           0.19     0.5968750
## label8           0.73           0.27     0.5164474
## label9           0.89           0.11     0.4688458
## label10          0.86           0.14     0.3996463
## label11          0.85           0.15     0.5000000
## label12          0.76           0.24     0.5330667
## label13          0.75           0.25     0.5938610
## label14          1.00           0.00            NA
getMultilabelBinaryPerformances(r$pred, measures = list(acc, mmce))
##         acc.test.mean mmce.test.mean
## label1     0.70293753      0.2970625
## label2     0.58047166      0.4195283
## label3     0.70211005      0.2978899
## label4     0.71410840      0.2858916
## label5     0.70335126      0.2966487
## label6     0.59329748      0.4067025
## label7     0.54613157      0.4538684
## label8     0.53371949      0.4662805
## label9     0.29830368      0.7016963
## label10    0.44145635      0.5585436
## label11    0.46710799      0.5328920
## label12    0.52916839      0.4708316
## label13    0.53330575      0.4666942
## label14    0.01406703      0.9859330
```

3.13 Learning Curve Analysis

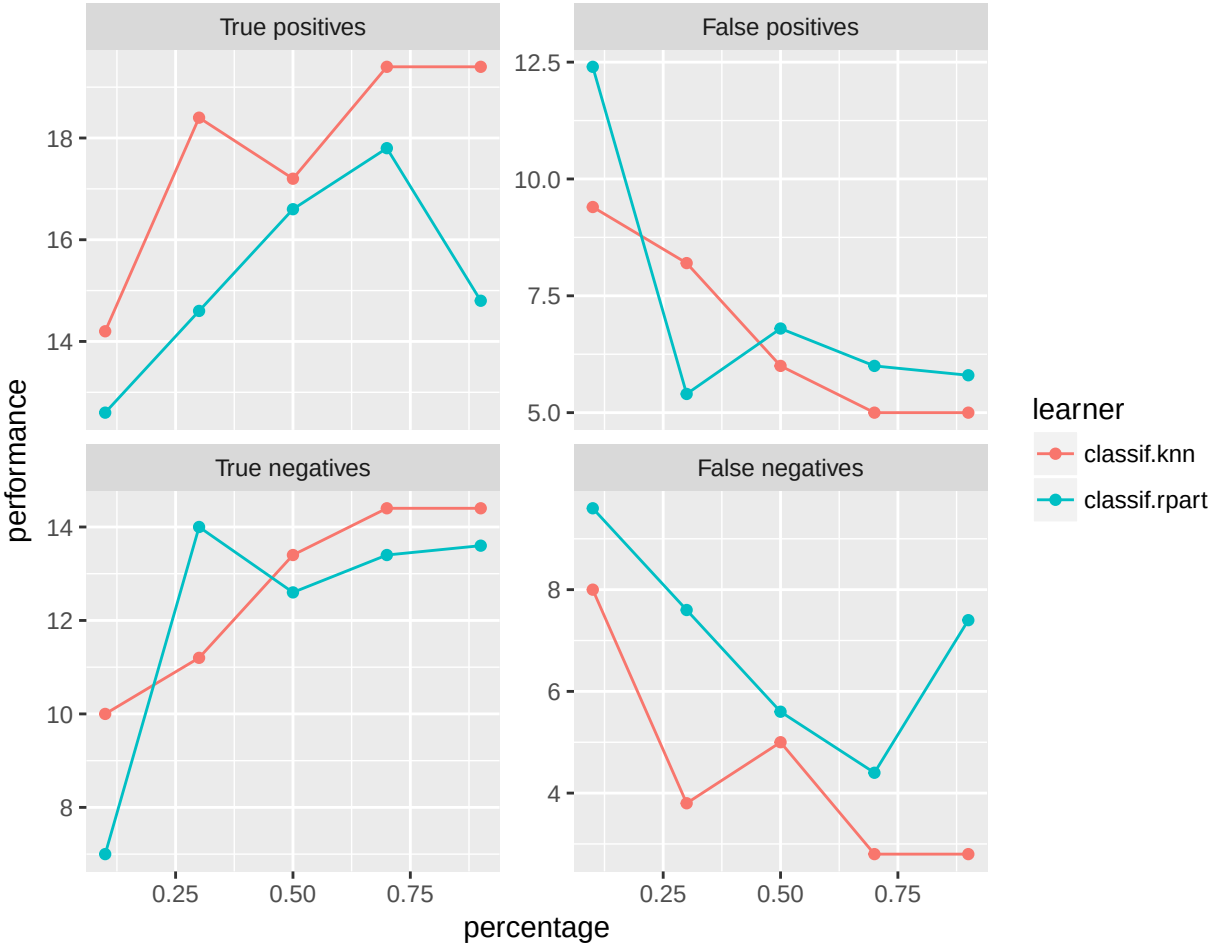
To analyze how the increase of observations in the training set improves the performance of a learner the *learning curve* is an appropriate visual tool. The experiment is conducted with an increasing subsample size and the performance is measured. In the plot the x-axis represents the relative subsample size whereas the y-axis represents the performance.

Note that this function internally uses `benchmark()` in combination with `makeDownsampleWrapper()`, so for every run new observations are drawn. Thus the results are noisy. To reduce noise increase the number of resampling iterations. You can define the resampling method in the `resampling` argument of `generateLearningCurveData()`. It is also possible to pass a ResampleInstance (`makeResampleInstance()`) (which is a result of `makeResampleInstance()`) to make resampling consistent for all passed learners and each step of increasing the number of observations.

3.13.1 Plotting the learning curve

The `mlr` function `generateLearningCurveData()` can generate the data for *learning curves* for multiple learners and multiple performance measures at once. With `plotLearningCurve()` the result of `generateLearningCurveData()` can be plotted using `ggplot2`. `plotLearningCurve()` has an argument `facet` which can be either `"measure"` or `"learner"`. By default `facet = "measure"` and facetted subplots are created for each measure input to `generateLearningCurveData()`. If `facet = "measure"` learners are mapped to color, and vice versa.

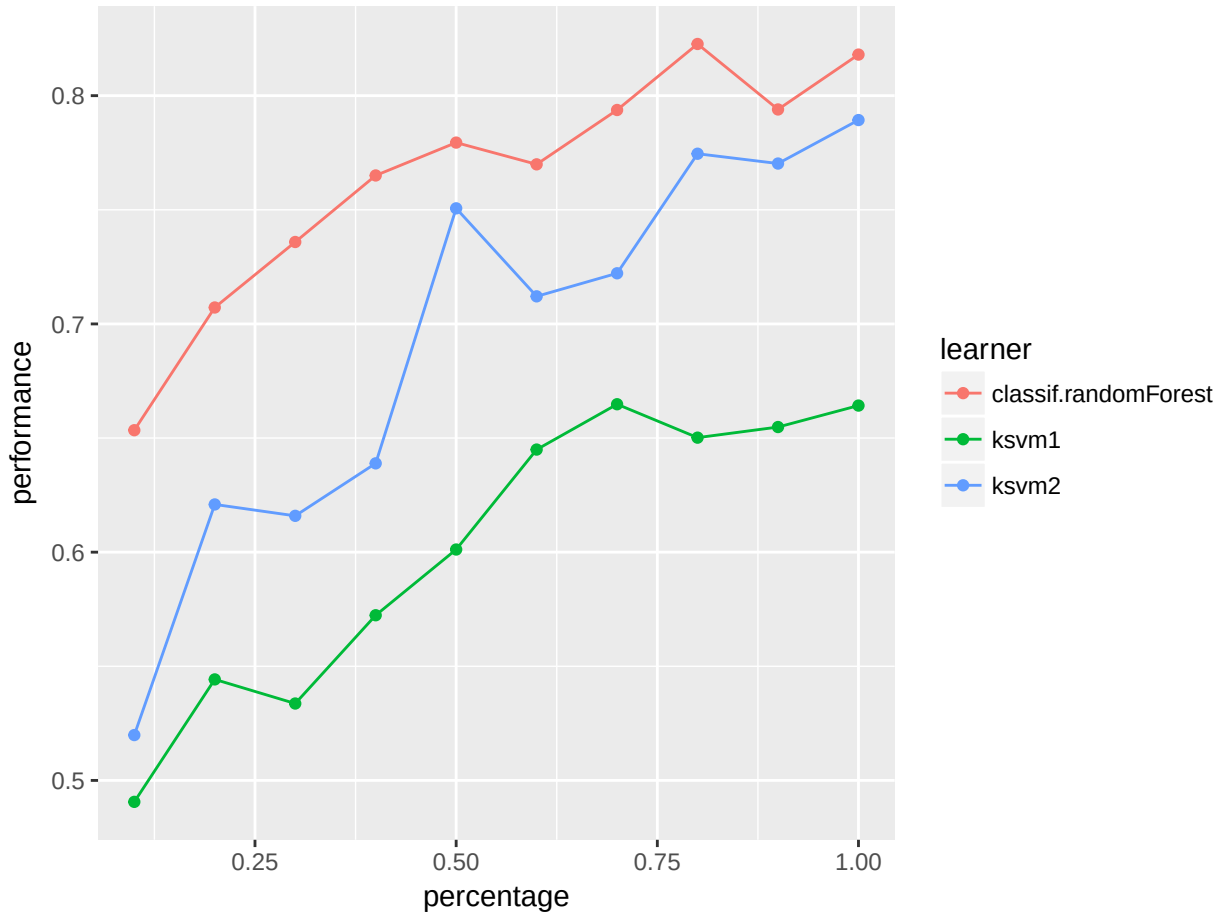
```
r = generateLearningCurveData(
  learners = c("classif.rpart", "classif.knn"),
  task = sonar.task,
  percs = seq(0.1, 1, by = 0.2),
  measures = list(tp, fp, tn, fn),
  resampling = makeResampleDesc(method = "CV", iters = 5),
  show.info = FALSE)
plotLearningCurve(r)
```



What happens in `generateLearningCurveData()` is the following: Each learner will be internally wrapped in a `DownsampleWrapper` (`makeDownsampleWrapper()`). To measure the performance at the first step of `percs`, say `0.1`, first the data will be split into a *training* and a *test set* according to the given *resampling strategy*. Then a random sample containing 10% of the observations of the *training set* will be drawn and used to train the learner. The performance will be measured on the *complete test set*. These steps will be repeated as defined by the given *resampling method* and for each value of `percs`.

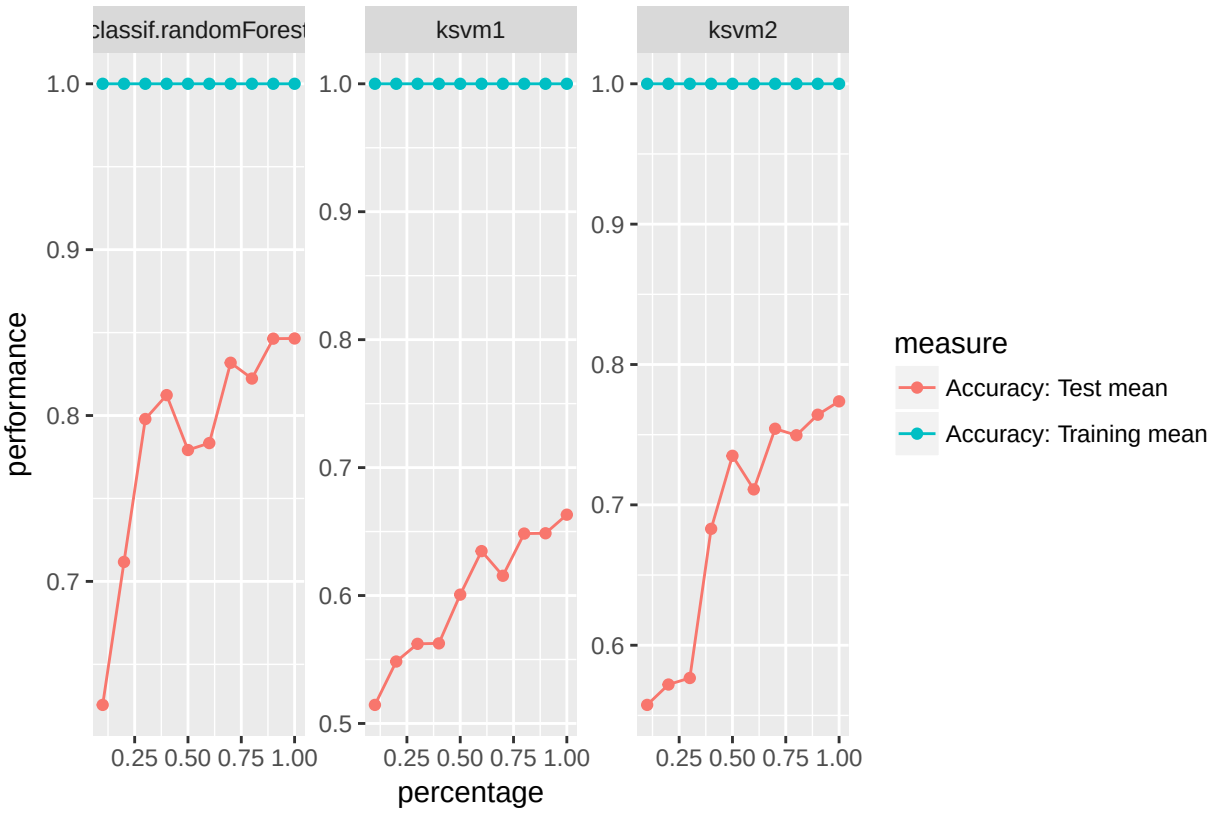
In the first example we simply passed a vector of learner names to `generateLearningCurveData()`. As usual, you can also create the learners beforehand and provide a `list` of Learner (`makeLearner()`) objects, or even pass a mixed `list` of Learner (`makeLearner()`) objects and strings. Make sure that all learners have unique `ids`.

```
lrns = list(
  makeLearner(cl = "classif.ksvm", id = "ksvm1", sigma = 0.2, C = 2),
  makeLearner(cl = "classif.ksvm", id = "ksvm2", sigma = 0.1, C = 1),
  "classif.randomForest"
)
rin = makeResampleDesc(method = "CV", iters = 5)
lc = generateLearningCurveData(learners = lrns, task = sonar.task,
  percs = seq(0.1, 1, by = 0.1), measures = acc,
  resampling = rin, show.info = FALSE)
plotLearningCurve(lc)
```



We can display performance on the train set as well as the test set:

```
rin2 = makeResampleDesc(method = "CV", iters = 5, predict = "both")
lc2 = generateLearningCurveData(learners = lrns, task = sonar.task,
  percs = seq(0.1, 1, by = 0.1),
  measures = list(acc, setAggregation(acc, train.mean)), resampling = rin2,
  show.info = FALSE)
plotLearningCurve(lc2, facet = "learner")
```



There is also an experimental `ggvis` plotting function, `plotLearningCurveGGVIS()`. Instead of the `facet` argument to `plotLearningCurve()` there is an argument `interaction` which plays a similar role. As subplots are not available in `ggvis`, measures or learners are mapped to an interactive sidebar which allows selection of the displayed measures or learners. The other feature is mapped to color.

```
plotLearningCurveGGVIS(lc2, interaction = "measure")
plotLearningCurveGGVIS(lc2, interaction = "learner")
```

3.14 Exploring Learner Predictions

Learners use features to learn a prediction function and make predictions, but the effect of those features is often not apparent. `mlr` can estimate the partial dependence of a learned function on a subset of the feature space using `generatePartialDependenceData()`.

Partial dependence plots reduce the potentially high dimensional function estimated by the learner, and display a marginalized version of this function in a lower dimensional space. For example suppose $Y = f(X) + \epsilon$, where $\mathbb{E}[\epsilon|X] = 0$. With (X, Y) pairs drawn independently from this statistical model, a learner may estimate $\hat{f}$, which, if X is high dimensional, can be uninterpretable. Suppose we want to approximate the relationship between some subset of X. We partition X into two sets, X_s and X_c such that $X = X_s \cup X_c$, where X_s is a subset of X of interest.

The partial dependence of f on X_s is

$$f_{X_s} = \mathbb{E}_{X_c} f(X_s, X_c).$$

X_c is integrated out. We use the following estimator:

$$\hat{f}_{X_s} = \frac{1}{N}\sum_{i=1}^{N}\hat{f}(X_s, x_{ic}).$$

The individual conditional expectation of an observation can also be estimated using the above algorithm absent the averaging, giving $\hat{f}^{(i)}_{X_s}$. This allows the discovery of features of $\hat{f}$ that may be obscured by an aggregated summary of $\hat{f}$.

The partial derivative of the partial dependence function, $\frac{\partial \hat{f}_{X_s}}{\partial X_s}$, and the individual conditional expectation function, $\frac{\partial \hat{f}^{(i)}_{X_s}}{\partial X_s}$, can also be computed. For regression and survival tasks the partial derivative of a single feature X_s is the gradient of the partial dependence function, and for classification tasks where the learner can output class probabilities the Jacobian. Note that if the learner produces discontinuous partial dependence (e.g., piecewise constant functions such as decision trees, ensembles of decision trees, etc.) the derivative will be 0 (where the function is not changing) or trending towards positive or negative infinity (at the discontinuities where the derivative is undefined). Plotting the partial dependence function of such learners may give the impression that the function is not discontinuous because the prediction grid is not composed of all discontinuous points in the predictor space. This results in a line interpolating that makes the function appear to be piecewise linear (where the derivative would be defined except at the boundaries of each piece).

The partial derivative can be informative regarding the additivity of the learned function in certain features. If $\hat{f}^{(i)}_{X_s}$ is an additive function in a feature X_s, then its partial derivative will not depend on any other features (X_c) that may have been used by the learner. Variation in the estimated partial derivative indicates that there is a region of interaction between X_s and X_c in $\hat{f}$. Similarly, instead of using the mean to estimate the expected value of the function at different values of X_s, instead computing the variance can highlight regions of interaction between X_s and X_c.

See Goldstein, Kapelner, Bleich, and Pitkin (2014) for more details and their package `ICEbox` for the original implementation. The algorithm works for any supervised learner with classification, regression, and survival tasks.

3.14.1 Generating partial dependences

Our implementation, following `mlr`'s visualization pattern, consists of the above mentioned function `generatePartialDependenceData()`, as well as two visualization functions, `plotPartialDependence()` and `plotPartialDependenceGGVIS()`. The former generates input (objects of class `PartialDependenceData()`) for the latter.

The first step executed by `generatePartialDependenceData()` is to generate a feature grid for every element of the character vector `features` passed. The data are given by the `input` argument, which can be a `Task()` or a `data.frame`. The feature grid can be generated in several ways. A uniformly spaced grid of length `gridsize` (default 10) from the empirical minimum to the empirical maximum is created by default, but arguments `fmin` and `fmax` may be used to override the empirical default (the lengths of `fmin` and `fmax` must match the length of `features`). Alternatively the feature data can be resampled, either by using a bootstrap or by subsampling.

```
lrn.classif = makeLearner("classif.ksvm", predict.type = "prob")
fit.classif = train(lrn.classif, iris.task)
pd = generatePartialDependenceData(fit.classif, iris.task, "Petal.Width")
pd
## PartialDependenceData
## Task: iris-example
## Features: Petal.Width
## Target: setosa, versicolor, virginica
## Derivative: FALSE
```

```
## Interaction: FALSE
## Individual: FALSE
##     Class Probability Petal.Width
## 1: setosa   0.5089315   0.1000000
## 2: setosa   0.4833071   0.3666667
## 3: setosa   0.4229569   0.6333333
## 4: setosa   0.3186628   0.9000000
## 5: setosa   0.2011831   1.1666667
## 6: setosa   0.1356411   1.4333333
## ... (#rows: 30, #cols: 3)
```

As noted above, X_s does not have to be unidimensional. If it is not, the `interaction` flag must be set to `TRUE`. Then the individual feature grids are combined using the Cartesian product, and the estimator above is applied, producing the partial dependence for every combination of unique feature values. If the `interaction` flag is `FALSE` (the default) then by default X_s is assumed unidimensional, and partial dependencies are generated for each feature separately. The resulting output when `interaction = FALSE` has a column for each feature, and `NA` where the feature was not used.

```
pd.lst = generatePartialDependenceData(fit.classif, iris.task, c("Petal.Width", "Petal.Length"), FALSE)
head(pd.lst$data)
##     Class Probability Petal.Width Petal.Length
## 1: setosa   0.5089315   0.1000000           NA
## 2: setosa   0.4833071   0.3666667           NA
## 3: setosa   0.4229569   0.6333333           NA
## 4: setosa   0.3186628   0.9000000           NA
## 5: setosa   0.2011831   1.1666667           NA
## 6: setosa   0.1356411   1.4333333           NA
tail(pd.lst$data)
##        Class Probability Petal.Width Petal.Length
## 1: virginica   0.2499415          NA     3.622222
## 2: virginica   0.3437488          NA     4.277778
## 3: virginica   0.4571984          NA     4.933333
## 4: virginica   0.6114234          NA     5.588889
## 5: virginica   0.6843610          NA     6.244444
## 6: virginica   0.6361217          NA     6.900000
pd.int = generatePartialDependenceData(fit.classif, iris.task, c("Petal.Width", "Petal.Length"), TRUE)
pd.int
## PartialDependenceData
## Task: iris-example
## Features: Petal.Width, Petal.Length
## Target: setosa, versicolor, virginica
## Derivative: FALSE
## Interaction: TRUE
## Individual: FALSE
##     Class Probability Petal.Width Petal.Length
## 1: setosa   0.5936306         0.1     1.000000
## 2: setosa   0.5986001         0.1     1.655556
## 3: setosa   0.5613686         0.1     2.311111
## 4: setosa   0.4595510         0.1     2.966667
## 5: setosa   0.3409719         0.1     3.622222
## 6: setosa   0.2873570         0.1     4.277778
## ... (#rows: 300, #cols: 4)
```

At each step in the estimation of $\hat{f}_{X_s}$ a set of predictions of length N is generated. By default the mean prediction is used. For classification where `predict.type = "prob"` this entails the mean class probabilities.

However, other summaries of the predictions may be used. For regression and survival tasks the function used here must either return one number or three, and, if the latter, the numbers must be sorted lowest to highest. For classification tasks the function must return a number for each level of the target feature.

As noted, the `fun` argument can be a function which returns three numbers (sorted low to high) for a regression task. This allows further exploration of relative feature importance. If a feature is relatively important, the bounds are necessarily tighter because the feature accounts for more of the variance of the predictions, i.e., it is "used" more by the learner. More directly setting `fun = var` identifies regions of interaction between X_s and X_c.

```
lrn.regr = makeLearner("regr.ksvm")
fit.regr = train(lrn.regr, bh.task)
pd.regr = generatePartialDependenceData(fit.regr, bh.task, "lstat", fun = median)
pd.regr
## PartialDependenceData
## Task: BostonHousing-example
## Features: lstat
## Target: medv
## Derivative: FALSE
## Interaction: FALSE
## Individual: FALSE
##        medv     lstat
## 1: 24.90884  1.730000
## 2: 23.73483  5.756667
## 3: 22.35572  9.783333
## 4: 20.71322 13.810000
## 5: 19.62132 17.836667
## 6: 19.04824 21.863333
## ... (#rows: 10, #cols: 2)
pd.ci = generatePartialDependenceData(fit.regr, bh.task, "lstat",
  fun = function(x) quantile(x, c(.25, .5, .75)))
pd.ci
## PartialDependenceData
## Task: BostonHousing-example
## Features: lstat
## Target: medv
## Derivative: FALSE
## Interaction: FALSE
## Individual: FALSE
##        medv Function     lstat
## 1: 21.37860 medv.25%  1.730000
## 2: 20.82492 medv.25%  5.756667
## 3: 19.92989 medv.25%  9.783333
## 4: 18.71068 medv.25% 13.810000
## 5: 16.52942 medv.25% 17.836667
## 6: 14.97075 medv.25% 21.863333
## ... (#rows: 30, #cols: 3)
pd.classif = generatePartialDependenceData(fit.classif, iris.task, "Petal.Length", fun = median)
pd.classif
## PartialDependenceData
## Task: iris-example
## Features: Petal.Length
## Target: setosa, versicolor, virginica
## Derivative: FALSE
## Interaction: FALSE
```

```
## Individual: FALSE
##     Class Probability Petal.Length
## 1: setosa  0.28179723     1.000000
## 2: setosa  0.27637842     1.655556
## 3: setosa  0.25405460     2.311111
## 4: setosa  0.19895270     2.966667
## 5: setosa  0.11451587     3.622222
## 6: setosa  0.04227993     4.277778
## ... (#rows: 30, #cols: 3)
```

In addition to bounds based on a summary of the distribution of the conditional expectation of each observation, learners which can estimate the variance of their predictions can also be used. The argument `bounds` is a numeric vector of length two which is added (so the first number should be negative) to the point prediction to produce a confidence interval for the partial dependence. The default is the .025 and .975 quantiles of the Gaussian distribution.

```
fit.se = train(makeLearner("regr.randomForest", predict.type = "se"), bh.task)
pd.se = generatePartialDependenceData(fit.se, bh.task, c("lstat", "crim"))
head(pd.se$data)
##       lower     medv    upper     lstat crim
## 1: 12.52356 31.33547 50.14739  1.730000   NA
## 2: 14.28674 26.30966 38.33258  5.756667   NA
## 3: 13.46318 23.54457 33.62596  9.783333   NA
## 4: 14.11382 22.06483 30.01584 13.810000   NA
## 5: 12.83159 20.37902 27.92645 17.836667   NA
## 6: 11.68656 19.71489 27.74322 21.863333   NA
tail(pd.se$data)
##       lower     medv    upper lstat     crim
## 1: 10.61874 22.03558 33.45241    NA 39.54849
## 2: 10.55490 22.01391 33.47291    NA 49.43403
## 3: 10.51112 21.99129 33.47146    NA 59.31957
## 4: 10.46239 21.97804 33.49370    NA 69.20512
## 5: 10.47418 21.98144 33.48869    NA 79.09066
## 6: 10.47487 21.98205 33.48923    NA 88.97620
```

As previously mentioned if the aggregation function is not used, i.e., it is the identity, then the conditional expectation of $\hat{f}_{X_s}^{(i)}$ is estimated. If `individual = TRUE` then `generatePartialDependenceData()` returns n partial dependence estimates made at each point in the prediction grid constructed from the features.

```
pd.ind.regr = generatePartialDependenceData(fit.regr, bh.task, "lstat", individual = TRUE)
pd.ind.regr
## PartialDependenceData
## Task: BostonHousing-example
## Features: lstat
## Target: medv
## Derivative: FALSE
## Interaction: FALSE
## Individual: TRUE
##        medv n     lstat
## 1: 22.18048 1  1.730000
## 2: 21.40916 1  5.756667
## 3: 20.72219 1  9.783333
## 4: 20.14669 1 13.810000
## 5: 19.63830 1 17.836667
## 6: 19.14623 1 21.863333
```

```
## ... (#rows: 5060, #cols: 3)
```

The resulting output, particularly the element `data` in the returned object, has an additional column `idx` which gives the index of the observation to which the row pertains.

For classification tasks this index references both the class and the observation index.

```
pd.ind.classif = generatePartialDependenceData(fit.classif, iris.task, "Petal.Length", individual = TRU
pd.ind.classif
## PartialDependenceData
## Task: iris-example
## Features: Petal.Length
## Target: setosa, versicolor, virginica
## Derivative: FALSE
## Interaction: FALSE
## Individual: TRUE
##     Class Probability n Petal.Length
## 1: setosa   0.9676110 1     1.000000
## 2: setosa   0.9761459 1     1.655556
## 3: setosa   0.9350573 1     2.311111
## 4: setosa   0.7452187 1     2.966667
## 5: setosa   0.4663795 1     3.622222
## 6: setosa   0.3302177 1     4.277778
## ... (#rows: 4500, #cols: 4)
```

Partial derivatives can also be computed for individual partial dependence estimates and aggregate partial dependence. This is restricted to a single feature at a time. The derivatives of individual partial dependence estimates can be useful in finding regions of interaction between the feature for which the derivative is estimated and the features excluded.

```
pd.regr.der = generatePartialDependenceData(fit.regr, bh.task, "lstat", derivative = TRUE)
head(pd.regr.der$data)
##          medv     lstat
## 1: -0.2299870  1.730000
## 2: -0.3544788  5.756667
## 3: -0.4251045  9.783333
## 4: -0.4317926 13.810000
## 5: -0.3800545 17.836667
## 6: -0.2852035 21.863333
pd.regr.der.ind = generatePartialDependenceData(fit.regr, bh.task, "lstat", derivative = TRUE,
  individual = TRUE)
head(pd.regr.der.ind$data)
##          medv   n     lstat
## 1: -0.6202023 396  1.730000
## 2: -0.9378079 396  5.756667
## 3: -1.0859810 396  9.783333
## 4: -1.0250696 396 13.810000
## 5: -0.7841616 396 17.836667
## 6: -0.4433710 396 21.863333
pd.classif.der = generatePartialDependenceData(fit.classif, iris.task, "Petal.Width", derivative = TRUE
head(pd.classif.der$data)
##     Class Probability Petal.Width
## 1: setosa -0.03937965   0.1000000
## 2: setosa -0.15635472   0.3666667
## 3: setosa -0.30429931   0.6333333
```

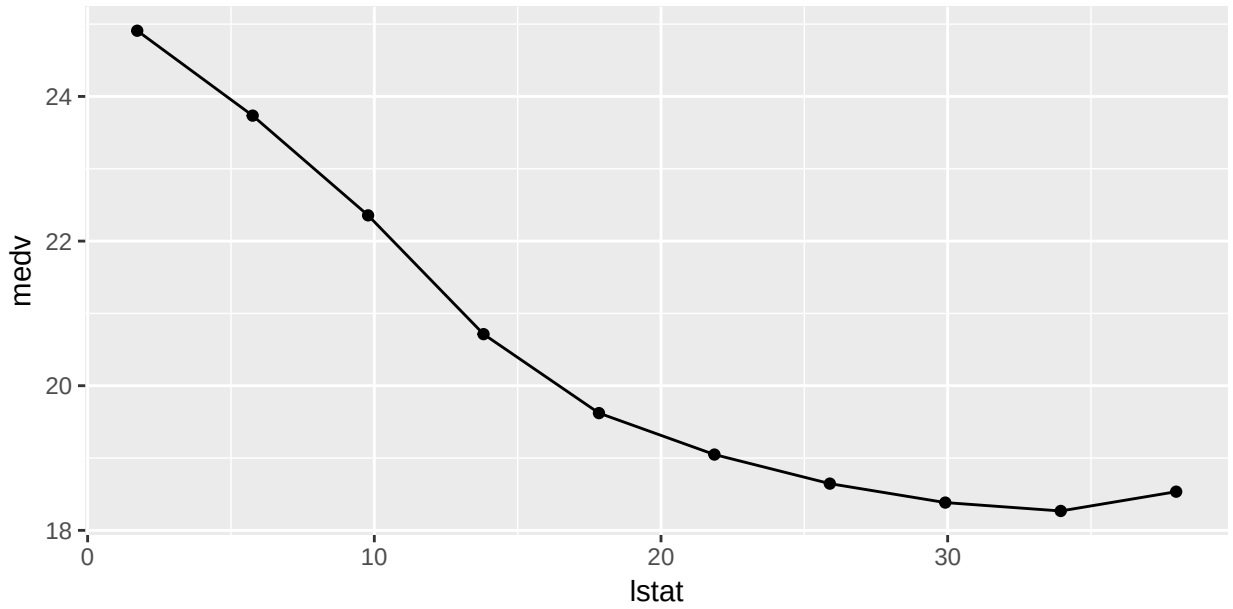
```
## 4: setosa -0.46283192   0.9000000
## 5: setosa -0.36263766   1.1666667
## 6: setosa -0.14153015   1.4333333
pd.classif.der.ind = generatePartialDependenceData(fit.classif, iris.task, "Petal.Width", derivative = T
  individual = TRUE)
head(pd.classif.der.ind$data)
##     Class Probability  n Petal.Width
## 1: setosa -0.19409978 58   0.1000000
## 2: setosa -0.63154325 58   0.3666667
## 3: setosa -0.41765112 58   0.6333333
## 4: setosa -0.09139630 58   0.9000000
## 5: setosa  0.01082549 58   1.1666667
## 6: setosa  0.10499747 58   1.4333333
```

3.14.2 Plotting partial dependences

Results from `generatePartialDependenceData()` and `generateFunctionalANOVAData()` can be visualized with `plotPartialDependence()` and `plotPartialDependenceGGVIS()`.

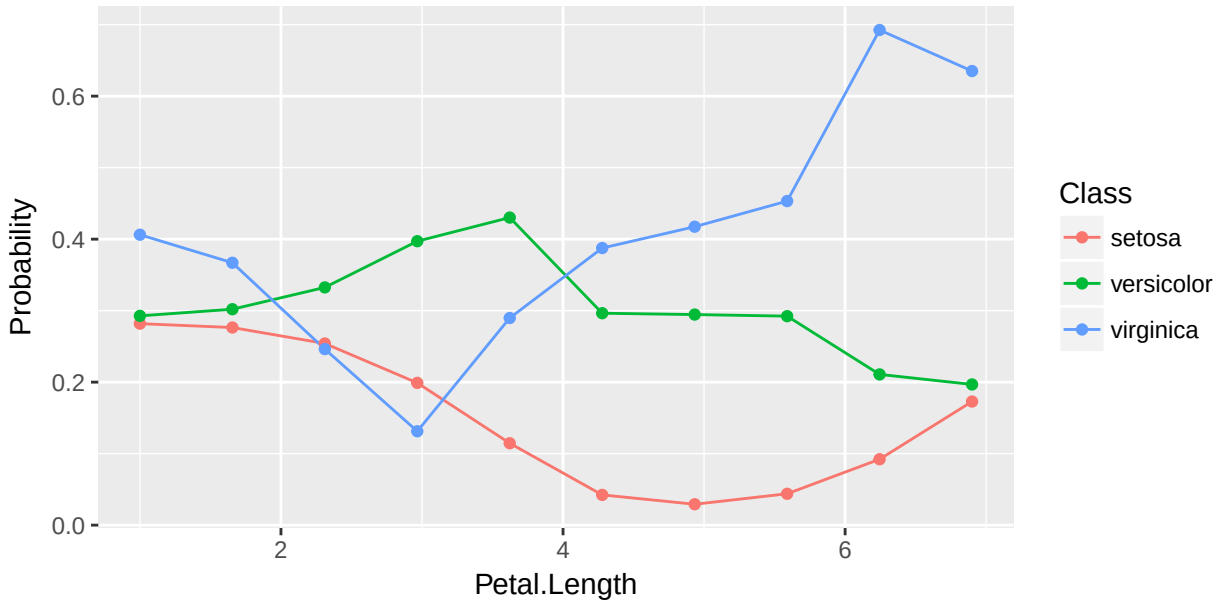
With one feature and a regression task the output is a line plot, with a point for each point in the corresponding feature's grid.

```
plotPartialDependence(pd.regr)
```



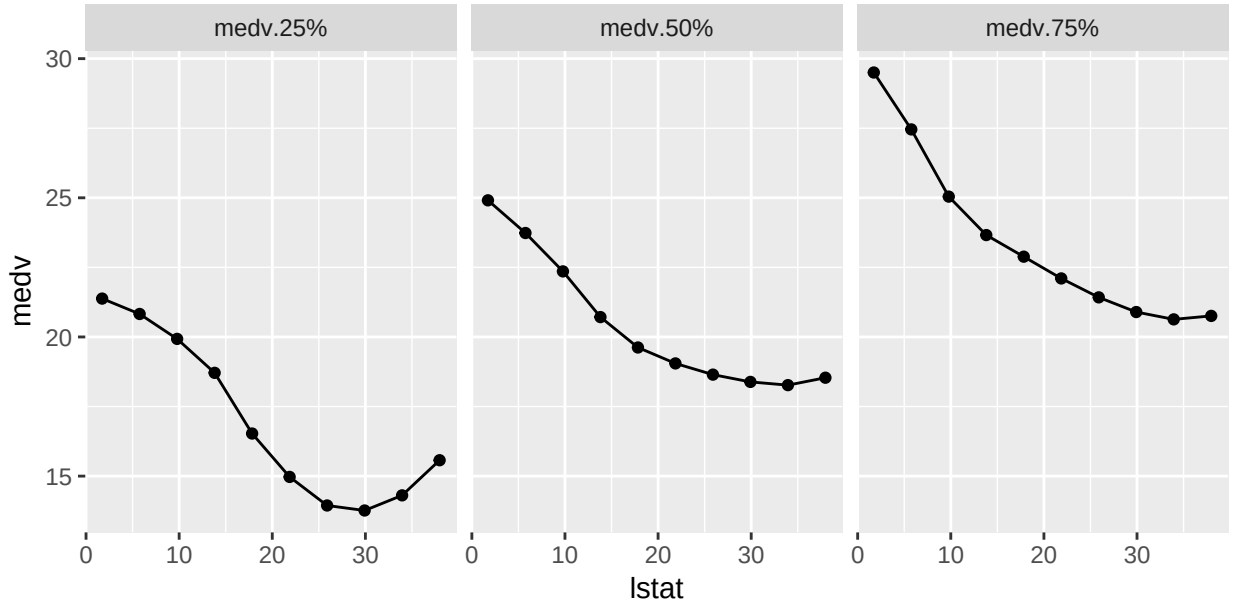
With a classification task, a line is drawn for each class, which gives the estimated partial probability of that class for a particular point in the feature grid.

```
plotPartialDependence(pd.classif)
```



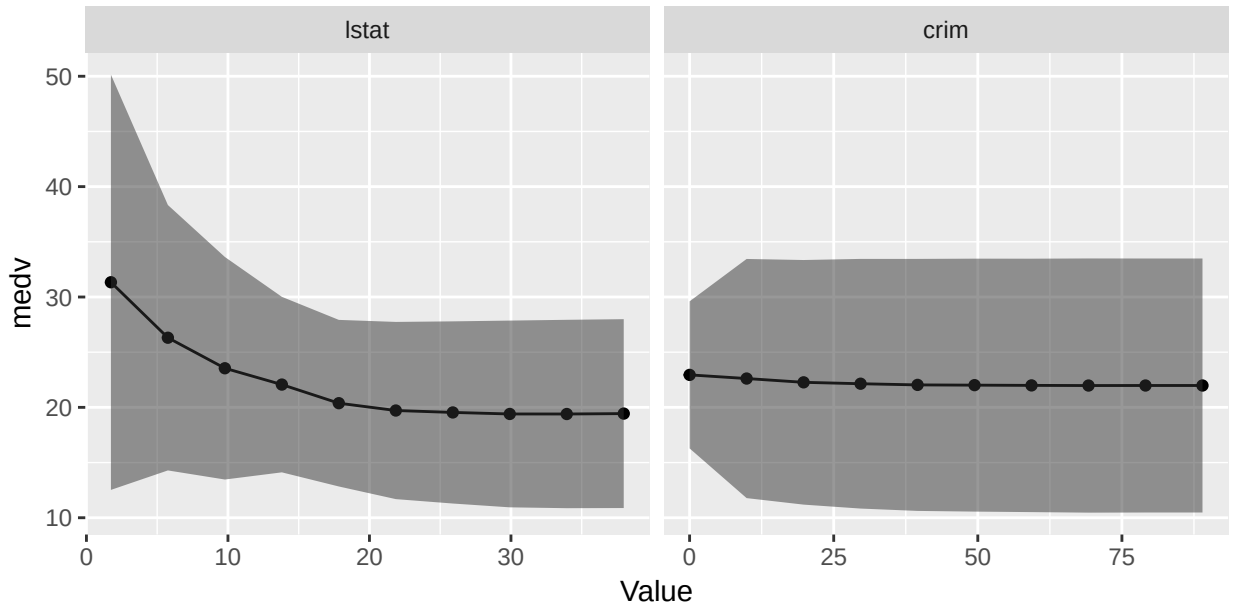
For regression tasks, when the `fun` argument of `generatePartialDependenceData()` is used, the bounds will automatically be displayed using a gray ribbon.

```
plotPartialDependence(pd.ci)
```



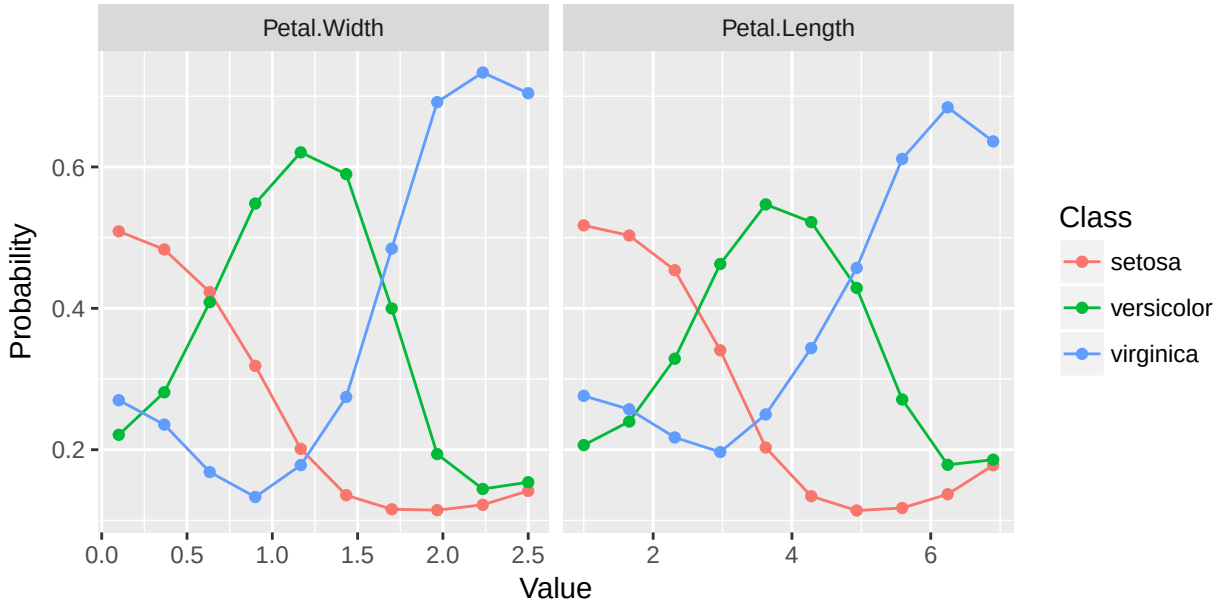
The same goes for plots of partial dependences where the learner has `predict.type = "se"`.

```
plotPartialDependence(pd.se)
```



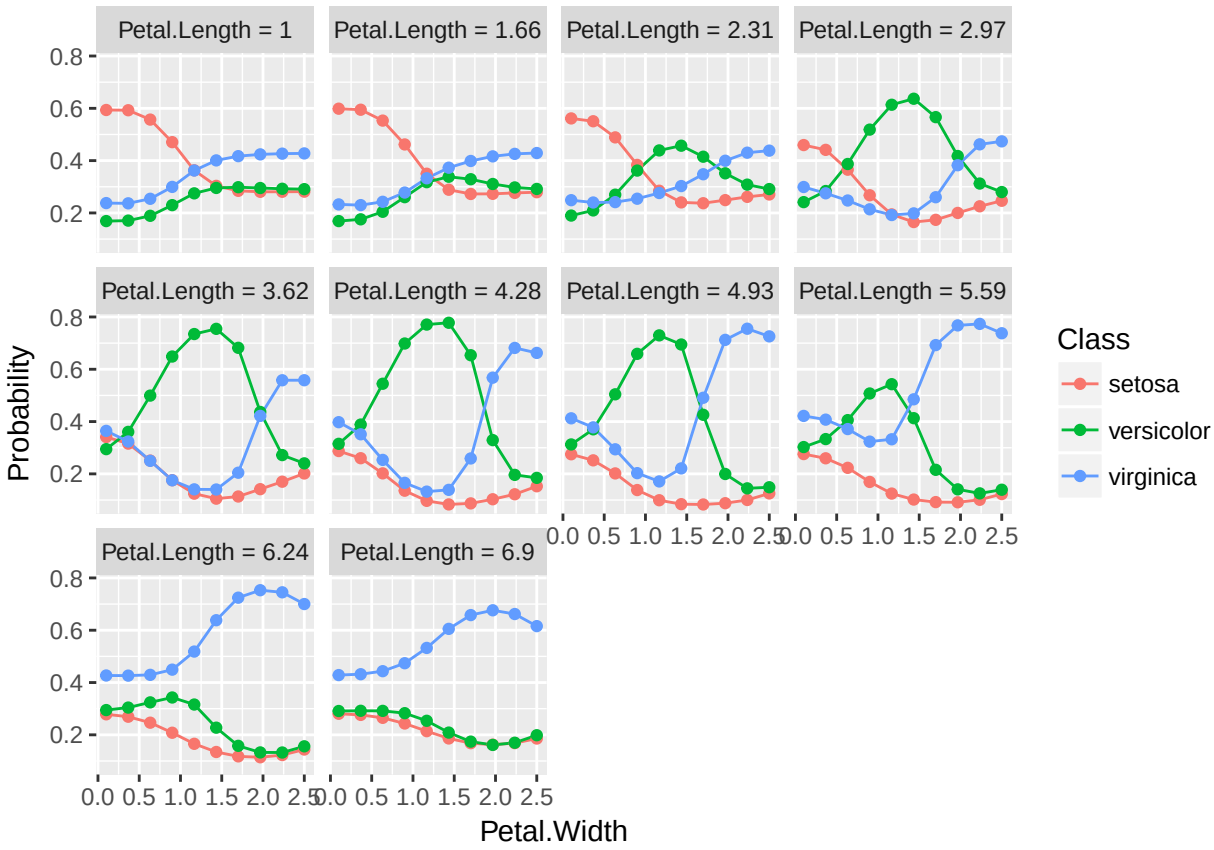
When multiple features are passed to `generatePartialDependenceData()` but `interaction = FALSE`, facetting is used to display each estimated bivariate relationship.

```
plotPartialDependence(pd.lst)
```



When `interaction = TRUE` in the call to `generatePartialDependenceData()`, one variable must be chosen to be used for facetting, and a subplot for each value in the chosen feature's grid is created, wherein the other feature's partial dependences within the facetting feature's value are shown. Note that this type of plot is limited to two features.

```
plotPartialDependence(pd.int, facet = "Petal.Length")
```

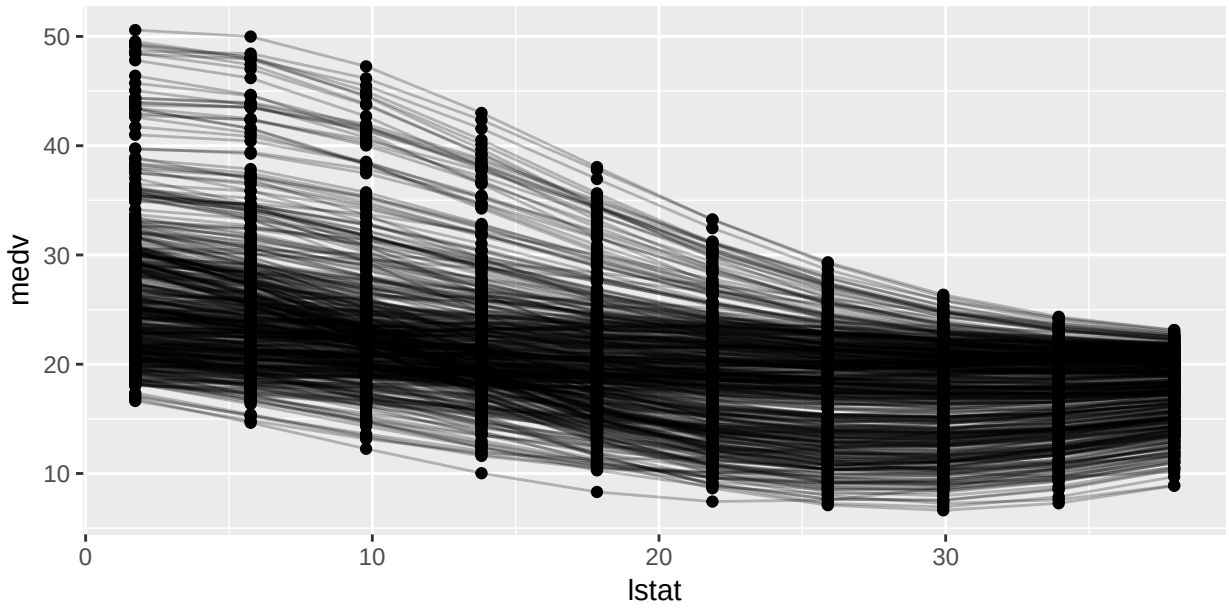


`plotPartialDependenceGGVIS()` can be used similarly, however, since `ggvis` currently lacks subplotting/facetting capabilities, the argument `interact` maps one feature to an interactive sidebar where the user can select a value of one feature.

```
plotPartialDependenceGGVIS(pd.int, interact = "Petal.Length")
```

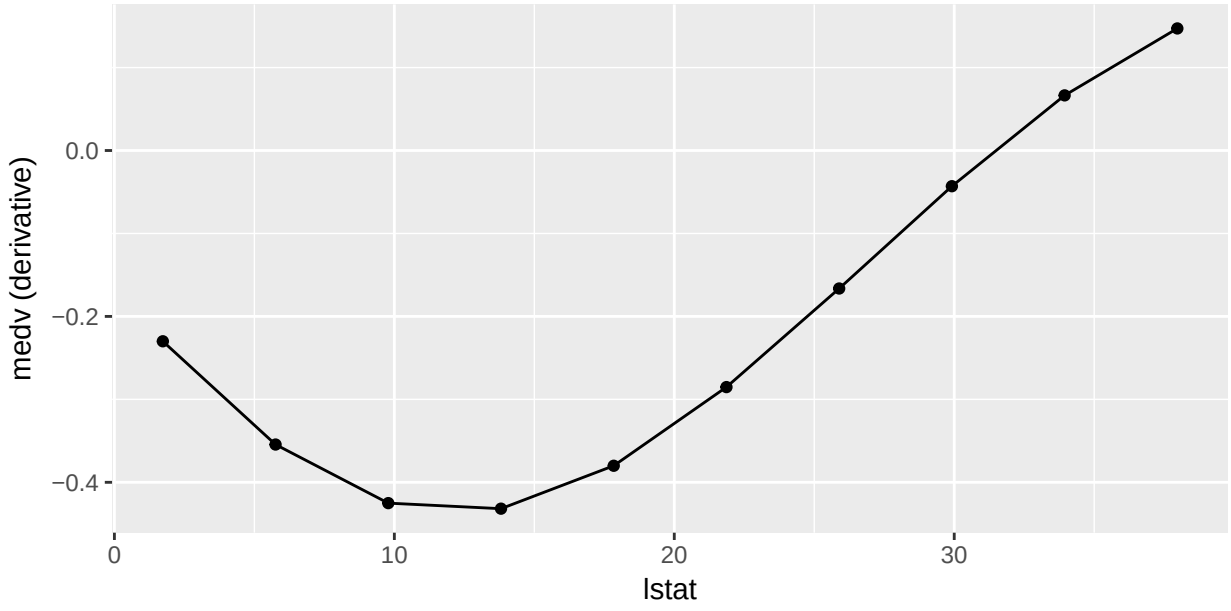
When `individual = TRUE` each individual conditional expectation curve is plotted.

```
plotPartialDependence(pd.ind.regr)
```



Plotting partial derivative functions works the same as partial dependence. Below are estimates of the derivative of the mean aggregated partial dependence function, and the individual partial dependence functions for a regression and a classification task respectively.

```
plotPartialDependence(pd.regr.der)
```



3.15 Classifier Calibration

A classifier is "calibrated" when the predicted probability of a class matches the expected frequency of that class. `mlr` can visualize this by plotting estimated class probabilities (which are discretized) against the observed frequency of said class in the data using `generateCalibrationData()` and `plotCalibration()`.

`generateCalibrationData()` takes as input `Prediction()`, `ResampleResult()`, `BenchmarkResult()`, or a named list of `Prediction()` or `ResampleResult()` objects on a classification (multiclass or binary) task with learner(s) that are capable of outputting probabiliites (i.e., learners must be constructed with `predict.type = "prob"`). The result is an object of class `CalibrationData` (`generateCalibrationData()`) which has elements `proportion`, `data`, and `task`. `proportion` gives the proportion of observations labelled with a given class for each predicted probability bin (e.g., for observations which are predicted to have class "A" with probability $(0, 0.1]$, what is the proportion of said observations which have class "A"?).

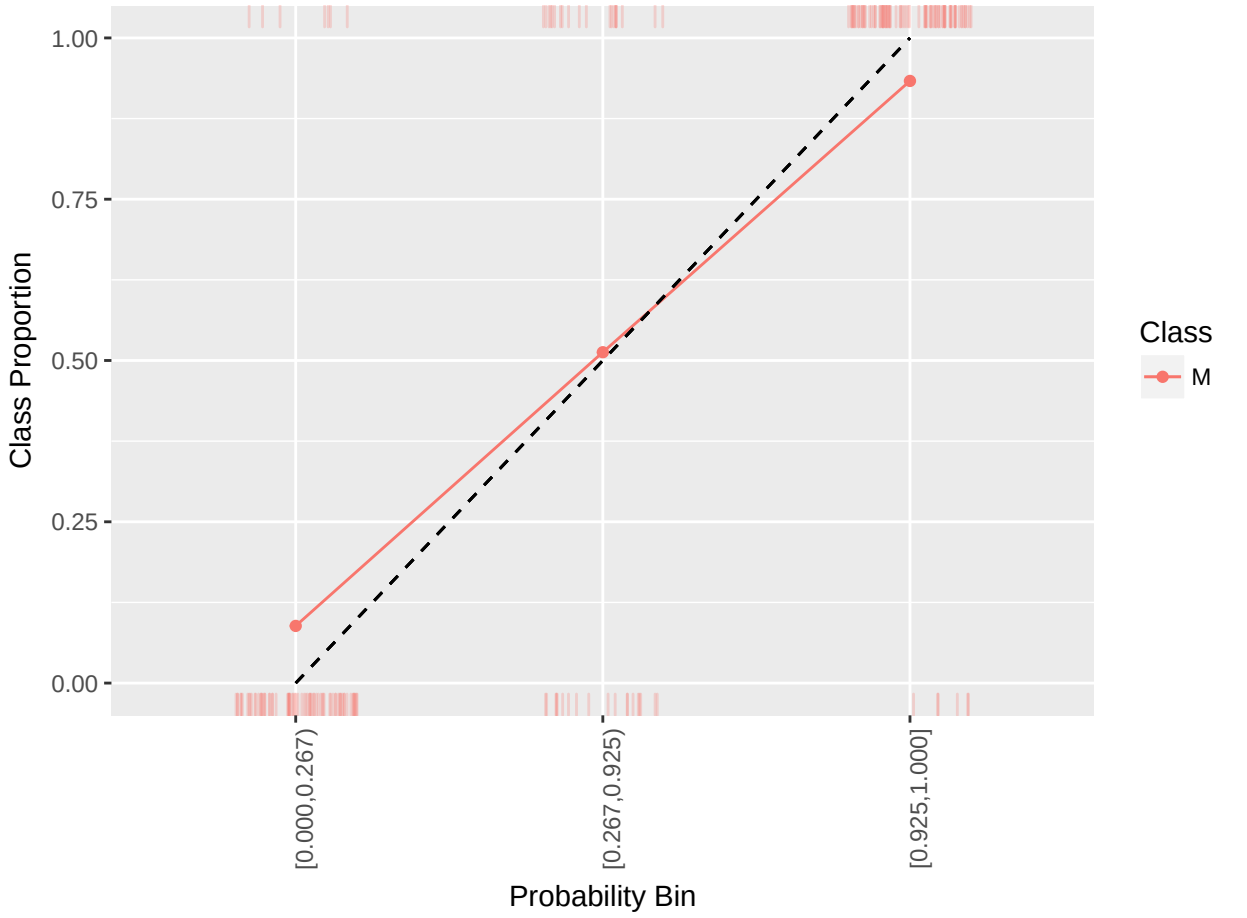
```
lrn = makeLearner("classif.rpart", predict.type = "prob")
mod = train(lrn, task = sonar.task)
pred = predict(mod, task = sonar.task)
cal = generateCalibrationData(pred)
cal$proportion
##      Learner       bin Class Proportion
## 1 prediction (0.1,0.2]     M  0.1060606
## 2 prediction (0.7,0.8]     M  0.7333333
## 3 prediction   [0,0.1]     M  0.0000000
## 4 prediction   (0.9,1]     M  0.9333333
## 5 prediction (0.2,0.3]     M  0.2727273
## 6 prediction (0.4,0.5]     M  0.4615385
## 7 prediction (0.8,0.9]     M  0.0000000
## 8 prediction (0.5,0.6]     M  0.0000000
```

The manner in which the predicted probabilities are discretized is controlled by two arguments: `breaks` and `groups`. By default `breaks = "Sturges"` which uses the Sturges algorithm in `graphics::hist()`. This argument can specify other algorithms available in `graphics::hist()`, it can be a numeric vector specifying breakpoints for `base::cut()`, or a single integer specifying the number of bins to create (which are evenly spaced). Alternatively, `groups` can be set to a positive integer value (by default `groups = NULL`) in which case `Hmisc::cut2()` is used to create bins with an approximately equal number of observations in each bin.

```
cal = generateCalibrationData(pred, groups = 3)
cal$proportion
##      Learner           bin Class Proportion
## 1 prediction [0.000,0.267)     M 0.08860759
## 2 prediction [0.267,0.925)     M 0.51282051
## 3 prediction [0.925,1.000]     M 0.93333333
```

`generateCalibrationData()` objects can be plotted using `plotCalibration()`. `plotCalibration()` by default plots a reference line which shows perfect calibration and a "rag" plot, which is a rug plot on the top and bottom of the graph, where the top pertains to "positive" cases, where the predicted class matches the observed class, and the bottom pertains to "negative" cases, where the predicted class does not match the observed class. Perfect classifier performance would result in all the positive cases clustering in the top right (i.e., the correct classes are predicted with high probability) and the negative cases clustering in the bottom left.

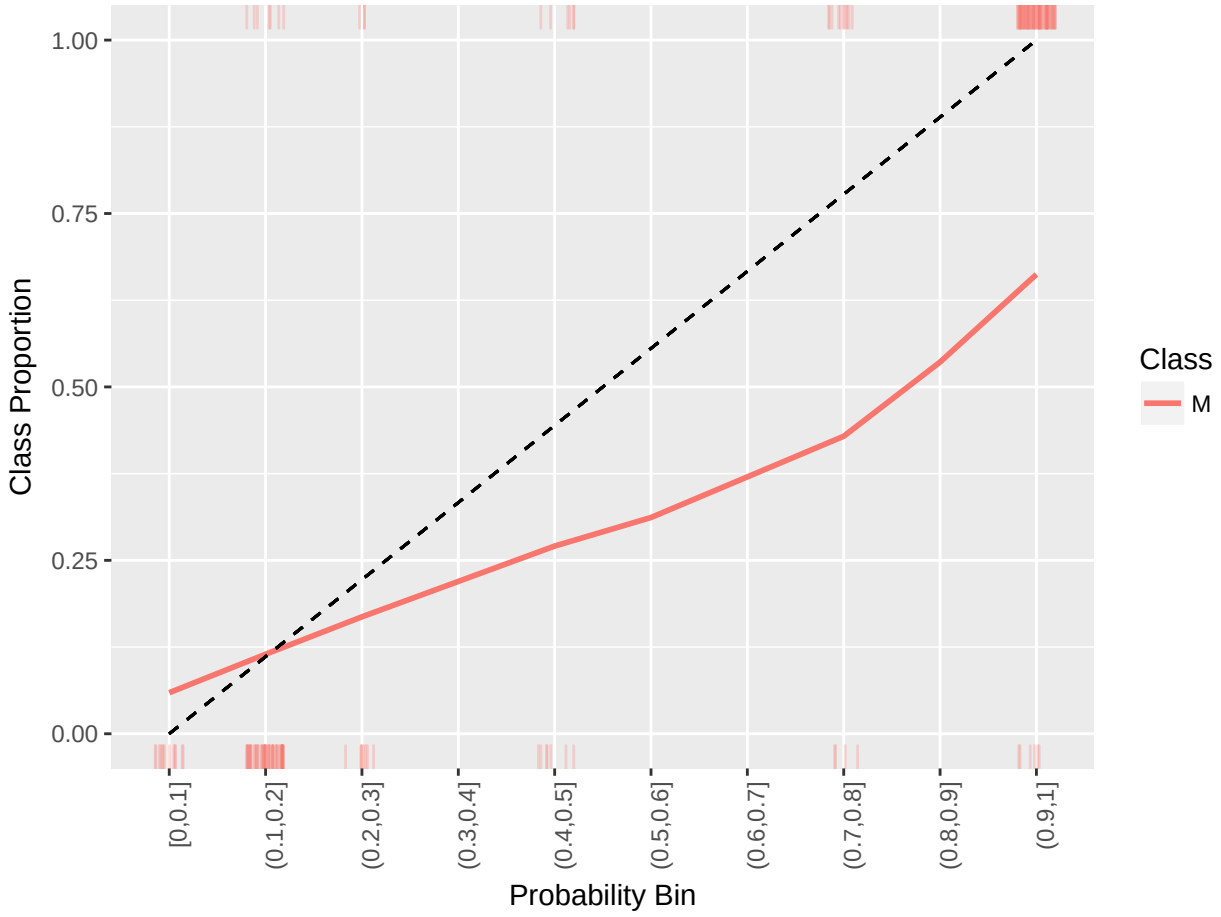
```
plotCalibration(cal)
```



Because of the discretization of the probabilities, sometimes it is advantageous to smooth the calibration plot. Though `smooth = FALSE` by default, setting this option to `TRUE` replaces the estimated proportions with a

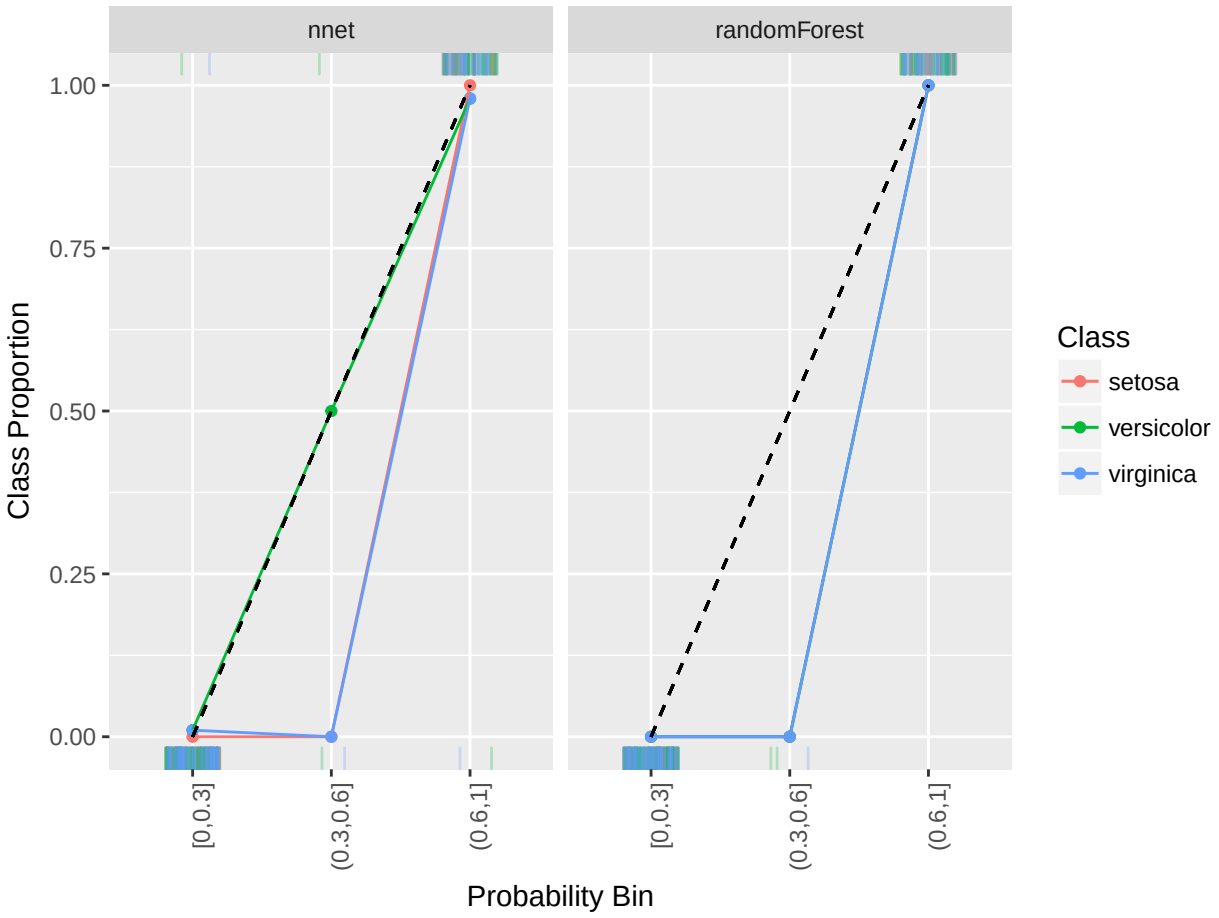
loess smoother.

```
cal = generateCalibrationData(pred)
plotCalibration(cal, smooth = TRUE)
```



All of the above functionality works with multi-class classification as well.

```
lrns = list(
  makeLearner("classif.randomForest", predict.type = "prob"),
  makeLearner("classif.nnet", predict.type = "prob", trace = FALSE)
)
mod = lapply(lrns, train, task = iris.task)
pred = lapply(mod, predict, task = iris.task)
names(pred) = c("randomForest", "nnet")
cal = generateCalibrationData(pred, breaks = c(0, .3, .6, 1))
plotCalibration(cal)
```



3.16 Evaluating Hyperparameter Tuning

As mentioned on the tuning tutorial page, tuning a machine learning algorithm typically involves:

- the hyperparameter search space:

```
### ex: create a search space for the C hyperparameter from 0.01 to 0.1
ps = makeParamSet(
  makeNumericParam("C", lower = 0.01, upper = 0.1)
)
```

- the optimization algorithm (aka tuning method):

```
### ex: random search with 100 iterations
ctrl = makeTuneControlRandom(maxit = 100L)
```

- an evaluation method, i.e., a resampling strategy and a performance measure:

```
### ex: 2-fold CV
rdesc = makeResampleDesc("CV", iters = 2L)
```

After tuning, you may want to evaluate the tuning process in order to answer questions such as:

- How does varying the value of a hyperparameter change the performance of the machine learning algorithm?
- What's the relative importance of each hyperparameter?
- How did the optimization algorithm (prematurely) converge?

`mlr` provides methods to generate and plot the data in order to evaluate the effect of hyperparameter tuning.

3.16.1 Generating hyperparameter tuning data

`mlr` separates the generation of the data from the plotting of the data in case the user wishes to use the data in a custom way downstream.

The `generateHyperParsEffectData()` method takes the tuning result along with 2 additional arguments: `trafo` and `include.diagnostics`. The `trafo` argument will convert the hyperparameter data to be on the transformed scale in case a transformation was used when creating the parameter (as in the case below). The `include.diagnostics` argument will tell `mlr` whether to include the eol and any error messages from the learner.

Below we perform random search on the `C` parameter for SVM on the famous Pima Indians (`mlbench::PimaIndiansDiabetes()`) dataset. We generate the hyperparameter effect data so that the `C` parameter is on the transformed scale and we do not include diagnostic data:

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x)
)
ctrl = makeTuneControlRandom(maxit = 100L)
rdesc = makeResampleDesc("CV", iters = 2L)
res = tuneParams("classif.ksvm", task = pid.task, control = ctrl,
  measures = list(acc, mmce), resampling = rdesc, par.set = ps, show.info = FALSE)
generateHyperParsEffectData(res, trafo = T, include.diagnostics = FALSE)
## HyperParsEffectData:
## Hyperparameters: C
## Measures: acc.test.mean,mmce.test.mean
## Optimizer: TuneControlRandom
## Nested CV Used: FALSE
## Snapshot of data:
##             C acc.test.mean mmce.test.mean iteration exec.time
## 1  0.09534198     0.6901042      0.3098958         1     0.128
## 2 14.88261592     0.7226562      0.2773438         2     0.135
## 3 13.22676934     0.7213542      0.2786458         3     0.130
## 4  0.25207598     0.7591146      0.2408854         4     0.123
## 5  0.07327737     0.6640625      0.3359375         5     0.118
## 6 15.56780810     0.7200521      0.2799479         6     0.119
```

As a reminder from the resampling tutorial, if we wanted to generate data on the training set as well as the validation set, we only need to make a few minor changes:

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x)
)
ctrl = makeTuneControlRandom(maxit = 100L)
rdesc = makeResampleDesc("CV", iters = 2L, predict = "both")
res = tuneParams("classif.ksvm", task = pid.task, control = ctrl,
  measures = list(acc, setAggregation(acc, train.mean), mmce, setAggregation(mmce,
    train.mean)), resampling = rdesc, par.set = ps, show.info = FALSE)
generateHyperParsEffectData(res, trafo = T, include.diagnostics = FALSE)
## HyperParsEffectData:
## Hyperparameters: C
## Measures: acc.test.mean,acc.train.mean,mmce.test.mean,mmce.train.mean
## Optimizer: TuneControlRandom
## Nested CV Used: FALSE
```

```
## Snapshot of data:
##            C acc.test.mean acc.train.mean mmce.test.mean mmce.train.mean
## 1 27.3182789     0.7304688      0.9557292      0.2695312      0.04427083
## 2  0.3813421     0.7565104      0.8125000      0.2434896      0.18750000
## 3  0.5809515     0.7682292      0.8307292      0.2317708      0.16927083
## 4 14.4907180     0.7473958      0.9166667      0.2526042      0.08333333
## 5 10.8330588     0.7486979      0.9192708      0.2513021      0.08072917
## 6  2.8072090     0.7617188      0.8776042      0.2382812      0.12239583
##   iteration exec.time
## 1         1     0.101
## 2         2     0.100
## 3         3     0.100
## 4         4     0.121
## 5         5     0.104
## 6         6     0.099
```

In the example below, we perform grid search on the `C` parameter for SVM on the Pima Indians dataset using nested cross validation. We generate the hyperparameter effect data so that the `C` parameter is on the untransformed scale and we do not include diagnostic data. As you can see below, nested cross validation is supported without any extra work by the user, allowing the user to obtain an unbiased estimator for the performance.

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x)
)
ctrl = makeTuneControlGrid()
rdesc = makeResampleDesc("CV", iters = 2L)
lrn = makeTuneWrapper("classif.ksvm", control = ctrl,
  measures = list(acc, mmce), resampling = rdesc, par.set = ps, show.info = FALSE)
res = resample(lrn, task = pid.task, resampling = cv2, extract = getTuneResult, show.info = FALSE)
generateHyperParsEffectData(res)
## HyperParsEffectData:
## Hyperparameters: C
## Measures: acc.test.mean,mmce.test.mean
## Optimizer: TuneControlGrid
## Nested CV Used: TRUE
## Snapshot of data:
##            C acc.test.mean mmce.test.mean iteration exec.time
## 1 -5.0000000     0.6614583      0.3385417         1     0.050
## 2 -3.8888889     0.6614583      0.3385417         2     0.050
## 3 -2.7777778     0.6848958      0.3151042         3     0.048
## 4 -1.6666667     0.7031250      0.2968750         4     0.050
## 5 -0.5555556     0.7317708      0.2682292         5     0.049
## 6  0.5555556     0.7213542      0.2786458         6     0.053
##   nested_cv_run
## 1             1
## 2             1
## 3             1
## 4             1
## 5             1
## 6             1
```

After generating the hyperparameter effect data, the next step is to visualize it. `mlr` has several methods built-in to visualize the data, meant to support the needs of the researcher and the engineer in industry. The next few sections will walk through the visualization support for several use-cases.

3.16.2 Visualizing the effect of a single hyperparameter

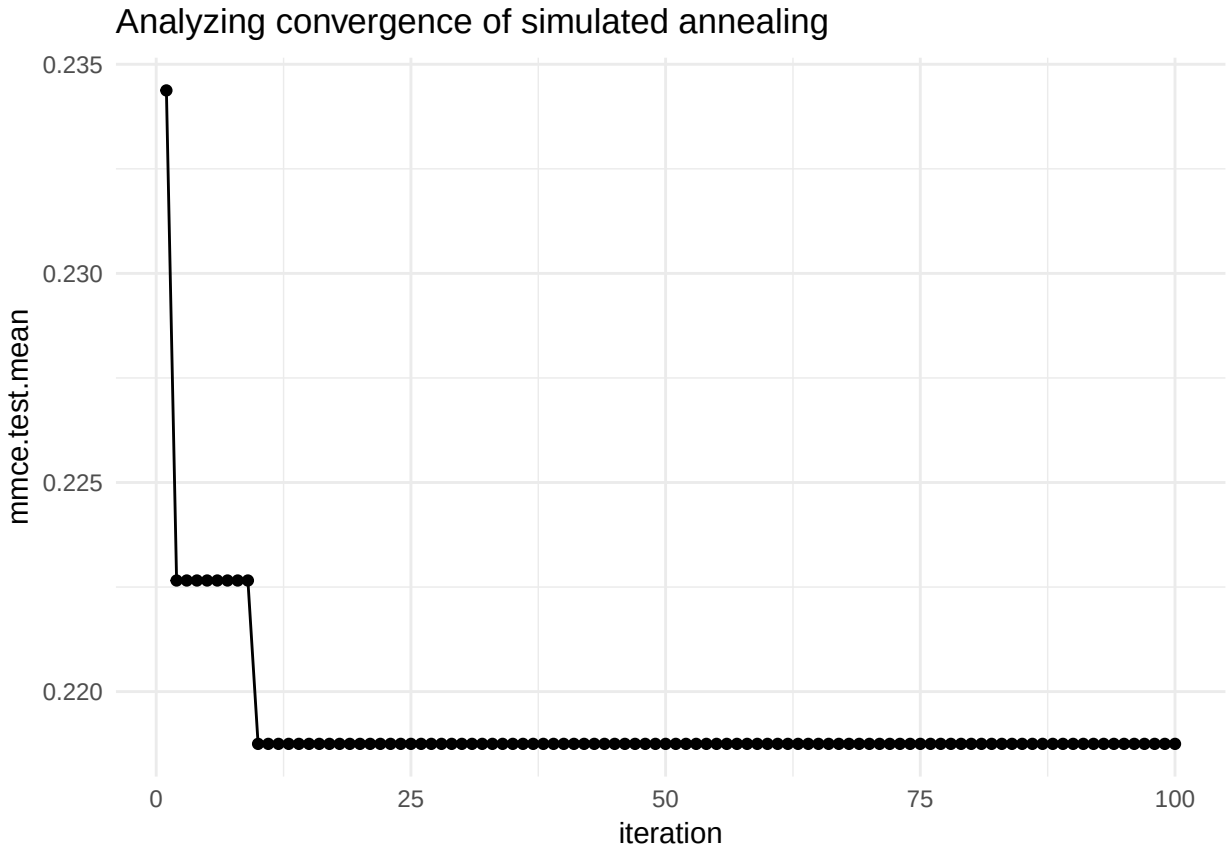
In a situation when the user is tuning a single hyperparameter for a learner, the user may wish to plot the performance of the learner against the values of the hyperparameter.

In the example below, we tune the number of clusters against the silhouette score on the Pima dataset. We specify the x-axis with the `x` argument and the y-axis with the `y` argument. If the `plot.type` argument is not specified, `mlr` will attempt to plot a scatterplot by default. Since `plotHyperParsEffect()` returns a `ggplot2::ggplot()` object, we can easily customize it to our liking!

```
library("clusterSim")
ps = makeParamSet(
  makeDiscreteParam("centers", values = 3:10)
)
ctrl = makeTuneControlGrid()
rdesc = makeResampleDesc("Holdout")
res = tuneParams("cluster.kmeans", task = mtcars.task, control = ctrl,
  measures = silhouette, resampling = rdesc, par.set = ps, show.info = FALSE)
data = generateHyperParsEffectData(res)
plt = plotHyperParsEffect(data, x = "centers", y = "silhouette.test.mean")
### add our own touches to the plot
plt + geom_point(colour = "red") +
  ggtitle("Evaluating Number of Cluster Centers on mtcars") +
  scale_x_continuous(breaks = 3:10) +
  theme_bw()
```

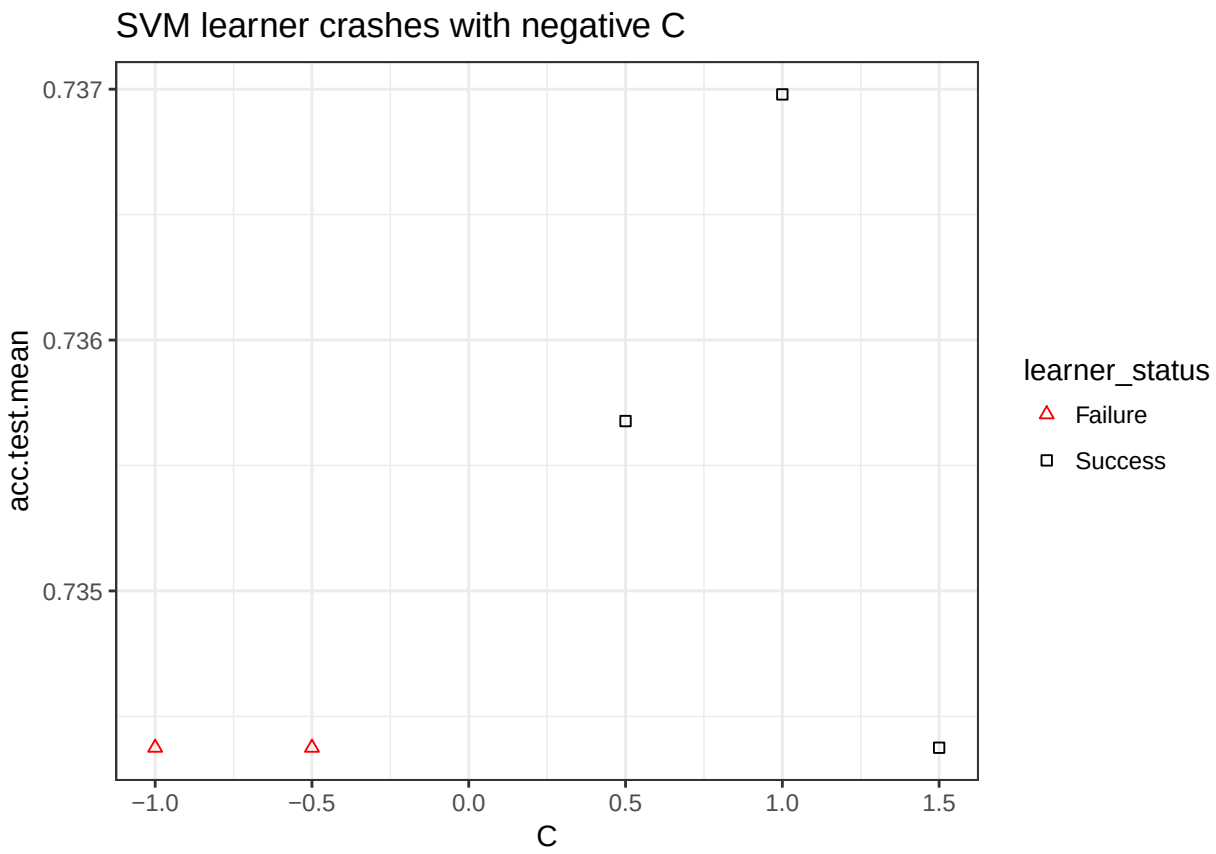
In the example below, we tune SVM with the `C` hyperparameter on the Pima dataset. We will use simulated annealing optimizer, so we are interested in seeing if the optimization algorithm actually improves with iterations. By default, `mlr` only plots improvements to the global optimum.

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x)
)
ctrl = makeTuneControlGenSA(budget = 100L)
rdesc = makeResampleDesc("Holdout")
res = tuneParams("classif.ksvm", task = pid.task, control = ctrl,
  resampling = rdesc, par.set = ps, show.info = FALSE)
data = generateHyperParsEffectData(res)
plt = plotHyperParsEffect(data, x = "iteration", y = "mmce.test.mean",
  plot.type = "line")
plt + ggtitle("Analyzing convergence of simulated annealing") +
  theme_minimal()
```



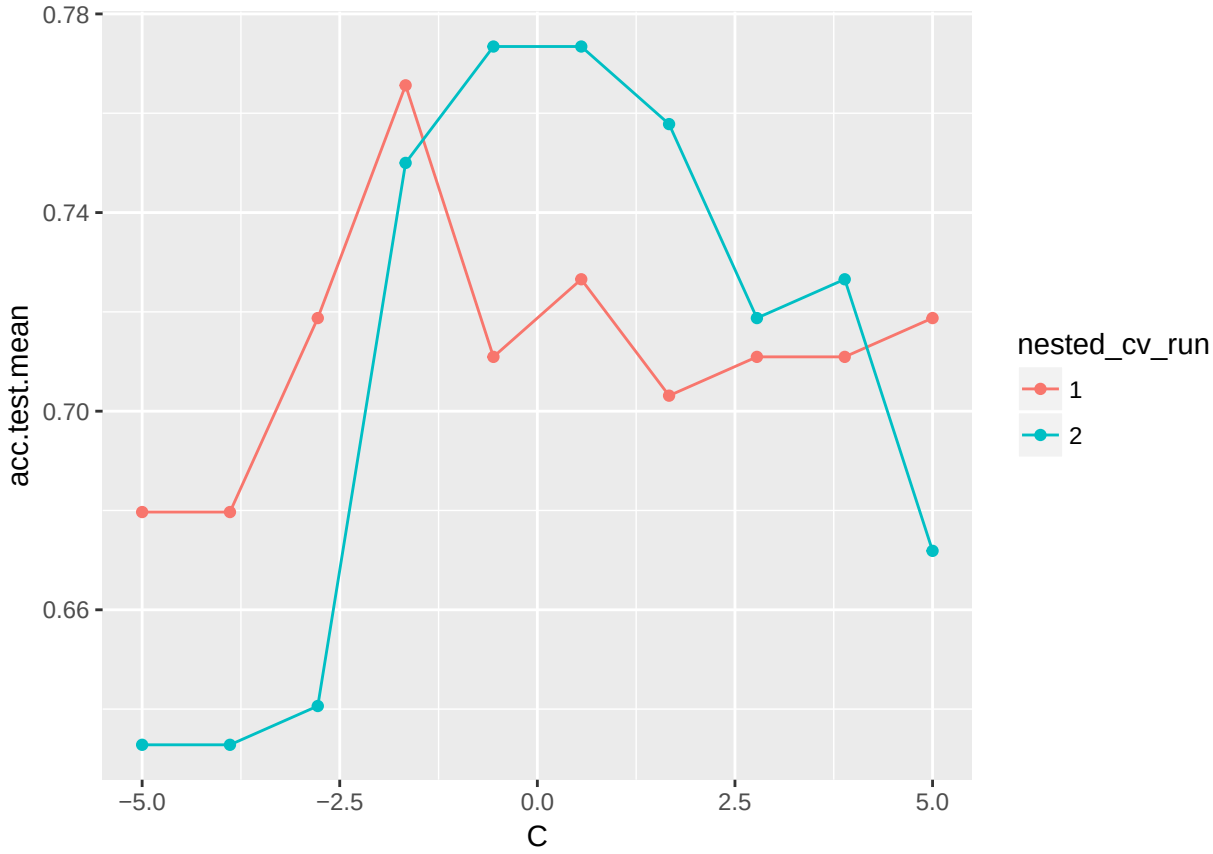
In the case of a learner crash, `mlr` will impute the crash with the worst value graphically and indicate the point. In the example below, we give the `C` parameter negative values, which will result in a learner crash for SVM.

```
ps = makeParamSet(
  makeDiscreteParam("C", values = c(-1, -0.5, 0.5, 1, 1.5))
)
ctrl = makeTuneControlGrid()
rdesc = makeResampleDesc("CV", iters = 2L)
res = tuneParams("classif.ksvm", task = pid.task, control = ctrl,
  measures = list(acc, mmce), resampling = rdesc, par.set = ps, show.info = FALSE)
data = generateHyperParsEffectData(res)
plt = plotHyperParsEffect(data, x = "C", y = "acc.test.mean")
plt + ggtitle("SVM learner crashes with negative C") +
  theme_bw()
```



The example below uses nested cross validation with an outer loop of 2 runs. `mlr` indicates each run within the visualization.

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x)
)
ctrl = makeTuneControlGrid()
rdesc = makeResampleDesc("Holdout")
lrn = makeTuneWrapper("classif.ksvm", control = ctrl,
  measures = list(acc, mmce), resampling = rdesc, par.set = ps, show.info = FALSE)
res = resample(lrn, task = pid.task, resampling = cv2, extract = getTuneResult, show.info = FALSE)
data = generateHyperParsEffectData(res)
plotHyperParsEffect(data, x = "C", y = "acc.test.mean", plot.type = "line")
```

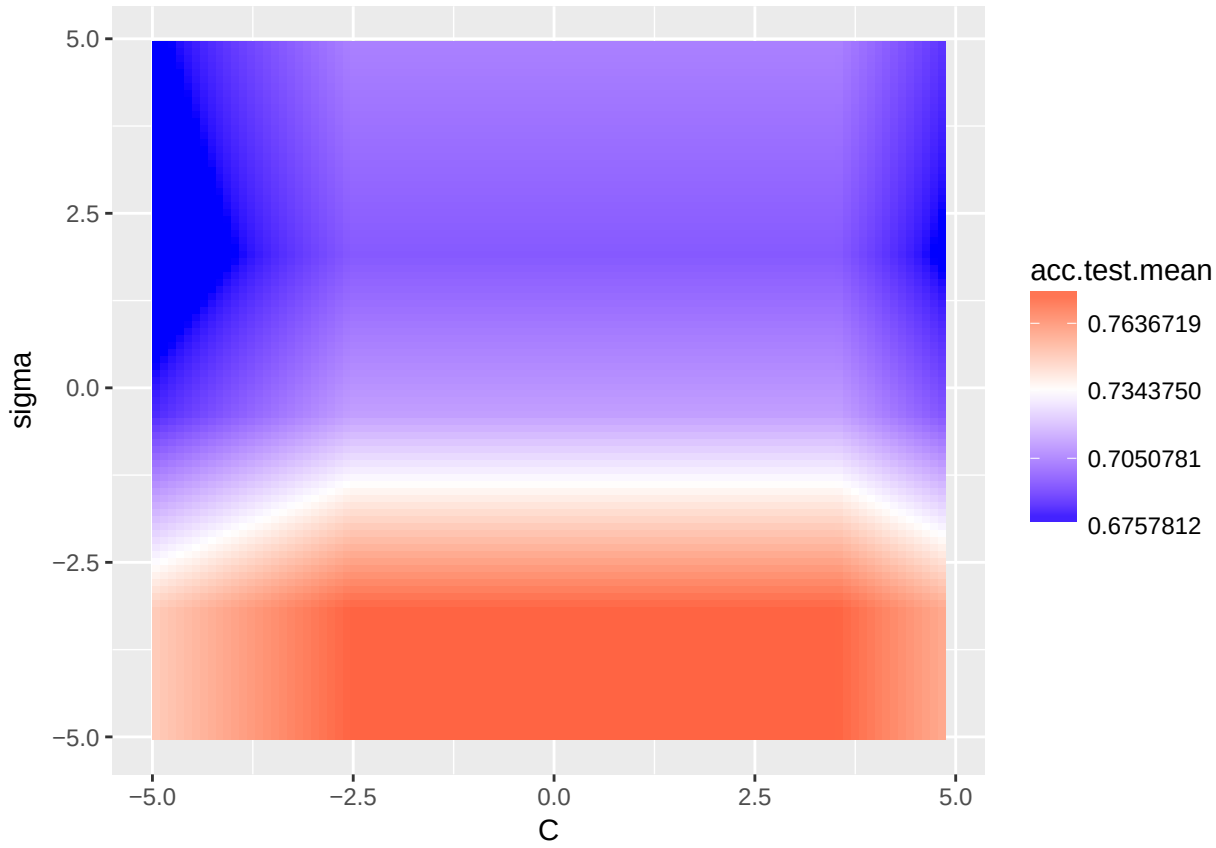


3.16.3 Visualizing the effect of 2 hyperparameters

In the case of tuning 2 hyperparameters simultaneously, `mlr` provides the ability to plot a heatmap and contour plot in addition to a scatterplot or line.

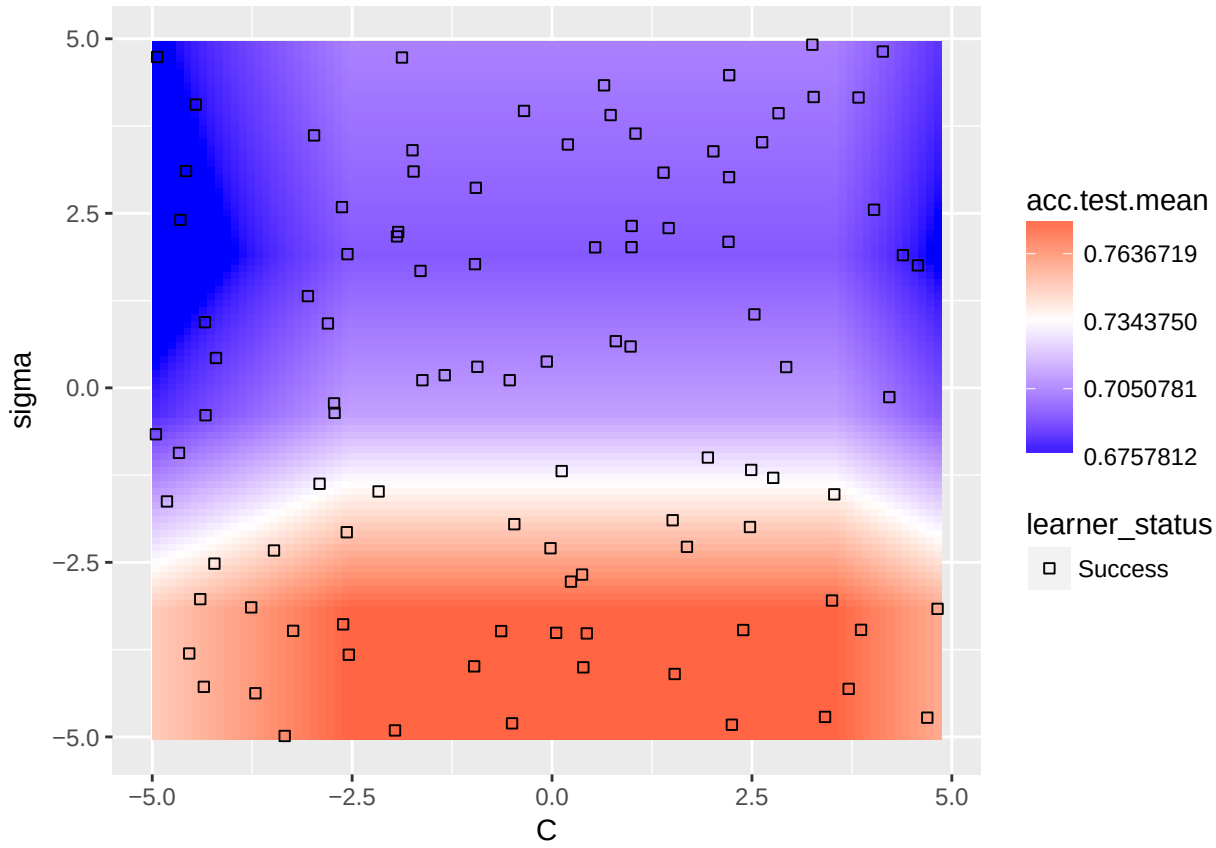
In the example below, we tune the `C` and `sigma` parameters for SVM on the Pima dataset. We use interpolation to produce a regular grid for plotting the heatmap. The `interpolation` argument accepts any regression learner from `mlr` to perform the interpolation. The `z` argument will be used to fill the heatmap or color lines, depending on the `plot.type` used.

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x),
  makeNumericParam("sigma", lower = -5, upper = 5, trafo = function(x) 2^x))
ctrl = makeTuneControlRandom(maxit = 100L)
rdesc = makeResampleDesc("Holdout")
learn = makeLearner("classif.ksvm", par.vals = list(kernel = "rbfdot"))
res = tuneParams(learn, task = pid.task, control = ctrl, measures = acc,
  resampling = rdesc, par.set = ps, show.info = FALSE)
data = generateHyperParsEffectData(res)
plt = plotHyperParsEffect(data, x = "C", y = "sigma", z = "acc.test.mean",
  plot.type = "heatmap", interpolate = "regr.earth")
min_plt = min(data$data$acc.test.mean, na.rm = TRUE)
max_plt = max(data$data$acc.test.mean, na.rm = TRUE)
med_plt = mean(c(min_plt, max_plt))
plt + scale_fill_gradient2(breaks = seq(min_plt, max_plt, length.out = 5),
  low = "blue", mid = "white", high = "red", midpoint = med_plt)
```



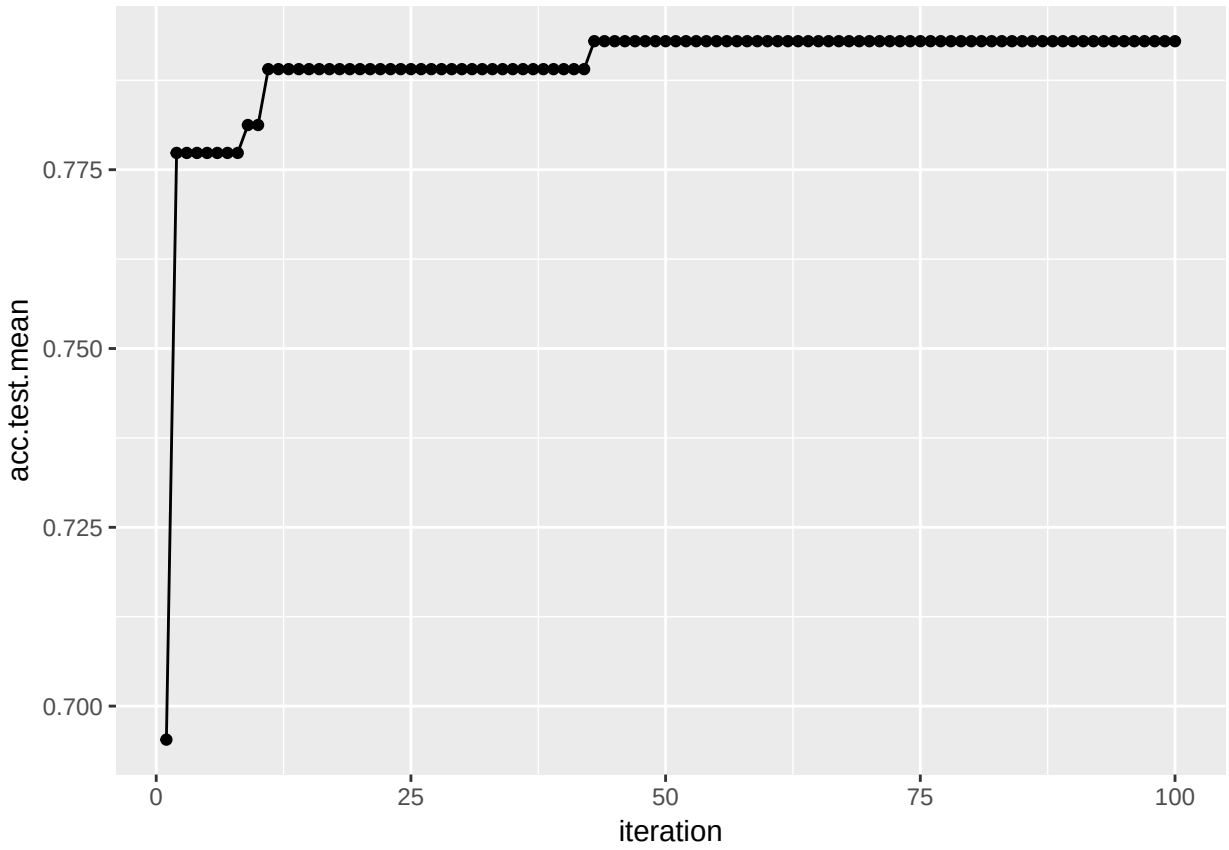
We can use the `show.experiments` argument in order to visualize which points were specifically passed to the learner in the original experiment and which points were interpolated by `mlr`:

```
plt = plotHyperParsEffect(data, x = "C", y = "sigma", z = "acc.test.mean",
  plot.type = "heatmap", interpolate = "regr.earth", show.experiments = TRUE)
plt + scale_fill_gradient2(breaks = seq(min_plt, max_plt, length.out = 5),
  low = "blue", mid = "white", high = "red", midpoint = med_plt)
```



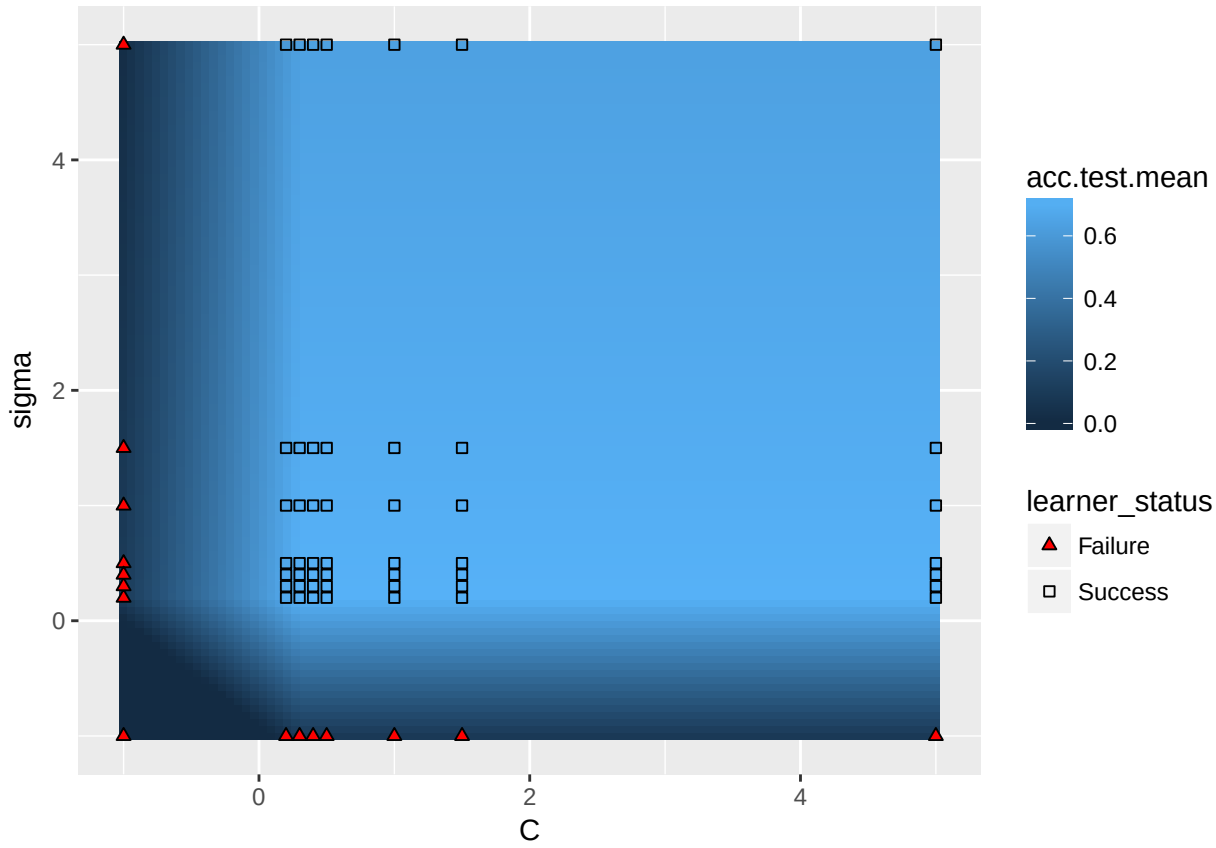
We can also visualize how long the optimizer takes to reach an optima for the same example:

```
plotHyperParsEffect(data, x = "iteration", y = "acc.test.mean",
  plot.type = "line")
```



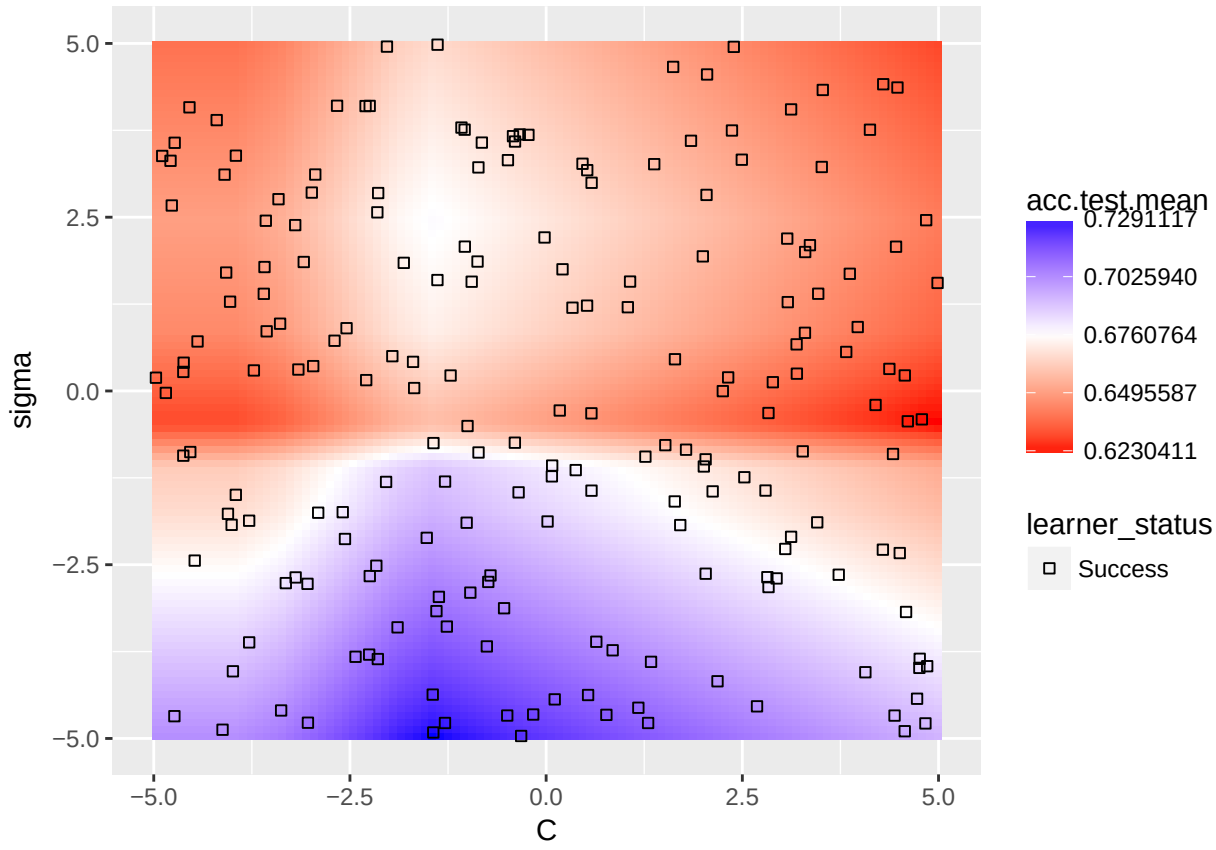
In the case where we are tuning 2 hyperparameters and we have a learner crash, `mlr` will indicate the respective points and impute them with the worst value. In the example below, we tune `C` and `sigma`, forcing `C` to be negative for some instances which will crash SVM. We perform interpolation to get a regular grid in order to plot a heatmap. We can see that the interpolation creates axis parallel lines resulting from the learner crashes.

```
ps = makeParamSet(
  makeDiscreteParam("C", values = c(-1, 0.5, 1.5, 1, 0.2, 0.3, 0.4, 5)),
  makeDiscreteParam("sigma", values = c(-1, 0.5, 1.5, 1, 0.2, 0.3, 0.4, 5)))
ctrl = makeTuneControlGrid()
rdesc = makeResampleDesc("Holdout")
learn = makeLearner("classif.ksvm", par.vals = list(kernel = "rbfdot"))
res = tuneParams(learn, task = pid.task, control = ctrl, measures = acc,
  resampling = rdesc, par.set = ps, show.info = FALSE)
data = generateHyperParsEffectData(res)
plotHyperParsEffect(data, x = "C", y = "sigma", z = "acc.test.mean",
  plot.type = "heatmap", interpolate = "regr.earth")
```



A slightly more complicated example is using nested cross validation while simultaneously tuning 2 hyperparameters. In order to plot a heatmap in this case, `mlr` will aggregate each of the nested runs by a user-specified function. The default function is `mean`. As expected, we can still take advantage of interpolation.

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x),
  makeNumericParam("sigma", lower = -5, upper = 5, trafo = function(x) 2^x))
ctrl = makeTuneControlRandom(maxit = 100)
rdesc = makeResampleDesc("Holdout")
learn = makeLearner("classif.ksvm", par.vals = list(kernel = "rbfdot"))
lrn = makeTuneWrapper(learn, control = ctrl, measures = list(acc, mmce),
  resampling = rdesc, par.set = ps, show.info = FALSE)
res = resample(lrn, task = pid.task, resampling = cv2, extract = getTuneResult, show.info = FALSE)
data = generateHyperParsEffectData(res)
plt = plotHyperParsEffect(data, x = "C", y = "sigma", z = "acc.test.mean",
  plot.type = "heatmap", interpolate = "regr.earth", show.experiments = TRUE,
  nested.agg = mean)
min_plt = min(plt$data$acc.test.mean, na.rm = TRUE)
max_plt = max(plt$data$acc.test.mean, na.rm = TRUE)
med_plt = mean(c(min_plt, max_plt))
plt + scale_fill_gradient2(breaks = seq(min_plt, max_plt, length.out = 5),
  low = "red", mid = "white", high = "blue", midpoint = med_plt)
```



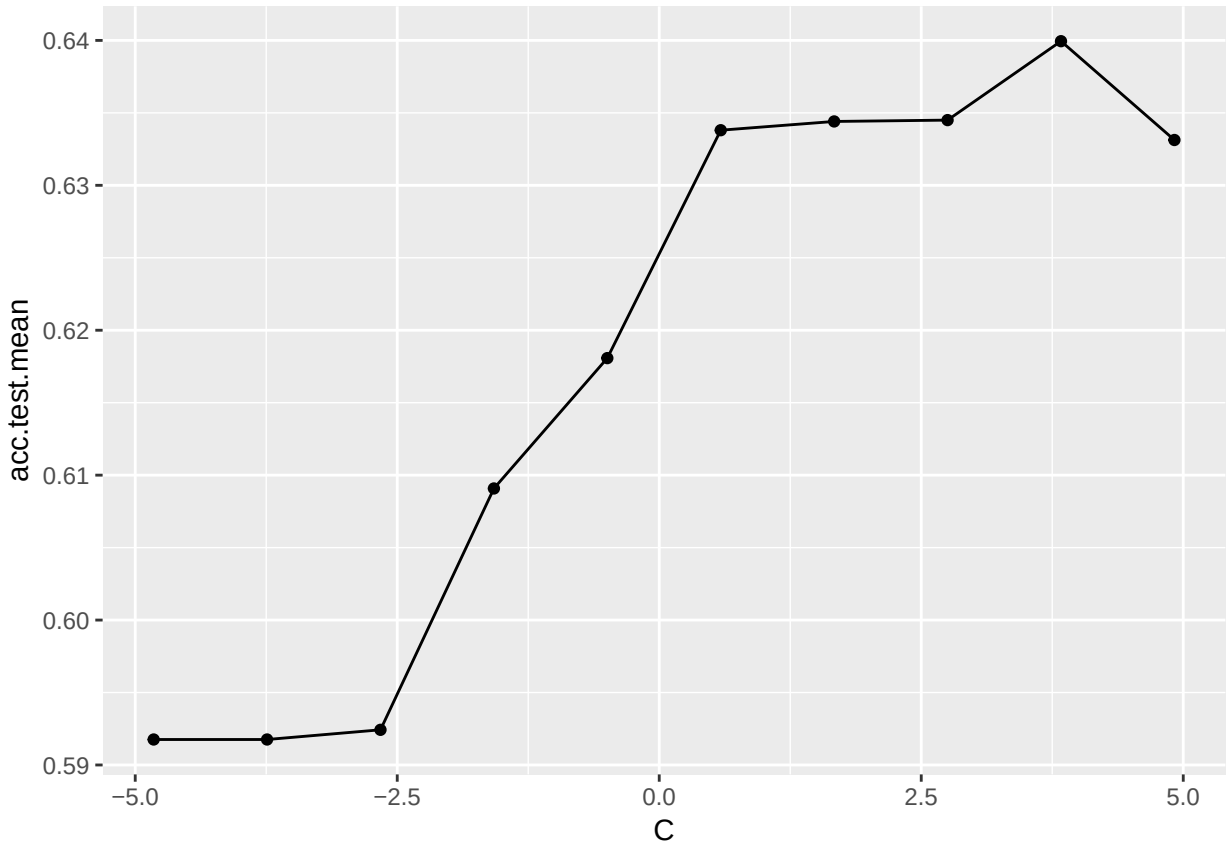
3.16.4 Visualizing the effects of more than 2 hyperparameters

In order to visualize the result when tuning 3 or more hyperparameters simultaneously we can take advantage of partial dependence plots to show how the performance depends on a one- or two-dimensional subset of the hyperparameters. Below we tune three hyperparameters `C`, `sigma`, and `degree` of an SVM with Bessel kernel and set the `partial.dep` flag to `TRUE` to indicate that we intend to calculate partial dependences.

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x),
  makeNumericParam("sigma", lower = -5, upper = 5, trafo = function(x) 2^x),
  makeDiscreteParam("degree", values = 2:5))
ctrl = makeTuneControlRandom(maxit = 100L)
rdesc = makeResampleDesc("Holdout", predict = "both")
learn = makeLearner("classif.ksvm", par.vals = list(kernel = "besseldot"))
res = tuneParams(learn, task = pid.task, control = ctrl,
  measures = list(acc, setAggregation(acc, train.mean)), resampling = rdesc,
  par.set = ps, show.info = FALSE)
data = generateHyperParsEffectData(res, partial.dep = TRUE)
```

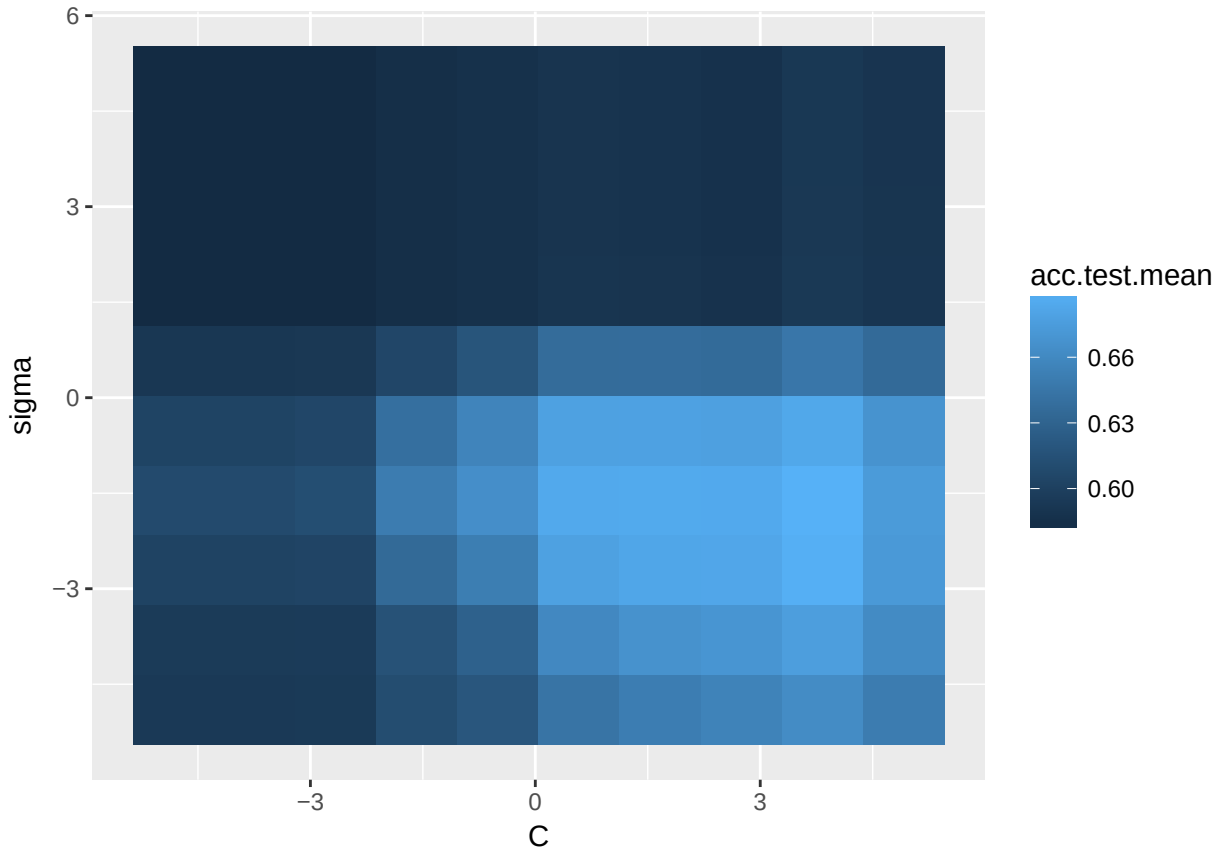
You can generate a plot for a single hyperparameter like `C` as shown below. The `partial.dep.learn` can be any regression Learner (`makeLearner()`) in `mlr` and is used to regress the attained performance values on the values of the 3 hyperparameters visited during tuning. The fitted model serves as basis for calculating partial dependences.

```
plotHyperParsEffect(data, x = "C", y = "acc.test.mean", plot.type = "line",
  partial.dep.learn = "regr.randomForest")
```



We can also look at two hyperparameters simultaneously, for example `C` and `sigma`.

```
plotHyperParsEffect(data, x = "C", y = "sigma", z = "acc.test.mean",
  plot.type = "heatmap", partial.dep.learn = "regr.randomForest")
```



3.17 Out-of-Bag Predictions

Some learners like random forest use bagging. Bagging means that the learner consists of an ensemble of several base learners and each base learner is trained with a different random subsample or bootstrap sample from all observations. A prediction made for an observation in the original data set using only base learners not trained on this particular observation is called out-of-bag (OOB) prediction. These predictions are not prone to overfitting, as each prediction is only made by learners that did not use the observation for training.

To get a list of learners that provide OOB predictions, you can call `listLearners(obj = NA, properties = "oobpreds")`.

```
listLearners(obj = NA, properties = "oobpreds")[c("class", "package")]
## Warning in listLearners.character(obj = NA_character_, properties, quiet, : The following learners c
## classif.mxff,regr.mxff
## Check ?learners to see which packages you need or install mlr with all suggestions.
##                       class         package
## 1    classif.randomForest    randomForest
## 2 classif.randomForestSRC randomForestSRC
## 3          classif.ranger          ranger
## 4          classif.rFerns          rFerns
## 5       regr.randomForest    randomForest
## 6    regr.randomForestSRC randomForestSRC
## ... (#rows: 8, #cols: 2)
```

In `mlr` function `getOOBPreds()` can be used to extract these observations from the trained models. These predictions can be used to evaluate the performance of a given learner like in the following example.

```
lrn = makeLearner("classif.ranger", predict.type = "prob", predict.threshold = 0.6)
mod = train(lrn, sonar.task)
oob = getOOBPreds(mod, sonar.task)
oob
## Prediction: 208 observations
## predict.type: prob
## threshold: M=0.60,R=0.40
## time: NA
##   id truth    prob.M    prob.R response
## 1  1     R 0.5356531 0.4643469        R
## 2  2     R 0.5169507 0.4830493        R
## 3  3     R 0.6706219 0.3293781        M
## 4  4     R 0.4956371 0.5043629        R
## 5  5     R 0.5456107 0.4543893        R
## 6  6     R 0.4267494 0.5732506        R
## ... (#rows: 208, #cols: 5)
performance(oob, measures = list(auc, mmce))
##       auc      mmce
## 0.9395375 0.1682692
```

As the predictions that are used are out-of-bag, this evaluation strategy is very similar to common resampling strategies like 10-fold cross-validation, but much faster, as only one training instance of the model is required.

3.18 Handling of Spatial Data

3.18.1 Introduction

Spatial data is different from non-spatial data by having a spatial reference information attached to each observation. This information is usually stored as coordinates, often named `x` and `y`. Coordinates are either stored in UTM (Universal Transverse Mercator) or latitude/longitude format.

Treating spatial data sets like non-spatial ones leads to overoptimistic results in predictive accuracy of models (Brenning 2005). This is due to the underlying spatial autocorrelation in the data. Spatial autocorrelation does occur in all spatial data sets. Magnitude varies depending on the characteristics of the data set. The closer observations are located to each other, the more similar they are.

If common validation procedures like cross-validation are applied to such data sets, they assume independence of the observation upfront to provide unbiased estimates. However, this assumption is violated in the spatial case due to spatial autocorrelation. Subsequently, non-spatial cross-validation will fail to provide accurate performance estimates.

By doing a random sampling of the data set (i.e., non-spatial sampling), training and test set data are often located directly next to each other (in geographical space). Hence, the test set will contain observations which are somewhat similar (due to spatial autocorrelation) to observations in the training set. This leads to the effect that the model, which was trained on the training set, performs quite well on the test data because it already knows it to some degree.

To reduce this bias on the resulting predictive accuracy estimate, Brenning 2005 suggested using spatial partitioning in favor of random partitioning (see Figure 1). Here, spatial clusters are equal to the number of folds chosen. These spatially disjoint subsets of the data introduce a spatial distance between training and test set. This reduces the influence of spatial autocorrelation and subsequently also the overoptimistic predictive accuracy estimates. The example in Figure 1 shows a five-fold nested cross-validation setting and exhibits the difference between spatial and non-spatial partitioning. The nested approach is used when hyperparameter tuning is performed.

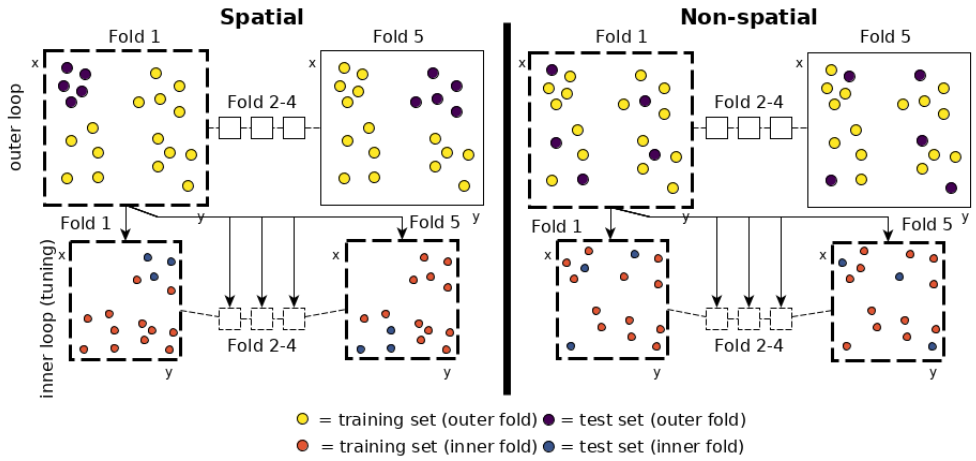


Figure 3: Nested Spatial and Non-Spatial Cross-Validation

3.18.2 How to use spatial partitioning in mlr

Spatial partitioning can be used when performing cross-validation. In any `resample()` call you can choose `SpCV` or `SpRepCV` to use it. While `SpCV` will perform a spatial cross-validation with only one repetition, `SpRepCV` gives you the option to choose any number of repetitions. As a rule of thumb, usually 100 repetitions are used with the aim to reduce variance introduced by partitioning.

There are some prerequisites for this:

When specifying the task, you need to provide spatial coordinates through argument `coordinates`. The supplied `data.frame` needs to have the same number of rows as the data and at least two dimensions need to be supplied. This means that a 3-D partitioning might also work but we have not tested this explicitly. Coordinates need to be numeric so it is suggested to use a UTM projection. If this applies, the coordinates will be used for spatial partitioning if `SpCV` or `SpRepCV` is selected as resampling strategy.

3.18.3 Examples

The `spatial.task` data set serves as an example data set for spatial modeling tasks in `mlr`. The task argument `coordinates` is a `data.frame` with two coordinates that will later be used for the spatial partitioning of the data set.

In this example, the "Random Forest" algorithm (package ranger) is used to model a binomial response variable.

For performance assessment, a repeated spatial cross-validation with 5 folds and 5 repetitions is chosen.

3.18.3.1 Spatial Cross-Validation

```
data("spatial.task")
spatial.task
## Supervised task: ecuador
## Type: classif
## Target: slides
## Observations: 751
## Features:
##    numerics     factors     ordered functionals
```

```
##          10           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: TRUE
## Classes: 2
## FALSE  TRUE
##   251   500
## Positive class: TRUE
learner.rf = makeLearner("classif.ranger", predict.type = "prob")

resampling = makeResampleDesc("SpRepCV", fold = 5, reps = 5)

set.seed(123)
out = resample(learner = learner.rf, task = spatial.task,
  resampling = resampling, measures = list(auc))
## Resampling: repeated spatial cross-validation
## Measures:             auc
## [Resample] iter 1:    0.6750295
## [Resample] iter 2:    0.5390011
## [Resample] iter 3:    0.7126168
## [Resample] iter 4:    0.7179386
## [Resample] iter 5:    0.4481074
## [Resample] iter 6:    0.6661747
## [Resample] iter 7:    0.5231959
## [Resample] iter 8:    0.7140047
## [Resample] iter 9:    0.7230064
## [Resample] iter 10:   0.4368742
## [Resample] iter 11:   0.6793610
## [Resample] iter 12:   0.6912488
## [Resample] iter 13:   0.5822304
## [Resample] iter 14:   0.8494331
## [Resample] iter 15:   0.6187330
## [Resample] iter 16:   0.7044860
## [Resample] iter 17:   0.6549153
## [Resample] iter 18:   0.6441667
## [Resample] iter 19:   0.5603976
## [Resample] iter 20:   0.5034305
## [Resample] iter 21:   0.6673554
## [Resample] iter 22:   0.4422466
## [Resample] iter 23:   0.7228560
## [Resample] iter 24:   0.7178289
## [Resample] iter 25:   0.5420875
##
## Aggregated Result: auc.test.mean=0.6294690
##
mean(out$measures.test$auc)
## [1] 0.629469
```

We can check for the introduced spatial autocorrelation bias here by performing the same modeling task using a non-spatial partitioning setting. To do so, we simply choose `RepCV` instead of `SpRepCV`. There is no need to remove `coordinates` from the task as it is only used if `SpCV` or `SpRepCV` is selected as the resampling strategy.

3.18.3.2 Non-Spatial Cross-Validation

```
learner.rf = makeLearner("classif.ranger", predict.type = "prob")

resampling = makeResampleDesc("RepCV", fold = 5, reps = 5)

set.seed(123)
out = resample(learner = learner.rf, task = spatial.task,
  resampling = resampling, measures = list(auc))
## Resampling: repeated cross-validation
## Measures:             auc
## [Resample] iter 1:    0.7362637
## [Resample] iter 2:    0.7651485
## [Resample] iter 3:    0.8119974
## [Resample] iter 4:    0.6807436
## [Resample] iter 5:    0.7441992
## [Resample] iter 6:    0.7769076
## [Resample] iter 7:    0.8383069
## [Resample] iter 8:    0.7276557
## [Resample] iter 9:    0.7341821
## [Resample] iter 10:   0.7563874
## [Resample] iter 11:   0.7542955
## [Resample] iter 12:   0.7972408
## [Resample] iter 13:   0.7444000
## [Resample] iter 14:   0.7083333
## [Resample] iter 15:   0.7405476
## [Resample] iter 16:   0.7296736
## [Resample] iter 17:   0.7212000
## [Resample] iter 18:   0.7715856
## [Resample] iter 19:   0.7898859
## [Resample] iter 20:   0.7915686
## [Resample] iter 21:   0.7391717
## [Resample] iter 22:   0.7454031
## [Resample] iter 23:   0.8092320
## [Resample] iter 24:   0.7267977
## [Resample] iter 25:   0.7643745
##
## Aggregated Result: auc.test.mean=0.7562201
##
mean(out$measures.test$auc)
## [1] 0.7562201
```

The introduced bias (caused by spatial autocorrelation) in performance in this example is around 0.12 AUROC.

3.18.4 Notes

- Some models are more affected by spatial autocorrelation than others. In general, it can be said that the more flexible a model is, the more it will profit from underlying spatial autocorrelation. Simpler models (e.g., GLM) will show less overoptimistic performance estimates.
- The concept of spatial cross-validation was originally implemented in package sperrorest. This package comes with even more partitioning options and the ability to visualize the spatial grouping of folds. We plan to integrate more functions from sperrorest into `mlr` so stay tuned!

- For more detailed information, see Brenning 2005 and Brenning2012.

4 Extending

4.1 Integrating Another Learner

In order to integrate a learning algorithm into `mlr` some interface code has to be written. Three functions are mandatory for each learner.

- First, define a new learner class with a name, description, capabilities, parameters, and a few other things. (An object of this class can then be generated by `makeLearner()`.)
- Second, you need to provide a function that calls the learner function and builds the model given data (which makes it possible to invoke training by calling `mlr`'s `train()` function).
- Finally, a prediction function that returns predicted values given new data is required (which enables invoking prediction by calling `mlr`'s `predict.WrappedModel()` function).

Technically, integrating a learning method means introducing a new S3 `class` and implementing the corresponding methods for the generic functions `RLearner()`, `trainLearner()`, and `predictLearner()`. Therefore we start with a quick overview of the involved classes and constructor functions.

4.1.1 Classes, constructors, and naming schemes

As you already know `makeLearner()` generates an object of class Learner (`makeLearner()`).

```
class(makeLearner(cl = "classif.lda"))
## [1] "classif.lda"     "RLearnerClassif" "RLearner"        "Learner"
class(makeLearner(cl = "regr.lm"))
## [1] "regr.lm"      "RLearnerRegr" "RLearner"     "Learner"
class(makeLearner(cl = "surv.coxph"))
## [1] "surv.coxph"   "RLearnerSurv" "RLearner"     "Learner"
class(makeLearner(cl = "cluster.kmeans"))
## [1] "cluster.kmeans"  "RLearnerCluster" "RLearner"        "Learner"
class(makeLearner(cl = "multilabel.rFerns"))
## [1] "multilabel.rFerns"  "RLearnerMultilabel" "RLearner"
## [4] "Learner"
```

The first element of each class attribute vector is the name of the learner class passed to the `cl` argument of `makeLearner()`. Obviously, this adheres to the naming conventions

- `"classif.<R_method_name>"` for classification,
- `"multilabel.<R_method_name>"` for multilabel classification,
- `"regr.<R_method_name>"` for regression,
- `"surv.<R_method_name>"` for survival analysis, and
- `"cluster.<R_method_name>"` for clustering.

Additionally, there exist intermediate classes that reflect the type of learning problem, i.e., all classification learners inherit from `RLearnerClassif` (`RLearner()`), all regression learners from `RLearnerRegr` (`RLearner()`) and so on. Their superclasses are `RLearner()` and finally `Learner` (`makeLearner()`). For all these (sub)classes there exist constructor functions `makeRLearner` (`RLearner()`), `makeRLearnerClassif` (`RLearner()`), `makeRLearneRegr` (`RLearner()`) etc. that are called internally by `makeLearner()`.

A short side remark: As you might have noticed there does not exist a special learner class for cost-sensitive classification (costsens) with example-specific costs. This type of learning task is currently exclusively handled through wrappers like `makeCostSensWeightedPairsWrapper()`.

In the following we show how to integrate learners for the five types of learning tasks mentioned above. Defining a completely new type of learner that has special properties and does not fit into one of the existing schemes is of course possible, but much more advanced and not covered here.

We use a classification example to explain some general principles (so even if you are interested in integrating a learner for another type of learning task you might want to read the following section). Examples for other types of learning tasks are shown later on.

4.1.2 Classification

We show how the Linear Discriminant Analysis (`MASS::lda()`) from package `MASS` has been integrated into the classification learner `classif.lda` in `mlr` as an example.

4.1.2.1 Definition of the learner

The minimal information required to define a learner is the `mlr` name of the learner, its package, the parameter set, and the set of properties of your learner. In addition, you may provide a human-readable name, a short name and a note with information relevant to users of the learner.

First, name your learner. According to the naming conventions above the name starts with `classif.` and we choose `classif.lda`.

Second, we need to define the parameters of the learner. These are any options that can be set when running it to change how it learns, how input is interpreted, how and what output is generated, and so on. `mlr` provides a number of functions to define parameters, a complete list can be found in the documentation of `LearnerParam` (`ParamHelpers::LearnerParam()`) of the `ParamHelpers` package.

In our example, we have discrete and numeric parameters, so we use `makeDiscreteLearnerParam` (`ParamHelpers::LearnerParam()`) and `makeNumericLearnerParam` (`ParamHelpers::LearnerParam()`) to incorporate the complete description of the parameters. We include all possible values for discrete parameters and lower and upper bounds for numeric parameters. Strictly speaking it is not necessary to provide bounds for all parameters and if this information is not available they can be estimated, but providing accurate and specific information here makes it possible to tune the learner much better (see the section on tuning).

Next, we add information on the properties of the learner (see also the section on learners). Which types of features are supported (numerics, factors)? Are case weights supported? Are class weights supported? Can the method deal with missing values in the features and deal with NA's in a meaningful way (not `na.omit`)? Are one-class, two-class, multi-class problems supported? Can the learner predict posterior probabilities?

If the learner supports class weights the name of the relevant learner parameter can be specified via argument `class.weights.param`.

Below is the complete code for the definition of the LDA learner. It has one discrete parameter, `method`, and two continuous ones, `nu` and `tol`. It supports classification problems with two or more classes and can deal with numeric and factor explanatory variables. It can predict posterior probabilities.

```
makeRLearner.classif.lda = function() {
  makeRLearnerClassif(
    cl = "classif.lda",
    package = "MASS",
    par.set = makeParamSet(
      makeDiscreteLearnerParam(id = "method", default = "moment", values = c("moment", "mle", "mve", "t
      makeNumericLearnerParam(id = "nu", lower = 2, requires = quote(method == "t")),
      makeNumericLearnerParam(id = "tol", default = 1e-4, lower = 0),
      makeDiscreteLearnerParam(id = "predict.method", values = c("plug-in", "predictive", "debiased"),
        default = "plug-in", when = "predict"),
      makeLogicalLearnerParam(id = "CV", default = FALSE, tunable = FALSE)
```

```
    ),
    properties = c("twoclass", "multiclass", "numerics", "factors", "prob"),
    name = "Linear Discriminant Analysis",
    short.name = "lda",
    note = "Learner param 'predict.method' maps to 'method' in predict.lda."
  )
}
```

4.1.2.2 Creating the training function of the learner

Once the learner has been defined, we need to tell `mlr` how to call it to train a model. The name of the function has to start with `trainLearner.`, followed by the `mlr` name of the learner as defined above (`classif.lda` here). The prototype of the function looks as follows.

```
function(.learner, .task, .subset, .weights = NULL, ...) { }
```

This function must fit a model on the data of the task `.task` with regard to the subset defined in the integer vector `.subset` and the parameters passed in the `...` arguments. Usually, the data should be extracted from the task using `getTaskData()`. This will take care of any subsetting as well. It must return the fitted model. `mlr` assumes no special data type for the return value – it will be passed to the predict function we are going to define below, so any special code the learner may need can be encapsulated there.

For our example, the definition of the function looks like this. In addition to the data of the task, we also need the formula that describes what to predict. We use the function `getTaskFormula()` to extract this from the task.

```
trainLearner.classif.lda = function (.learner, .task, .subset, .weights = NULL, ...)
{
    f = getTaskFormula(.task)
    MASS::lda(f, data = getTaskData(.task, .subset), ...)
}
```

4.1.2.3 Creating the prediction method

Finally, the prediction function needs to be defined. The name of this function starts with `predictLearner.`, followed again by the `mlr` name of the learner. The prototype of the function is as follows.

```
function(.learner, .model, .newdata, ...) { }
```

It must predict for the new observations in the `data.frame .newdata` with the wrapped model `.model`, which is returned from the training function. The actual model the learner built is stored in the `$learner.model` member and can be accessed simply through `.model$learner.model`.

For classification, you have to return a factor of predicted classes if `.learner$predict.type` is `"response"`, or a matrix of predicted probabilities if `.learner$predict.type` is `"prob"` and this type of prediction is supported by the learner. In the latter case the matrix must have the same number of columns as there are classes in the task and the columns have to be named by the class names.

The definition for LDA looks like this. It is pretty much just a straight pass-through of the arguments to the `base::predict()` function and some extraction of prediction data depending on the type of prediction requested.

```
predictLearner.classif.lda = function (.learner, .model, .newdata, predict.method = "plug-in",
    ...)
{
    p = predict(.model$learner.model, newdata = .newdata, method = predict.method,
        ...)
```

```
    if (.learner$predict.type == "response")
        return(p$class)
    else return(p$posterior)
}
```

4.1.3 Regression

The main difference for regression is that the type of predictions are different (numeric instead of labels or probabilities) and that not all of the properties are relevant. In particular, whether one-, two-, or multi-class problems and posterior probabilities are supported is not applicable.

Apart from this, everything explained above applies. Below is the definition for the `earth::earth()` learner.

```
makeRLearner.regr.earth = function() {
  makeRLearnerRegr(
    cl = "regr.earth",
    package = "earth",
    par.set = makeParamSet(
      makeLogicalLearnerParam(id = "keepxy", default = FALSE, tunable = FALSE),
      makeNumericLearnerParam(id = "trace", default = 0, upper = 10, tunable = FALSE),
      makeIntegerLearnerParam(id = "degree", default = 1L, lower = 1L),
      makeNumericLearnerParam(id = "penalty"),
      makeIntegerLearnerParam(id = "nk", lower = 0L),
      makeNumericLearnerParam(id = "thres", default = 0.001),
      makeIntegerLearnerParam(id = "minspan", default = 0L),
      makeIntegerLearnerParam(id = "endspan", default = 0L),
      makeNumericLearnerParam(id = "newvar.penalty", default = 0),
      makeIntegerLearnerParam(id = "fast.k", default = 20L, lower = 0L),
      makeNumericLearnerParam(id = "fast.beta", default = 1),
      makeDiscreteLearnerParam(id = "pmethod", default = "backward",
        values = c("backward", "none", "exhaustive", "forward", "seqrep", "cv")),
      makeIntegerLearnerParam(id = "nprune")
    ),
    properties = c("numerics", "factors"),
    name = "Multivariate Adaptive Regression Splines",
    short.name = "earth",
    note = ""
  )
}
trainLearner.regr.earth = function (.learner, .task, .subset, .weights = NULL, ...)
{
    f = getTaskFormula(.task)
    earth::earth(f, data = getTaskData(.task, .subset), ...)
}
predictLearner.regr.earth = function (.learner, .model, .newdata, ...)
{
    predict(.model$learner.model, newdata = .newdata)[, 1L]
}
```

Again most of the data is passed straight through to/from the train/predict functions of the learner.

4.1.4 Survival analysis

For survival analysis, you have to return so-called linear predictors in order to compute the default measure for this task type, the cindex (for `.learner$predict.type == "response"`). For `.learner$predict.type == "prob"`, there is no substantially meaningful measure (yet). You may either ignore this case or return something like predicted survival curves (cf. example below).

There are three properties that are specific to survival learners: "rcens", "lcens" and "icens", defining the type(s) of censoring a learner can handle – right, left and/or interval censored.

Let's have a look at how the Cox Proportional Hazard Model (`survival::coxph()`) from package `survival` has been integrated into the survival learner `surv.coxph` in `mlr` as an example:

```
makeRLearner.surv.coxph = function() {
  makeRLearnerSurv(
    cl = "surv.coxph",
    package = "survival",
    par.set = makeParamSet(
      makeDiscreteLearnerParam(id = "ties", default = "efron", values = c("efron", "breslow", "exact")),
      makeLogicalLearnerParam(id = "singular.ok", default = TRUE),
      makeNumericLearnerParam(id = "eps", default = 1e-09, lower = 0),
      makeNumericLearnerParam(id = "toler.chol", default = .Machine$double.eps^0.75, lower = 0),
      makeIntegerLearnerParam(id = "iter.max", default = 20L, lower = 1L),
      makeNumericLearnerParam(id = "toler.inf", default = sqrt(.Machine$double.eps^0.75), lower = 0),
      makeIntegerLearnerParam(id = "outer.max", default = 10L, lower = 1L),
      makeLogicalLearnerParam(id = "model", default = FALSE, tunable = FALSE),
      makeLogicalLearnerParam(id = "x", default = FALSE, tunable = FALSE),
      makeLogicalLearnerParam(id = "y", default = TRUE, tunable = FALSE)
    ),
    properties = c("missings", "numerics", "factors", "weights", "prob", "rcens"),
    name = "Cox Proportional Hazard Model",
    short.name = "coxph",
    note = ""
  )
}
trainLearner.surv.coxph = function (.learner, .task, .subset, .weights = NULL, ...)
{
    f = getTaskFormula(.task)
    data = getTaskData(.task, subset = .subset)
    if (is.null(.weights)) {
        survival::coxph(formula = f, data = data, ...)
    }
    else {
        survival::coxph(formula = f, data = data, weights = .weights,
            ...)
    }
}
predictLearner.surv.coxph = function (.learner, .model, .newdata, ...)
{
    predict(.model$learner.model, newdata = .newdata, type = "lp",
        ...)
}
```

4.1.5 Clustering

For clustering, you have to return a numeric vector with the IDs of the clusters that the respective datum has been assigned to. The numbering should start at 1.

Below is the definition for the `FarthestFirst` (`RWeka::FarthestFirst()`) learner from the `RWeka` package. Weka starts the IDs of the clusters at 0, so we add 1 to the predicted clusters. RWeka has a different way of setting learner parameters; we use the special `Weka_control` function to do this.

```
makeRLearner.cluster.FarthestFirst = function() {
  makeRLearnerCluster(
    cl = "cluster.FarthestFirst",
    package = "RWeka",
    par.set = makeParamSet(
      makeIntegerLearnerParam(id = "N", default = 2L, lower = 1L),
      makeIntegerLearnerParam(id = "S", default = 1L, lower = 1L),
      makeLogicalLearnerParam(id = "output-debug-info", default = FALSE, tunable = FALSE)
    ),
    properties = c("numerics"),
    name = "FarthestFirst Clustering Algorithm",
    short.name = "farthestfirst"
  )
}
trainLearner.cluster.FarthestFirst = function (.learner, .task, .subset, .weights = NULL, ...)
{
    ctrl = RWeka::Weka_control(...)
    RWeka::FarthestFirst(getTaskData(.task, .subset), control = ctrl)
}
predictLearner.cluster.FarthestFirst = function (.learner, .model, .newdata, ...)
{
    as.integer(predict(.model$learner.model, .newdata, ...)) +
        1L
}
```

4.1.6 Multilabel classification

As stated in the multilabel section, multilabel classification methods can be divided into problem transformation methods and algorithm adaptation methods.

At this moment the only problem transformation method implemented in `mlr` is the binary relevance method (`makeMultilabelBinaryRelevanceWrapper()`). Integrating more of these methods requires good knowledge of the architecture of the `mlr` package.

The integration of an algorithm adaptation multilabel classification learner is easier and works very similar to the normal multiclass-classification. In contrast to the multiclass case, not all of the learner properties are relevant. In particular, whether one-, two-, or multi-class problems are supported is not applicable. Furthermore the prediction function output must be a matrix with each prediction of a label in one column and the names of the labels as column names. If `.learner$predict.type` is `"response"` the predictions must be logical. If `.learner$predict.type` is `"prob"` and this type of prediction is supported by the learner, the matrix must consist of predicted probabilities.

Below is the definition of the `rFerns::rFerns()` learner from the `rFerns` package, which does not support probability predictions.

```
makeRLearner.multilabel.rFerns = function() {
  makeRLearnerMultilabel(
```

```
    cl = "multilabel.rFerns",
    package = "rFerns",
    par.set = makeParamSet(
      makeIntegerLearnerParam(id = "depth", default = 5L),
      makeIntegerLearnerParam(id = "ferns", default = 1000L)
    ),
    properties = c("numerics", "factors", "ordered"),
    name = "Random ferns",
    short.name = "rFerns",
    note = ""
  )
}
trainLearner.multilabel.rFerns = function (.learner, .task, .subset, .weights = NULL, ...)
{
    d = getTaskData(.task, .subset, target.extra = TRUE)
    rFerns::rFerns(x = d$data, y = as.matrix(d$target), ...)
}
predictLearner.multilabel.rFerns = function (.learner, .model, .newdata, ...)
{
    as.matrix(predict(.model$learner.model, .newdata, ...))
}
```

4.1.7 Creating a new method for extracting feature importance values

Some learners, for example decision trees and random forests, can calculate feature importance values, which can be extracted from a fitted model (`makeWrappedModel()`) using function `getFeatureImportance()`.

If your newly integrated learner supports this you need to

- add `"featimp"` to the learner properties and
- implement a new S3 method for function `getFeatureImportanceLearner()` (which later is called internally by `getFeatureImportance()`) in order to make this work.

This method takes the `Learner()` `.learner`, the WrappedModel (`makeWrappedModel()`) `.model` and potential further arguments and calculates or extracts the feature importance. It must return a named vector of importance values.

Below are two simple examples. In case of `"classif.rpart"` the feature importance values can be easily extracted from the fitted model.

```
getFeatureImportanceLearner.classif.rpart = function (.learner, .model, ...)
{
    mod = getLearnerModel(.model, more.unwrap = TRUE)
    mod$variable.importance
}
```

For the `randomForestSRC::rfsrc()` from package `randomForestSRC` function `randomForestSRC::vimp()` is called.

```
getFeatureImportanceLearner.classif.randomForestSRC = function (.learner, .model, ...)
{
    mod = getLearnerModel(.model, more.unwrap = TRUE)
    randomForestSRC::vimp(mod, ...)$importance[, "all"]
}
```

4.1.8 Creating a new method for extracting out-of-bag predictions

Many ensemble learners generate out-of-bag predictions (OOB predictions) automatically. `mlr` provides the function `getOOBPreds()` to access these predictions in the `mlr` framework.

If your newly integrated learner is able to calculate OOB predictions and you want to be able to access them in `mlr` via `getOOBPreds()` you need to

- add `"oobpreds"` to the learner properties and
- implement a new S3 method for function `getOOBPredsLearner()` (which later is called internally by `getOOBPreds()`).

This method takes the Learner (`makeLearner()`) `.learner` and the WrappedModel (`makeWrappedModel()`) `.model` and extracts the OOB predictions. It must return the predictions in the same format as the `predictLearner()` function.

```
getOOBPredsLearner.classif.randomForest = function (.learner, .model)
{
    if (.learner$predict.type == "response") {
        m = getLearnerModel(.model, more.unwrap = TRUE)
        unname(m$predicted)
    }
    else {
        getLearnerModel(.model, more.unwrap = TRUE)$votes
    }
}
```

4.1.9 Registering your learner

If your interface code to a new learning algorithm exists only locally, i.e., it is not (yet) merged into `mlr` or does not live in an extra package with a proper namespace you might want to register the new S3 methods to make sure that these are found by, e.g., `listLearners()`. You can do this as follows:

```
registerS3method("makeRLearner", "<awesome_new_learner_class>", makeRLearner.<awesome_new_learner_class
registerS3method("trainLearner", "<awesome_new_learner_class>", trainLearner.<awesome_new_learner_class
registerS3method("predictLearner", "<awesome_new_learner_class>", predictLearner.<awesome_new_learner_cl
```

If you have written more methods, for example in order to extract feature importance values or out-of-bag predictions these also need to be registered in the same manner, for example:

```
registerS3method("getFeatureImportanceLearner", "<awesome_new_learner_class>",
  getFeatureImportanceLearner.<awesome_new_learner_class>)
```

For the new learner to work with parallelization, you may have to export the new methods explicitly:

```
parallelExport("trainLearner.<awesome_new_learner_class>", "predictLearner.<awesome_new_learner_class>"
```

4.1.10 Further information for developers

If you haven't written a learner interface for private use only, but intend to send a pull request to have it included in the `mlr` package there are a few things to take care of, most importantly unit testing!

For general information about contributing to the package, unit testing, version control setup and the like please also read the coding guidelines in the mlr Wiki.

- The R file containing the interface code should adhere to the naming convention `RLearner_<type>_<learner_name>.R`, e.g., `RLearner_classif_lda.R`, see for example https://github.com/mlr-org/mlr/blob/master/R/

RLearner_classif_lda.R and contain the necessary roxygen `@export` tags to register the S3 methods in the NAMESPACE.

- The learner interfaces should work out of the box without requiring any parameters to be set, e.g., `train("classif.lda", iris.task)` should run. Sometimes, this makes it necessary to change or set some additional defaults as explained above and – very important – informing the user about this in the `note`.
- The parameter set of the learner should be as complete as possible.
- Every learner interface must be unit tested.

4.1.11 Unit testing

The tests make sure that we get the same results when the learner is invoked through the `mlr` interface and when using the original functions. If you are not familiar or want to learn more about unit testing and package `testthat` have a look at the Testing chapter in Hadley Wickham's R packages.

In `mlr` all unit tests are in the following directory: https://github.com/mlr-org/mlr/tree/master/tests/testthat. For each learner interface there is an individual file whose name follows the scheme `test_<type>_<learner_name>.R`, for example https://github.com/mlr-org/mlr/blob/master/tests/testthat/test_classif_lda.R.

Below is a snippet from the tests of the lda interface https://github.com/mlr-org/mlr/blob/master/tests/testthat/test_classif_lda.R.

```
test_that("classif_lda", {
  requirePackagesOrSkip("MASS", default.method = "load")

  set.seed(getOption("mlr.debug.seed"))
  m = MASS::lda(formula = multiclass.formula, data = multiclass.train)
  set.seed(getOption("mlr.debug.seed"))
  p = predict(m, newdata = multiclass.test)

  testSimple("classif.lda", multiclass.df, multiclass.target, multiclass.train.inds, p$class)
  testProb("classif.lda", multiclass.df, multiclass.target, multiclass.train.inds, p$posterior)
})
```

The tests make use of numerous helper objects and helper functions. All of these are defined in the `helper_` files in https://github.com/mlr-org/mlr/blob/master/tests/testthat/.

In the above code the first line just loads package `MASS` or skips the test if the package is not available. The objects `multiclass.formula`, `multiclass.train`, `multiclass.test` etc. are defined in https://github.com/mlr-org/mlr/blob/master/tests/testthat/helper_objects.R. We tried to choose fairly self-explanatory names: For example `multiclass` indicates a multi-class classification problem, `multiclass.train` contains data for training, `multiclass.formula` a `formula` object etc.

The test fits an lda model on the training set and makes predictions on the test set using the original functions `MASS::lda()` and `MASS:predict.lda()`. The helper functions `testSimple` and `testProb` perform training and prediction on the same data using the `mlr` interface – `testSimple` for `predict.type = "response` and `testProbs` for `predict.type = "prob"` – and check if the predicted class labels and probabilities coincide with the outcomes `p$class` and `p$posterior`.

In order to get reproducible results seeding is required for many learners. The `"mlr.debug.seed"` works as follows: When invoking the tests the option `"mlr.debug.seed"` is set (see https://github.com/mlr-org/mlr/blob/master/tests/testthat/helper_zzz.R), and `set.seed(getOption("mlr.debug.seed"))` is used to specify the seed. Internally, `mlr`'s train and predict.WrappedModel functions check if the `"mlr.debug.seed"` option is set and if yes, also specify the seed.

Note that the option `"mlr.debug.seed"` is only set for testing, so no seeding happens in normal usage of `mlr`.

Let's look at a second example. Many learners have parameters that are commonly changed or tuned and it is important to make sure that these are passed through correctly. Below is a snippet from https://github.com/mlr-org/mlr/blob/master/tests/testthat/test_regr_randomForest.R.

```
test_that("regr_randomForest", {
  requirePackagesOrSkip("randomForest", default.method = "load")

  parset.list = list(
    list(),
    list(ntree = 5, mtry = 2),
    list(ntree = 5, mtry = 4),
    list(proximity = TRUE, oob.prox = TRUE),
    list(nPerm = 3)
  )

  old.predicts.list = list()

  for (i in 1:length(parset.list)) {
    parset = parset.list[[i]]
    pars = list(formula = regr.formula, data = regr.train)
    pars = c(pars, parset)
    set.seed(getOption("mlr.debug.seed"))
    m = do.call(randomForest::randomForest, pars)
    set.seed(getOption("mlr.debug.seed"))
    p = predict(m, newdata = regr.test, type = "response")
    old.predicts.list[[i]] = p
  }

  testSimpleParsets("regr.randomForest", regr.df, regr.target,
    regr.train.inds, old.predicts.list, parset.list)
})
```

All tested parameter configurations are collected in the `parset.list`. In order to make sure that the default parameter configuration is tested the first element of the `parset.list` is an empty `list` (`base::list()`). Then we simply loop over all parameter settings and store the resulting predictions in `old.predicts.list`. Again the helper function `testSimpleParsets` does the same using the `mlr` interface and compares the outcomes.

Additional to tests for individual learners we also have general tests that loop through all integrated learners and make for example sure that learners have the correct properties (e.g. a learner with property `"factors"` can cope with `factor` (`base::factor()`) features, a learner with property `"weights"` takes observation weights into account properly etc.). For example https://github.com/mlr-org/mlr/blob/master/tests/testthat/test_learners_all_classif.R runs through all classification learners. Similar tests exist for all types of learning methods like regression, cluster and survival analysis as well as multilabel classification.

In order to run all tests for, e.g., classification learners on your machine you can invoke the tests from within **R** by

```
devtools::test("mlr", filter = "classif")
```

or from the command line using Michel's rt tool

```
rtest --filter=classif
```

4.2 Integrating Another Measure

In some cases, you might want to evaluate a `Prediction()` or `ResamplePrediction()` with a `Measure` (`makeMeasure()`) which is not yet implemented in `mlr`. This could be either a performance measure which is not listed in the Appendix or a measure that uses a misclassification cost matrix.

4.2.1 Performance measures and aggregation schemes

Performance measures in `mlr` are objects of class `Measure` (`makeMeasure()`). For example the mse (mean squared error) looks as follows.

```
str(mse)
## List of 10
##  $ id        : chr "mse"
##  $ minimize  : logi TRUE
##  $ properties: chr [1:3] "regr" "req.pred" "req.truth"
##  $ fun       :function (task, model, pred, feats, extra.args)
##  $ extra.args: list()
##  $ best      : num 0
##  $ worst     : num Inf
##  $ name      : chr "Mean of squared errors"
##  $ note      : chr "Defined as: mean((response - truth)^2)"
##  $ aggr      :List of 4
##   ..$ id        : chr "test.mean"
##   ..$ name      : chr "Test mean"
##   ..$ fun       :function (task, perf.test, perf.train, measure, group, pred)
##   ..$ properties: chr "req.test"
##   ..- attr(*, "class")= chr "Aggregation"
##  - attr(*, "class")= chr "Measure"
mse$fun
## function (task, model, pred, feats, extra.args)
## {
##     measureMSE(pred$data$truth, pred$data$response)
## }
## <bytecode: 0x13c4ce60>
## <environment: namespace:mlr>
measureMSE
## function (truth, response)
## {
##     mean((response - truth)^2)
## }
## <bytecode: 0x10d53110>
## <environment: namespace:mlr>
```

See the `Measure` (`makeMeasure()`) documentation page for a detailed description of the object slots.

At the core is slot `$fun` which contains the function that calculates the performance value. The actual work is done by function `measureMSE` (`measures()`). Similar functions, generally adhering to the naming scheme `measure` followed by the capitalized measure ID, exist for most performance measures. See the [`measures()`] help page for a complete list.

Just as `Task()` and Learner (`makeLearner()`) objects each `Measure` (`makeMeasure()`) has an identifier `$id` which is for example used to annotate results and plots. For plots there is also the option to use the longer measure `$name` instead. See the tutorial page on visualization for more information.

Moreover, a `Measure` (`makeMeasure()`) includes a number of `$properties` that indicate for which types of learning problems it is suitable and what information is required to calculate it. Obviously, most measures need the `Prediction()` object (`"req.pred"`) and, for supervised problems, the true values of the target variable(s) (`"req.truth"`). You can use functions `getMeasureProperties` (`MeasureProperties()`) and `hasMeasureProperties` (`MeasureProperties()`) to determine the properties of a `Measure` (`makeMeasure()`). Moreover, `listMeasureProperties()` shows all measure properties currently available in `mlr`.

```
listMeasureProperties()
##  [1] "classif"       "classif.multi" "multilabel"    "regr"
##  [5] "surv"          "cluster"       "costsens"      "req.pred"
##  [9] "req.truth"     "req.task"      "req.feats"     "req.model"
## [13] "req.prob"
```

Additional to its properties, each `Measure` (`makeMeasure()`) knows its extreme values `$best` and `$worst` and if it wants to be minimized or maximized (`$minimize`) during tuning or feature selection.

For resampling slot `$aggr` specifies how the overall performance across all resampling iterations is calculated. Typically, this is just a matter of aggregating the performance values obtained on the test sets `perf.test` or the training sets `perf.train` by a simple function. The by far most common scheme is `test.mean` (`aggregations()`), i.e., the unweighted mean of the performances on the test sets.

```
str(test.mean)
## List of 4
##  $ id        : chr "test.mean"
##  $ name      : chr "Test mean"
##  $ fun       :function (task, perf.test, perf.train, measure, group, pred)
##  $ properties: chr "req.test"
##  - attr(*, "class")= chr "Aggregation"
test.mean$fun
## function (task, perf.test, perf.train, measure, group, pred)
## mean(perf.test)
## <bytecode: 0xce02578>
## <environment: namespace:mlr>
```

All aggregation schemes are objects of class `Aggregation()` with the function in slot `$fun` doing the actual work. The `$properties` member indicates if predictions (or performance values) on the training or test data sets are required to calculate the aggregation.

You can change the aggregation scheme of a `Measure` (`makeMeasure()`) via function `setAggregation()`. See the tutorial page on resampling for some examples and the `?aggregations()` help page for all available aggregation schemes.

You can construct your own `Measure` (`makeMeasure()`) and `Aggregation()` objects via functions `makeMeasure()`, `makeCostMeasure()`, `makeCustomResampledMeasure()` and `makeAggregation()`. Some examples are shown in the following.

4.2.2 Constructing a performance measure

Function `makeMeasure()` provides a simple way to construct your own performance measure.

Below this is exemplified by re-implementing the mean misclassification error mmce. We first write a function that computes the measure on the basis of the true and predicted class labels. Note that this function must have certain formal arguments listed in the documentation of `makeMeasure()`. Then the `Measure` (`makeMeasure()`) object is created and we work with it as usual with the `performance()` function.

See the **R** documentation of `makeMeasure()` for more details on the various parameters.

```
### Define a function that calculates the misclassification rate
my.mmce.fun = function(task, model, pred, feats, extra.args) {
  tb = table(getPredictionResponse(pred), getPredictionTruth(pred))
  1 - sum(diag(tb)) / sum(tb)
}

### Generate the Measure object
my.mmce = makeMeasure(
  id = "my.mmce", name = "My Mean Misclassification Error",
  properties = c("classif", "classif.multi", "req.pred", "req.truth"),
  minimize = TRUE, best = 0, worst = 1,
  fun = my.mmce.fun
)

### Train a learner and make predictions
mod = train("classif.lda", iris.task)
pred = predict(mod, task = iris.task)

### Calculate the performance using the new measure
performance(pred, measures = my.mmce)
## my.mmce
##    0.02
### Apparently the result coincides with the mlr implementation
performance(pred, measures = mmce)
## mmce
## 0.02
```

4.2.3 Constructing a measure for ordinary misclassification costs

For in depth explanations and details see the tutorial page on cost-sensitive classification.

To create a measure that involves ordinary, i.e., class-dependent misclassification costs you can use function `makeCostMeasure()`. You first need to define the cost matrix. The rows indicate true and the columns predicted classes and the rows and columns have to be named by the class labels. The cost matrix can then be wrapped in a `Measure` (`makeMeasure()`) object and predictions can be evaluated as usual with the `performance()` function.

See the **R** documentation of function `makeCostMeasure()` for details on the various parameters.

```
### Create the cost matrix
costs = matrix(c(0, 2, 2, 3, 0, 2, 1, 1, 0), ncol = 3)
rownames(costs) = colnames(costs) = getTaskClassLevels(iris.task)

### Encapsulate the cost matrix in a Measure object
my.costs = makeCostMeasure(
  id = "my.costs", name = "My Costs",
  costs = costs,
  minimize = TRUE, best = 0, worst = 3
)

### Train a learner and make a prediction
mod = train("classif.lda", iris.task)
pred = predict(mod, newdata = iris)
```

```
### Calculate the average costs
performance(pred, measures = my.costs)
##   my.costs
## 0.02666667
```

4.2.4 Creating an aggregation scheme

It is possible to create your own aggregation scheme using function `makeAggregation()`. You need to specify an identifier `id`, the `properties`, and write a function that does the actual aggregation. Optionally, you can `name` your aggregation scheme.

Possible settings for `properties` are `"req.test"` and `"req.train"` if predictions on either the training or test sets are required, and the vector `c("req.train", "req.test")` if both are needed.

The aggregation function must have a certain signature detailed in the documentation of `makeAggregation()`. Usually, you will only need the performance values on the test sets `perf.test` or the training sets `perf.train`. In rare cases, e.g., the `Prediction()` object `pred` or information stored in the `Task()` object might be required to obtain the aggregated performance. For an example have a look at the definition of function `test.join` (`aggregations()`).

4.2.5 Example: Evaluating the range of measures

Let's say you are interested in the range of the performance values obtained on individual test sets.

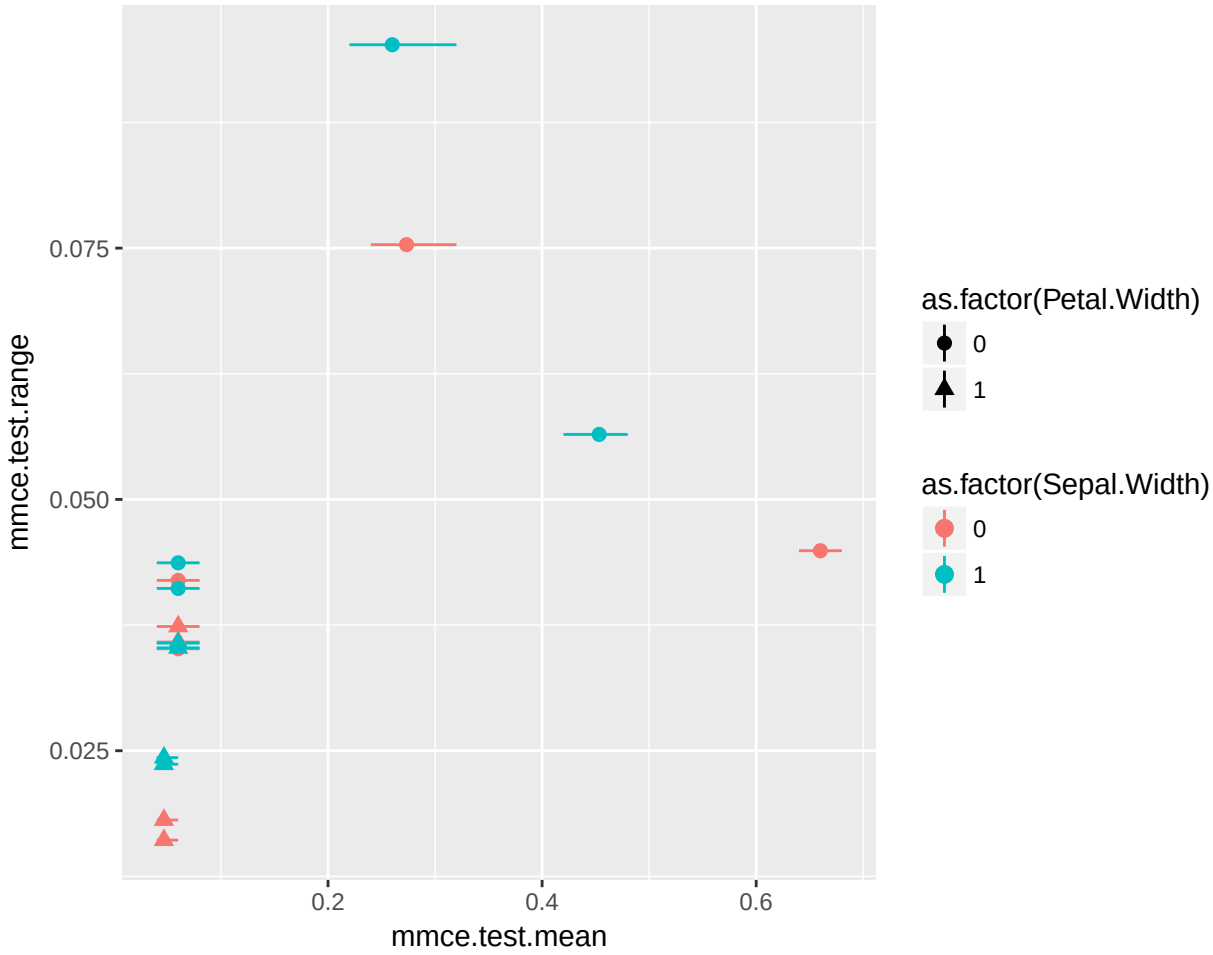
```
my.range.aggr = makeAggregation(id = "test.range", name = "Test Range",
  properties = "req.test",
  fun = function (task, perf.test, perf.train, measure, group, pred)
    diff(range(perf.test))
)
```

`perf.train` and `perf.test` are both numerical vectors containing the performances on the train and test data sets. In most cases (unless you are using bootstrap as resampling strategy or have set `predict = "both"` in `makeResampleDesc()`) the `perf.train` vector is empty.

Now we can run a feature selection based on the first measure in the provided list and see how the other measures turn out.

```
### mmce with default aggregation scheme test.mean
ms1 = mmce

### mmce with new aggregation scheme my.range.aggr
ms2 = setAggregation(ms1, my.range.aggr)

### Minimum and maximum of the mmce over test sets
ms1min = setAggregation(ms1, test.min)
ms1max = setAggregation(ms1, test.max)

### Feature selection
rdesc = makeResampleDesc("CV", iters = 3)
res = selectFeatures("classif.rpart", iris.task, rdesc, measures = list(ms1, ms2, ms1min, ms1max),
  control = makeFeatSelControlExhaustive(), show.info = FALSE)

### Optimization path, i.e., performances for the 16 possible feature subsets
perf.data = as.data.frame(res$opt.path)
head(perf.data[1:8])
```

```
##   Sepal.Length Sepal.Width Petal.Length Petal.Width mmce.test.mean
## 1            0           0            0           0     0.66000000
## 2            1           0            0           0     0.27333333
## 3            0           1            0           0     0.45333333
## 4            0           0            1           0     0.06000000
## 5            0           0            0           1     0.04666667
## 6            1           1            0           0     0.26000000
##   mmce.test.range mmce.test.min mmce.test.max
## 1            0.04          0.64          0.68
## 2            0.08          0.24          0.32
## 3            0.06          0.42          0.48
## 4            0.04          0.04          0.08
## 5            0.02          0.04          0.06
## 6            0.10          0.22          0.32
pd = position_jitter(width = 0.005, height = 0)
p = ggplot(aes(x = mmce.test.range, y = mmce.test.mean, ymax = mmce.test.max, ymin = mmce.test.min,
  color = as.factor(Sepal.Width), pch = as.factor(Petal.Width)), data = perf.data) +
  geom_pointrange(position = pd) +
  coord_flip()
print(p)
```



The plot shows the range versus the mean misclassification error. The value on the y-axis thus corresponds to the length of the error bars. (Note that the points and error bars are jittered in y-direction.)

4.3 Creating an Imputation Method

Function `makeImputeMethod()` permits to create your own imputation method. For this purpose you need to specify a *learn* function that extracts the necessary information and an *impute* function that does the actual imputation. The *learn* and *impute* functions both have at least the following formal arguments:

- `data` is a `base::data.frame()` with missing values in some features.
- `col` indicates the feature to be imputed.
- `target` indicates the target variable(s) in a supervised learning task.

4.3.1 Example: Imputation using the mean

Let's have a look at function imputeMean (`imputations()`).

```
imputeMean = function ()
{
    makeImputeMethod(learn = function(data, target, col) mean(data[[col]],
        na.rm = TRUE), impute = simpleImpute)
}
```

imputeMean (`imputations()`) calls the unexported `mlr` function `simpleImpute` which is defined as follows.

```
simpleImpute = function (data, target, col, const)
{
    if (is.na(const))
        stopf("Error imputing column '%s'. Maybe all input data was missing?",
            col)
    x = data[[col]]
    if (is.logical(x) && !is.logical(const)) {
        x = as.factor(x)
    }
    if (is.factor(x) && const %nin% levels(x)) {
        levels(x) = c(levels(x), as.character(const))
    }
    replace(x, is.na(x), const)
}
```

The *learn* function calculates the mean of the non-missing observations in column `col`. The mean is passed via argument `const` to the *impute* function that replaces all missing values in feature `col`.

4.3.2 Writing your own imputation method

Now let's write a new imputation method: A frequently used simple technique for longitudinal data is *last observation carried forward* (LOCF). Missing values are replaced by the most recent observed value.

In the **R** code below the *learn* function determines the last observed value previous to each `NA` (`values`) as well as the corresponding number of consecutive `NA's` (`times`). The *impute* function generates a vector by replicating the entries in `values` according to `times` and replaces the `NA's` in feature `col`.

```
imputeLOCF = function() {
  makeImputeMethod(
    learn = function(data, target, col) {
      x = data[[col]]
      ind = is.na(x)
      dind = diff(ind)
      lastValue = which(dind == 1)  ## position of the last observed value previous to NA
```

```
      lastNA = which(dind == -1)    ## position of the last of potentially several consecutive NA's
      values = x[lastValue]         ## last observed value previous to NA
      times = lastNA - lastValue    ## number of consecutive NA's
      return(list(values = values, times = times))
    },
    impute = function(data, target, col, values, times) {
      x = data[[col]]
      replace(x, is.na(x), rep(values, times))
    }
  )
}
```

Note that this function is just for demonstration and is lacking some checks for real-world usage (for example 'What should happen if the first value in `x` is already missing?'). Below it is used to impute the missing values in features `Ozone` and `Solar.R` in the airquality (`datasets::airquality()`) data set.

```
data(airquality)
imp = impute(airquality, cols = list(Ozone = imputeLOCF(), Solar.R = imputeLOCF()),
  dummy.cols = c("Ozone", "Solar.R"))
head(imp$data, 10)
##    Ozone Solar.R Wind Temp Month Day Ozone.dummy Solar.R.dummy
## 1     41     190  7.4   67     5   1       FALSE         FALSE
## 2     36     118  8.0   72     5   2       FALSE         FALSE
## 3     12     149 12.6   74     5   3       FALSE         FALSE
## 4     18     313 11.5   62     5   4       FALSE         FALSE
## 5     18     313 14.3   56     5   5        TRUE          TRUE
## 6     28     313 14.9   66     5   6       FALSE          TRUE
## 7     23     299  8.6   65     5   7       FALSE         FALSE
## 8     19      99 13.8   59     5   8       FALSE         FALSE
## 9      8      19 20.1   61     5   9       FALSE         FALSE
## 10     8     194  8.6   69     5  10        TRUE         FALSE
```

4.4 Integrating Another Filter Method

A lot of feature filter methods are already integrated in `mlr` and a complete list is given in the Appendix or can be obtained using `listFilterMethods()`. You can easily add another filter, be it a brand new one or a method which is already implemented in another package, via function `makeFilter()`.

4.4.1 Filter objects

In `mlr` all filter methods are objects of class Filter (`makeFilter()`) and are registered in an environment called `.FilterRegister` (where `listFilterMethods()` looks them up to compile the list of available methods). To get to know their structure let's have a closer look at the `"rank.correlation"` filter which interfaces function `Rfast::correls()` in package `Rfast`.

```
filters = as.list(mlr:::.FilterRegister)
filters$rank.correlation
## Filter: 'rank.correlation'
## Packages: 'Rfast'
## Supported tasks: regr
## Supported features: numerics
str(filters$rank.correlation)
## List of 6
```

```
##  $ name              : chr "rank.correlation"
##  $ desc              : chr "Spearman's correlation between feature and target"
##  $ pkg               : chr "Rfast"
##  $ supported.tasks   : chr "regr"
##  $ supported.features: chr "numerics"
##  $ fun               :function (task, nselect, ...)
##  - attr(*, "class")= chr "Filter"
filters$rank.correlation$fun
## function (task, nselect, ...)
## {
##     d = getTaskData(task, target.extra = TRUE)
##     y = Rfast::correls(d$target, d$data, type = "spearman")
##     for (i in which(is.na(y[, "correlation"]))) {
##         y[i, "correlation"] = cor(d$target, d$data[, i], use = "complete.obs",
##             method = "spearman")
##     }
##     setNames(abs(y[, "correlation"]), getTaskFeatureNames(task))
## }
## <bytecode: 0x13186d68>
## <environment: namespace:mlr>
```

The core element is `$fun` which calculates the feature importance. For the `"rank.correlation"` filter it just extracts the data and formula from the `task` and passes them on to the `Rfast::correls()` function.

Additionally, each Filter (`makeFilter()`) object has a `$name`, which should be short and is for example used to annotate graphics (cp. `plotFilterValues()`), and a slightly more detailed description in slot `$desc`. If the filter method is implemented by another package its name is given in the `$pkg` member. Moreover, the supported task types and feature types are listed.

4.4.2 Writing a new filter method

You can integrate your own filter method using `makeFilter()`. This function generates a Filter (`makeFilter()`) object and also registers it in the `.FilterRegister` environment.

The arguments of `makeFilter()` correspond to the slot names of the Filter (`makeFilter()`) object above. Currently, feature filtering is only supported for supervised learning tasks and possible values for `supported.tasks` are `"regr"`, `"classif"` and `"surv"`. `supported.features` can be `"numerics"`, `"factors"` and `"ordered"`.

`fun` must be a function with at least the following formal arguments:

- `task` is a `mlr` learning `Task()`.
- `nselect` corresponds to the argument of `generateFilterValuesData()` of the same name and specifies the number of features for which to calculate importance scores. Some filter methods have the option to stop after a certain number of top-ranked features have been found in order to save time and ressources when the number of features is high. The majority of filter methods integrated in `mlr` doesn't support this and thus `nselect` is ignored in most cases. An exception is the minimum redundancy maximum relevance filter from package `mRMRe`.
- `...` for additional arguments.

`fun` must return a named vector of feature importance values. By convention the most important features receive the highest scores.

If you are making use of the `nselect` option `fun` can either return a vector of `nselect` scores or a vector as long as the total numbers of features in the task filled with `NAs` for all features whose scores weren't calculated.

When writing `fun` many of the getter functions for `Task()`s come in handy, particularly `getTaskData()`, `getTaskFormula()` and `getTaskFeatureNames()`. It's worth having a closer look at `getTaskData()` which provides many options for formatting the data and recoding the target variable.

As a short demonstration we write a totally meaningless filter that determines the importance of features according to alphabetical order, i.e., giving highest scores to features with names that come first (`decreasing = TRUE`) or last (`decreasing = FALSE`) in the alphabet.

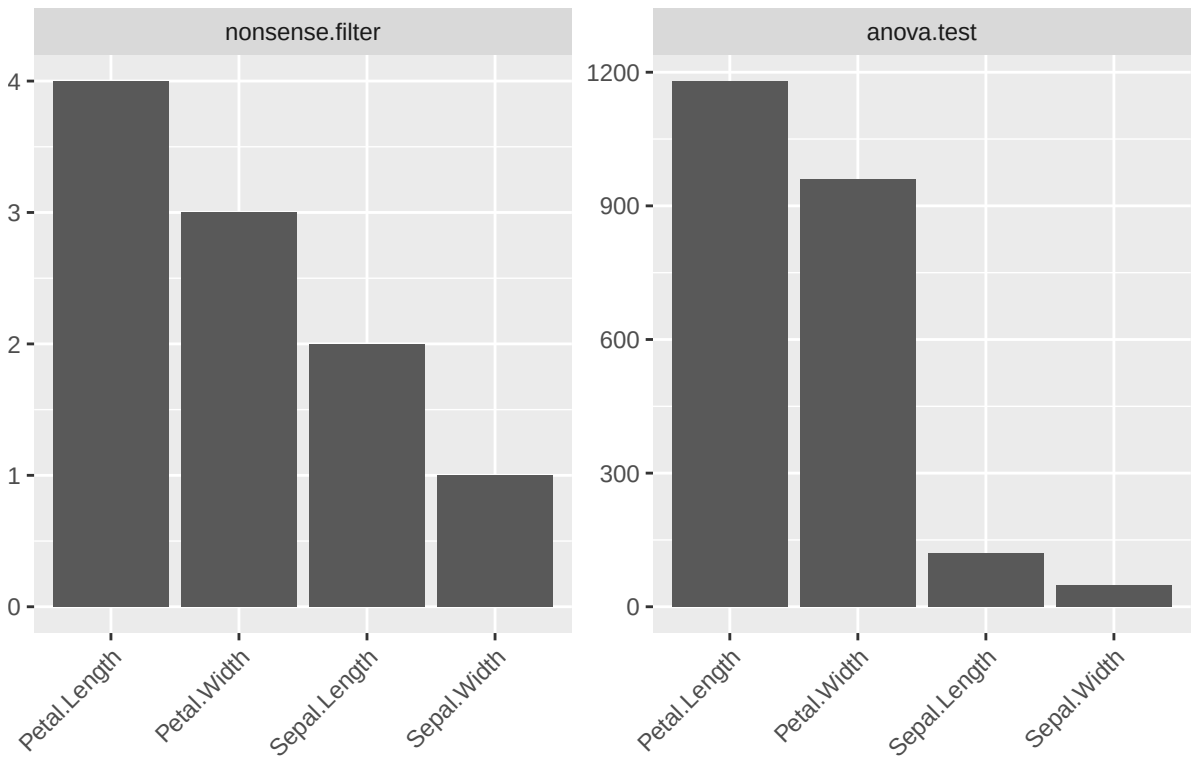
```
makeFilter(
  name = "nonsense.filter",
  desc = "Calculates scores according to alphabetical order of features",
  pkg = "",
  supported.tasks = c("classif", "regr", "surv"),
  supported.features = c("numerics", "factors", "ordered"),
  fun = function(task, nselect, decreasing = TRUE, ...) {
    feats = getTaskFeatureNames(task)
    imp = order(feats, decreasing = decreasing)
    names(imp) = feats
    imp
  }
)
## Filter: 'nonsense.filter'
## Packages: ''
## Supported tasks: classif,regr,surv
## Supported features: numerics,factors,ordered
```

The `nonsense.filter` is now registered in `mlr` and shown by `listFilterMethods()`.

```
listFilterMethods()$id
##  [1] anova.test                 auc
##  [3] carscore                   cforest.importance
##  [5] chi.squared                gain.ratio
##  [7] information.gain           kruskal.test
##  [9] linear.correlation         mrmr
## [11] nonsense.filter            oneR
## [13] permutation.importance     randomForest.importance
## [15] randomForestSRC.rfsrc      randomForestSRC.var.select
## [17] rank.correlation           relief
## [19] symmetrical.uncertainty    univariate.model.score
## [21] variance
## 24 Levels: anova.test auc carscore cforest.importance ... variance
```

You can use it like any other filter method already integrated in `mlr` (i.e., via the `method` argument of `generateFilterValuesData()` or the `fw.method` argument of `makeFilterWrapper()`; see also the page on feature selection.

```
d = generateFilterValuesData(iris.task, method = c("nonsense.filter", "anova.test"))
d
## FilterValues:
## Task: iris-example
##           name    type nonsense.filter anova.test
## 1 Sepal.Length numeric               2  119.26450
## 2  Sepal.Width numeric               1   49.16004
## 3 Petal.Length numeric               4 1180.16118
## 4  Petal.Width numeric               3  960.00715
plotFilterValues(d)
```




```
iris.task.filtered = filterFeatures(iris.task, method = "nonsense.filter", abs = 2)
iris.task.filtered
## Supervised task: iris-example
## Type: classif
## Target: Species
## Observations: 150
## Features:
##    numerics     factors     ordered functionals
##           2           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Has coordinates: FALSE
## Classes: 3
##     setosa versicolor  virginica
##         50         50         50
## Positive class: NA
getTaskFeatureNames(iris.task.filtered)
## [1] "Petal.Length" "Petal.Width"
```

You might also want to have a look at the source code of the filter methods already integrated in `mlr` for some more complex and meaningful examples.

5 Appendix

5.1 Example Tasks

For your convenience `mlr` provides pre-defined `Task()`s for each type of learning problem. These are used throughout this tutorial in order to get shorter and more readable code.

Type	Task	Description
classif	bc.task	Wisconsin Breast Cancer classification task.
	gunpoint.task	Gunpoint functional data classification task.
	iris.task	Iris classification task.
	phoneme.task	Phoneme functional data multilabel classification task.
	pid.task	PimaIndiansDiabetes classification task.
	sonar.task	Sonar classification task.
	spatial.task	J. Muenchow's Ecuador landslide data set
cluster	agri.task	European Union Agricultural Workforces clustering task.
	mtcars.task	Motor Trend Car Road Tests clustering task.
costsens	costiris.task	Iris cost-sensitive classification task.
multilabel	yeast.task	Yeast multilabel classification task.
regr	bh.task	Boston Housing regression task.
	fuelsubset.task	FuelSubset functional data regression task.
surv	lung.task	NCCTG Lung Cancer survival task.
	wpbc.task	Wisonsin Prognostic Breast Cancer (WPBC) survival task.

5.2 Integrated Learners

This page lists the learning methods already integrated in `mlr`.

Columns **Num.**, **Fac.**, **Ord.**, **NAs**, and **Weights** indicate if a method can cope with numerical, factor, and ordered factor predictors, if it can deal with missing values in a meaningful way (other than simply removing observations with missing values) and if observation weights are supported.

Column **Props** shows further properties of the learning methods specific to the type of learning task. See also `RLearner()` for details.

5.2.0.1 Classification (85)

For classification the following additional learner properties are relevant and shown in column **Props**:

- *prob*: The method can predict probabilities,
- *oneclass*, *twoclass*, *multiclass*: One-class, two-class (binary) or multi-class classification problems be handled,
- *class.weights*: Class weights can be handled.

Class / Short Name / Name	Package	Num	Fac	Ord	NAs	Wgts	Prob	Note
classif.ada *ada* ada Boosting	ada	X	X				prob	`xtrain` has been set to `0` by default for speed.
classif.ada_boostm1 *adaboostm1* ada Boosting M1	RWeka	X	X		X		prob	NAs are directly passed to WEKA with `na.action = na.pass`.
classif.bartMachine *bartmachine* Bayesian Additive Regression Trees	bartMachine	X	X		X		prob	`use_missing_data` has been set to `TRUE` by default to allow missing data support.
classif.binomial *binomial* Binomial Regression	stats	X	X			X	prob	Delegates to `glm` with freely choosable binomial link function via learner parameter `link`. We set 'model' to FALSE by default to save memory.
classif.blackboost *blackboost* Gradient Boosting With Regression Trees	mboost	X	X	X		X	prob	See `?ctree_control` for possible breakage for nominal features with missingness. `family` has been set to `Binomial` by default. For 'family' 'AUC' and 'AdaExp' probabilities cannot be predcited.

Class / Short Name / Name	Package	Num	Fac	Ord	NA	Weights	Prob	Note
classif.adabag *adabag* Adabag Boosting	adabag	X	X	X	X		prob	`xval` has been set to 0 by default for speed.
classif.bst *bst* Gradient Boosting	bst	X					two.class	Renamed parameter `learner` to `Learner` due to nameclash with `setHyperPars`. Default changes: `Learner = "ls"`, `xval = 0`, and `maxdepth = 1`.
classif.C50 *C50* C50	C50	X		X	X	X	prob	two.class multiclass
classif.cforest *cforest* Random forest based on conditional inference trees	party	X	X	X	X	X	prob	See `?ctree_control` for possible breakage for nominal features with missingness.
classif.clusterSVM *clusterSVM* Clustered Support Vector Machines	SwarmSVM	X					prob	`centers` set to `2` by default.

Class / Short Name / Name	Package	Num	Fac	Ord	NAs	Weights	Prob	Note
classif.ctree *ctree* Conditional Inference Trees	party	X	X	X	X		prob	See ?ctree_control for possible breakage for nominal features with missingness.
classif.cvglmnet *cvglmnet* GLM with Lasso or Elastic-net Regularization (Cross Validated Lambda)	glmnet	X					prob	The family parameter is set to `binomial` for two-class problems and to `multinomial` otherwise. Factors automatically get converted to dummy columns, ordered factors to integer. glmnet uses a global control object for its parameters. mlr resets all control parameters to their defaults before setting the specified parameters and after training. If you are setting glmnet.control parameters through glmnet.control, you need to save and re-set them after running the glmnet learner.
classif.dbndnn *dbn.dnn* Deep neural network with weights initialized by DBN	deepnet	X					prob	output activation function is `"softmax"` by default.

Class / Short Name / Name	Package	Num	Ex	Ord	NA	Weights	Prob	Note
classif.dcSVM *dcSVM* Divided-Conquer Support Vector Machines	SwarmSVM	X					twoclass	
classif.fda *fda* Flexible Discriminant Analysis	earth, stats	X					X prob	This learner performs flexible discriminant analysis using the earth algorithm. na.action is set to na.fail and only this is supported.
classif.evtree *evtree* Evolutionary learning of globally optimal trees	evtree	X	X		X		X prob	`pmutatemajor`, `pmutateminor`, `pcrossover`, `psplit`, and `pprune`, are scaled internally to sum to 100.
classif.extraTrees *extraTrees* Extremely Randomized Trees	extraTrees	X					X prob	twoclassmulticlass

Class / Short Name / Name	Package	Num	Fac	Ord	NAs	Weights	Prob	Note
classif.fdausc.glm *fdausc.glm* Generalized Linear Models classification on FDA	fdausc	X	X				prob	twoclass multiclass functionals $*classif.glm)||**classif.fdausc.kernel** *< br/ > *fdausc.kernel* < br/ >< br/ > Kernelclassificationon FDA|[fda.usc](http://www.rdocumentation.org/packages/fda.usc/)|||||prob < br/ > twoclass < br/ > multiclass < br/ > single.functional|Argumentdraw = FALSEisusedasdefault.|| **classif.fdausc.knn** *< br/ > *fdausc.knn* < br/ >< br/ > fdausc.knn|[fda.usc](http://www.rdocumentation.org/packages/fda.usc/)|||||X|prob < br/ > twoclass < br/ > multiclass < br/ > single.functional|Argumentdraw = FALSEisusedasdefault.||**classif.fdausc.np** < br/ > *fdausc.np* < br/ >< br/ > Nonparametricclassification on FDA|[fda.usc](http://www.rdocumentation.org/packages/fda.usc/)|||||prob < br/ > twoclass < br/ > multiclass < br/ > single.functional|Argumentdraw = FALSEisusedasdefault.Additionally, mod C[[1]] is set to quote(classif.np)
classif.featureless *featureless* Featureless classifier	featureless	X	X	X	X		prob	twoclass multiclass functionals
classif.fnn *fnn* Fast k-Nearest Neighbour	FNN	X						twoclass multiclass
classif.gamboost *gamboost* Gradient boosting with smooth components	mboost	X				X	prob	family has been set to `Binomial()` by default. For 'family' 'AUC' and 'AdaExp' probabilities cannot be predicted.

Class / Short Name / Name	Package	Num	Ens	Ord	NA	Wgts	Prob	Note
classif.gaterSVM *gaterSVM* Mixture of SVMs with Neural Network Gater Function	SwarmSVM	X						two class set to `3` and `max.iter` set to `1` by default.
classif.gausspr *gausspr* Gaussian Processes	kernlab	X					X	two class multiclass Kernel parameters have to be passed directly and not by using the `kpar` list in `gausspr`. Note that `fit` has been set to `FALSE` by default for speed.
classif.gbm *gbm* Gradient Boosting Machine	gbm	X	X		X	X		prob two class multiclass `keep.data` is set to `FALSE` to reduce memory requirements. Note on param 'distribution': gbm will select 'bernoulli' by default for 2 classes, and 'multinomial' for multiclass problems. The latter is the only setting that works for > 2 classes.
classif.geoDA *geoda* Geometric Predictive Discriminant Analysis	DiscriMiner							two class multiclass
classif.glmboost *glmboost* Boosting for GLMs	mboost	X				X		prob two class `family` has been set to `Binomial` by default. For 'family' 'AUC' and 'AdaExp' probabilities cannot be predcited.

Class / Short Name / Name	Package	Num	Fac	Ord	NA	Weights	Prob	One-class	Note
classif.glmnet *glmnet* GLM with Lasso or Elastic-net Regularization	glmnet	X	X			X	prob		The family parameter is set to `binomial` for two-class problems and to `multinomial` otherwise. Factors automatically get converted to dummy columns, ordered factors to integer. Parameter `s` (value of the regularization parameter used for predictions) is set to `0.1` by default, but needs to be tuned by the user. glmnet uses a global control object for its parameters. mlr resets all control parameters to their defaults before setting the specified parameters and after training. If you are setting glmnet.control parameters through glmnet.control, you need to save and re-set them after running the glmnet learner.
classif.h2o.deeplearning *h2o.dl* h2o.deeplearning	h2o	X	X		X	X	prob	two	class multi class
classif.h2o.gbm *h2o.gbm* h2o.gbm	h2o	X	X		X		prob	two	class multi class 'distribution' is set automatically to 'gaussian'.
classif.h2o.glm *h2o.glm* h2o.glm	h2o	X	X		X		prob	two	class 'family' is always set to 'binomial' to get a binary classifier.
classif.h2o.randomForest *h2o.rf* h2o.randomForest	h2o	X	X		X	X	prob	two	class multi class
classif.IBk *ibk* k-Nearest Neighbours	RWeka	X	X				prob	two	class multi class
classif.J48 *j48* J48 Decision Trees	RWeka	X	X	X			prob	two	class multi class NAs are directly passed to WEKA with `na.action = na.pass`.
classif.JRip *jrip* Propositional Rule Learner	RWeka	X	X	X			prob	two	class multi class NAs are directly passed to WEKA with `na.action = na.pass`.
classif.kknn *kknn* k-Nearest Neighbor	kknn	X	X				prob	two	class multi class

Class / Short Name / Name	Package	Num	Fac	Ord	NA	Wei	Prob	Note
classif.ksvm *ksvm* Support Vector Machines	kernlab	X					two-class multi-class	Kernel parameters have to be passed directly and not by using the `kpar` list in `ksvm`. Note that `fit` has been set to `FALSE` by default for speed.
classif.lda *lda* Linear Discriminant Analysis	MASS	X			X		two-class multi-class	Learner parameter `predict.method` maps to `method` in `predict.lda`.
classif.LiblineaRL1L2SVC *liblinl1l2svc* L1-Regularized L2-Loss Support Vector Classification	LiblineaR	X					two-class multi-class	class.weights
classif.LiblineaRL1LogReg *liblinl1logreg* L1-Regularized Logistic Regression	LiblineaR	X					two-class multi-class	class.weights

Class / Short Name / Name	Package	Native	Ensemble	Ordinal	Weights	Probs	Note
classif_liblinearL2L1SVC *liblinl2l1svc* L2-Regularized L1-Loss Support Vector Classification	liblinear				multiclass		class.weights
classif_liblinearL2LogReg *liblinl2logreg* L2-Regularized Logistic Regression	liblinear				multiclass		class.weights type = 0 (the default) is primal and type = 7 is dual problem.
classif_liblinearL2SVC *liblinl2svc* L2-Regularized L2-Loss Support Vector Classification	liblinear				multiclass		class.weights type = 2 (the default) is primal and type = 1 is dual problem.

Class / Short Name / Name	Package	Num	Fac	Ord	NA	Wts	Prob	Note
classif.LiblineaRMulticlassSVC *liblinmulticlasssvc* Support Vector Classification by Crammer and Singer	LiblineaR	N	N	N	N	Y	N	class.weights
classif.linDA *linda* Linear Discriminant Analysis	ipred	N	N	N	N	N	N	two.stage, validation = NULL by default to disable internal test set validation.
classif.logreg *logreg* Logistic Regression	stats	N	N	N	N	Y	Y	X prob Delegates to glm with family = binomial(link = 'logit'). We set 'model' to FALSE by default to save memory.

Class / Short Name / Name	Package	Num	Fac	Ord	NAs	Wgts	Prob	Note
classif.lqa *lqa* Fitting penalized Generalized Linear Models with the LQA algorithm	lqa	X					prob	`penalty` has been set to `"lasso"` and `lambda` to `0.1` by default. The parameters `lambda`, `gamma`, `alpha`, `oscar.c`, `a`, `lambda1` and `lambda2` are the tuning parameters of the `penalty` function being used, and correspond to the parameters as named in the respective help files. Parameter `c` for penalty method `oscar` has been named `oscar.c`. Parameters `lambda1` and `lambda2` correspond to the parameters named 'lambda_1' and 'lambda_2' of the penalty functions `enet`, `fused.lasso`, `icb`, `licb`, as well as `weighted.fusion`.
classif.lssvm *lssvm* Least Squares Support Vector Machine	kernlab	X					twoclass	`fast.method` has been set to `FALSE` by default for speed.
classif.lvq1 *lvq1* Learning Vector Quantization	class	X					twoclassmulticlass	
classif.mda *mda* Mixture Discriminant Analysis	mda	X					prob	`keep.fitted` has been set to `FALSE` by default for speed and we use `start.method = "lvq"` for more robust behavior / less technical crashes.

Class / Short Name / Name	Package	Num	Fac	Ord	NA	Weights	Prob	Note
classif.mlp *mlp* Multi-Layer Perceptron	RSNNS	X					prob	two class multi class
classif.multinom *multinom* Multinomial Regression	nnet	X	X		X		prob	two class multi class

Class / Short Name / Name	Package	Num	Ord	NAs	Weights	Prob	Note
classif.mxnet *mxff* Feed-forward Neural Network	mxnet	X	X			X	Default of `learning.rate` set to `0.1`. Default of `array.layout` set to `'rowmajor'`. Default of `verbose` is set to `FALSE`. If `symbol` is specified, it will be passed to mxnet ignoring almost all other architectural specifications, the exception being that when convolution is used in the symbol, `conv.layer1` has to be set to `TRUE` and `conv.data.shape` has to be specified. Default of `initializer` is set to NULL, which results in the default mxnet initializer being called when training a model. Number of output nodes is detected automatically. The upper bound for dropout is set to `1 - 1e-7` as in `mx.mlp` in the `mxnet` package. If `dropout.global` is `TRUE`, the same dropout rate `dropout.input` will be applied to the inputs and all the hidden layers. If `dropout.global` is `FALSE`, `dropout.input` will be applied to the inputs, and the different `dropout.layer` parameters to their respective layers. `batch.normalization` specifies whether batch normalization should be used in all hidden layers. If `batch.normalization` is set to `FALSE`, `batch.normalization1` specifies whether batch normalization should be used in the first hidden layer, `batch.normalization2` and `batch.normalization3` are defined accordingly. If `conv.layer1` is `FALSE`, the first layer is a `FullyConnected` layer and `num.layer1` gives the number of neurons. If `conv.layer1` is `TRUE`, then `num.layer1` gives the number of filters. In this case, `act1` is applied as an `Activation` layer afterwards (as is the case with a `FullyConnected` layer). This is the same for `conv.layer2` and `conv.layer3`. A `Convolution` layer cannot follow a `FullyConnected` layer. To stick with the example of the first layer, `conv.kernel1`, `conv.stride1`, `conv.dilate1` and `conv.pad1` correspond to the parameters of `mx.symbol.Convolution`. When a `Convolution` layer is constructed, a `Pooling` layer is constructed with it automatically. Again sticking to the example of the first layer, `pool.kernel1`, `pool.stride1`, `pool.pad1` and `pool.type1` correspond to the parameters in `mx.symbol.Pooling`. When convolution is used, `conv.data.shape` needs to be specified, which is a vector giving the dimensionality of the data (e.g. for MNIST `c(28, 28)` or `c(28, 28, 1)` and for `CIFAR10` `c(28, 28, 3)`). Furthermore, `array.layout` is set to `colmajor` if convolution is used, to enable compatability with `mxnet`. When using convolution, `mx.model.FeedForward.create` expects the array containing the data to have `4` dimensions. To allow for flexibility, `conv.data.shape` can have length `1` to `4`, the dimensions are taken in ascending order. For common cases, giving an `conv.data.shape` of length `2` or `3` is sufficient. `validation.ratio` gives the ratio of training data that will not be used for training but as validation data similar to the data provided in `eval.data`. If `eval.data` is specified, `validation.ratio` will be ignored. Note that `eval.data` is passed to `mx.model.FeedForward.create` unchanged to provide unconstrained usability of the underlying learner. In particular, this implies that `array.layout` is not adapted when using convolution, so `eval.data` needs to be provided in the right format. If `validation.ratio` is specified, it is sampled randomly using R's `sample`. If `early.stop.badsteps` is specified and `epoch.end.callback` is not specified, early stopping will be used using `mx.callback.early.stop` as `epoch.end.callback` with the learner's `eval.metric`. In this case, `early.stop.badsteps` gives the number of bad.steps in `mx.callback.early.stop` and `early.stop.maximize` gives the `maximize` parameter in `mx.callback.early.stop`. Please note that

Class / Short Name / Name	Package	Num	Fac	Ord	NA	Weights	Preds	Note

5.2.0.2 Regression (62)

Additional learner properties:

- *se*: Standard errors can be predicted.

Class / Short Name / Name	Package	Num	Fac	Ord	NA	Weights	Preds	Note
regr.bartMachine *bartMachine* Bayesian Additive Regression Trees	bartMachine	X	X	X	X			`use_missing_data` has been set to `TRUE` by default to allow missing data support.
regr.bcart *bcart* Bayesian CART	tgp	X	X				se	
regr.bgp *bgp* Bayesian Gaussian Process	tgp	X					se	

Class / Short Name / Name	Package	Num	Fac	Ord	NA	Weights	Preds	Note
regr.bgpllm *bgpllm* Bayesian Gaussian Process with jumps to the Limiting Linear Model	bgpllm	X					se	
regr.blackboost *blackboost* Gradient Boosting with Regression Trees	mboost	X	X	X				See `?ctree_control` for possible breakage for nominal features with missingness.
regr.blm *blm* Bayesian Linear Model	blm	X					se	

Class / Short Name / Name	Package	Num.	Ord.	NAs	Weights	Prob.	Note
regr.brnn *brnn* Bayesian regularization for feed-forward neural networks	brnn	X	X				
regr.bst *bst* Gradient Boosting	bst, rpart	X					Renamed parameter `learner` to `Learner` due to nameclash with `setHyperPars`. Default changes: `Learner = "ls"`, `xval = 0`, and `maxdepth = 1`.
regr.btgp *btgp* Bayesian Treed Gaussian Process	tgp	X	X				se
regr.btgpllm *btgpllm* Bayesian Treed Gaussian Process with jumps to the Limiting Linear Model	tgp	X	X				se

Class / Short Name / Name	Package	Num	Fac	Ord	NA	Weights	Prob	Note
regr.btlm *btlm* Bayesian Treed Linear Model	btlm	X	X				se	
regr.cforest *cforest* Random Forest Based on Conditional Inference Trees	party	X	X	X	X	X	featimp	See `?ctree_control` for possible breakage for nominal features with missingness.
regr.crs *crs* Regression Splines	crs	X	X			X	se	
regr.ctree *ctree* Conditional Inference Trees	party	X	X	X	X	X		See `?ctree_control` for possible breakage for nominal features with missingness.
regr.cubist *cubist* Cubist	Cubist	X	X		X			

Class / Short Name / Name	Package	Num.	Fac.	Ord.	NA	Weights	Prob.	Note
regr.cvglmnet *cvglmnet* GLM with Lasso or Elastic-net Regularization (Cross Validated Lambda)	glmnet	X	X			X		Factors automatically get converted to dummy columns, ordered factors to integer. glmnet uses a global control object for its parameters. mlr resets all control parameters to their defaults before setting the specified parameters and after training. If you are setting glmnet.control parameters through glmnet.control, you need to save and re-set them after running the glmnet learner.
regr.earth *earth* Multivariate Adaptive Regression Splines	earth	X	X					

Class / Short Name / Name	Package	Num.	Ord.	NA	Weights	Prob.	Note
regr.elmNN *elmNN* Extreme Learning Machine for Single Hidden Layer Feed-forward Neural Networks	nnet	X	X	X	X		`nhid` has been set to `1` and `actfun` has been set to `"sig"` by default.
regr.evtree *evtree* Evolutionary learning of globally optimal trees	evtree	X	X	X	X		`pmutatemajor`, `pmutateminor`, `pcrossover`, `psplit`, and `pprune`, are scaled internally to sum to 100.
regr.extraTrees *extraTrees* Extremely Randomized Trees	extraTrees	X			X		

Class / Short Name / Name	Package	Num.	Ord.	NAs	Weights	Prob.	Note
regr.FDboost *FDboost* Functional linear array regression boosting	FDboost	X	X				mboost functionals. Only allow one base learner for functional covariate and one base learner for scalar covariate, the parameters for these base learners are the same. Also we currently do not support interaction between scalar covariates
regr.featureless *featureless* Featureless regression		X	X	X			
regr.fnn *fnn* Fast k-Nearest Neighbor	FNN	X					
regr.frbs *frbs* Fuzzy Rule-based Systems	frbs	X					
regr.gamboost *gamboost* Gradient Boosting with Smooth Components	mboost	X	X		X		

Class / Short Name / Name	Package	Num	Fac	Ord	NA	Weights	Prob	Note
regr.gausspr *gausspr* Gaussian Processes	kernlab	X					se	Kernel parameters have to be passed directly and not by using the `kpar` list in `gausspr`. Note that `fit` has been set to `FALSE` by default for speed.
regr.gbm *gbm* Gradient Boosting Machine	gbm	X	X		X	X	featur	`keep.data` is set to FALSE to reduce memory requirements, `distribution` has been set to `"gaussian"` by default.
regr.glm *glm* Generalized Linear Regression	stats	X	X		X		se	'family' must be a character and every family has its own link, i.e. family = 'gaussian', link.gaussian = 'identity', which is also the default. We set 'model' to FALSE by default to save memory.
regr.glmboost *glmboost* Boosting for GLMs	mboost	X	X		X			
regr.glmnet *glmnet* GLM with Lasso or Elastic-net Regularization	glmnet	X	X		X			Factors automatically get converted to dummy columns, ordered factors to integer. Parameter `s` (value of the regularization parameter used for predictions) is set to `0.1` by default, but needs to be tuned by the user. glmnet uses a global control object for its parameters. mlr resets all control parameters to their defaults before setting the specified parameters and after training. If you are setting glmnet.control parameters through glmnet.control, you need to save and re-set them after running the glmnet learner.
regr.GPfit *GPfit* Gaussian Process	GPfit	X					se	(1) As the optimization routine assumes that the inputs are scaled to the unit hypercube [0,1]^d, the input gets scaled for each variable by default. If this is not wanted, scale = FALSE has to be set. (2) We replace the GPfit parameter 'corr = list(type = 'exponential',power = 1.95)'to be seperate parameters 'type' and 'power', in the case of corr = list(type = 'matern', nu = 0.5), the seperate parameters are 'type' and 'matern_nu_k = 0', and nu is computed by 'nu = (2 * matern_nu_k + 1) / 2 = 0.5'

Class / Short Name / Name	Package	Num.	Fac.	Ord.	NA's	Weights	Preds.	Note
regr.h2o.deeplearning *h2o.dl* h2o.deeplearning	h2o	X	X	X	X	X		
regr.h2o.gbm *h2o.gbm* h2o.gbm	h2o	X	X	X		X		'distribution' is set automatically to 'gaussian'.
regr.h2o.glm *h2o.glm* h2o.glm	h2o	X	X	X		X	X	'family' is always set to 'gaussian'.
regr.h2o.randomForest *h2o.rf* h2o.randomForest	h2o	X	X	X	X			
regr.IBk *ibk* K-Nearest Neighbours	RWeka	X						
regr.kknn *kknn* K-Nearest-Neighbor regression	kknn	X	X					
regr.km *km* Kriging	DiceKriging		X					se In predict, we currently always use `type = "SK"`. The extra parameter `jitter` (default is `FALSE`) enables adding a very small jitter (order 1e-12) to the x-values before prediction, as `predict.km` reproduces the exact y-values of the training data points, when you pass them in, even if the nugget effect is turned on. We further introduced `nugget.stability` which sets the `nugget` to `nugget.stability * var(y)` before each training to improve numerical stability. We recommend a setting of 10^-8
regr.ksvm *ksvm* Support Vector Machines	kernlab	X						Kernel parameters have to be passed directly and not by using the `kpar` list in `ksvm`. Note that `fit` has been set to `FALSE` by default for speed.
regr.laGP *laGP* Local Approximate Gaussian Process	laGP	X						se

Class / Short Name / Name	Package	Num.	Fac.	Ord.	NAs	Weights	Prob.	Note
regr.LiblineaRL2L1SVR *liblinl2l1svr* L2-Regularized L1-Loss Support Vector Regression	LiblineaR	X						Parameter `svr_eps` has been set to `0.1` by default.
regr.LiblineaRL2L2SVR *liblinl2l2svr* L2-Regularized L2-Loss Support Vector Regression	LiblineaR	X						`type = 11` (the default) is primal and `type = 12` is dual problem. Parameter `svr_eps` has been set to `0.1` by default.
regr.lm *lm* Simple Linear Regression	stats	X	X		X		se	
regr.mars *mars* Multivariate Adaptive Regression Splines	mda	X						

Class / Short Name / Name	Package	NaEa	Or	NA	We	Pl	Note
regr.mob	partykit	X	X	X	X	X	X
mob Model-based Recursive Partitioning Yielding a Tree with Fitted Models Associated with each Terminal Node							

Class / Short Name / Name	Package	Num.	Fac.	Ord.	NAs	Weights	Prob.	Note
regr.mxff *mxff* Feed-forward Neural Network	mxnet	X						Default of `learning.rate` set to `0.1`. Default of `array.layout` set to `'rowmajor'`. Default of `verbose` is set to `FALSE`. If `symbol` is specified, it will be passed to mxnet ignoring other architectural specifications. Default of `initializer` is set to NULL, which results in the default mxnet initializer being called when training a model. Number of output nodes is detected automatically. The upper bound for dropout is set to `1 - 1e-7` as in `mx.mlp` in the `mxnet` package. If `dropout.global` is `TRUE`, the same dropout rate `dropout.input` will be applied to the inputs and all the hidden layers. If `dropout.global` is `FALSE`, `dropout.input` will be applied to the inputs, and the different `dropout.layer` parameters to their respective layers. `dropout.mode` specifies if dropout should only be used in training or also for predictions, which allows stochastic predictions. This can be controlled for `se` with `dropout.predict.repls`. If `conv.layer1` is `FALSE`, the first layer is a `FullyConnected` layer and `num.layer1` gives the number of neurons. If `conv.layer1` is `TRUE`, then `num.layer1` gives the number of filters. In this case, `act1` is applied as an `Activation` layer afterwards (as is the case with a `FullyConnected` layer). This is the same for `conv.layer2` and `conv.layer3`. A `Convolution` layer cannot follow a `FullyConnected` layer. To stick with the example of the first layer, `conv.kernel1`, `conv.stride1`, `conv.dilate1` and `conv.pad1` correspond to the parameters of `mx.symbol.Convolution`. When a `Convolution` layer is constructed, a `Pooling` layer is constructed with it automatically. Again sticking to the example of the first layer, `pool.kernel1`, `pool.stride1`, `pool.pad1` and `pool.type1` correspond to the parameters in `mx.symbol.Pooling`. When convolution is used, `conv.data.shape` needs to be specified, which is a vector giving the dimensionality of the data (e.g. for MNIST `c(28, 28)` or `c(28, 28, 1)` and for CIFAR10 `c(28, 28, 3)`). Furthermore, `array.layout` is set to `colmajor` if convolution is used, to enable compatability with `mxnet`. When using convolution, `mx.model.FeedForward.create` expects the array containing the data to have `4` dimensions. To allow for flexibility, `conv.data.shape` can have length `1` to `4`, the dimensions are taken in ascending order. For common cases, giving an `conv.data.shape` of length `2` or `3` is sufficient. `validation.ratio` gives the ratio of training data that will not be used for training but as validation data similar to the data provided in `eval.data`. If `eval.data` is specified, `validation.ratio` will be ignored. Note that `eval.data` is passed to `mx.model.FeedForward.create` unchanged to provide unconstrained usability of the underlying learner. In particular, this implies that `array.layout` is not adapted when using convolution, so `eval.data` needs to be provided in the right format. If `validation.ratio` is specified, it is sampled randomly using R's `sample`. If `early.stop.badsteps` is specified and `epoch.end.callback` is not specified, early stopping will be used using `mx.callback.early.stop` as `epoch.end.callback` with the learner's `eval.metric`. In this case, `early.stop.badsteps` gives the number of `bad.steps` in `mx.callback.early.stop` and `early.stop.maximize` gives the `maximize` parameter in `mx.callback.early.stop`. Please note that when using `early.stop`, `badsteps`, `eval.metric` and either `eval.data` or `validation.ratio` should be specified. | | **regr.nnet** *nnet* Neural Network | [nnet](http://www.rdocumentation.org/packages/nnet/) | X | X | | | X | |

Class / Short Name / Name	Packages	Num	Fac	Ord	NA	Weights	Props	Note

5.2.0.3 Survival analysis (12)

Additional learner properties:

- *prob*: Probabilities can be predicted,
- *rcens*, *lcens*, *icens*: The learner can handle right, left and/or interval censored data.

Class / Short Name / Name	Packages	Num	Fac	Ord	NA	Weights	Props	Note
surv.cforest *crf* Random Forest based on Conditional Inference Trees	partysurvival	X	X	X	X	X	featimp	See `?ctree_control` for possible breakage for nominal features with missingness.
surv.CoxBoost *coxboost* Cox Proportional Hazards Model with Componentwise Likelihood based Boosting	CoxBoost	X	X	X		X		Factors automatically get converted to dummy columns, ordered factors to integer.
surv.coxph *coxph* Cox Proportional Hazard Model	survival	X	X			X		
surv.cv.CoxBoost *cv.CoxBoost* Cox Proportional Hazards Model with Componentwise Likelihood based Boosting, tuned for the optimal number of boosting steps	CoxBoost	X	X			X		Factors automatically get converted to dummy columns, ordered factors to integer.
surv.cvglmnet *cvglmnet* GLM with Regularization (Cross Validated Lambda)	glmnet	X	X	X		X		Factors automatically get converted to dummy columns, ordered factors to integer.

Class / Short Name / Name	Packages	Num	Fac	Ord	NA	Weights	Props	Note
surv.gamboost *gamboost* Gradient boosting with smooth components	survivalmboost	X	X	X		X		`family` has been set to `CoxPH()` by default.
surv.gbm *gbm* Gradient Boosting Machine	gbm	X	X		X	X	featim	`keep.data` is set to FALSE to reduce memory requirements.
surv.glmboost *glmboost* Gradient Boosting with Componentwise Linear Models	survivalmboost	X	X	X		X		`family` has been set to `CoxPH()` by default.
surv.glmnet *glmnet* GLM with Regularization	glmnet	X	X	X		X		Factors automatically get converted to dummy columns, ordered factors to integer. Parameter `s` (value of the regularization parameter used for predictions) is set to `0.1` by default, but needs to be tuned by the user. glmnet uses a global control object for its parameters. mlr resets all control parameters to their defaults before setting the specified parameters and after training. If you are setting glmnet.control parameters through glmnet.control, you need to save and re-set them after running the glmnet learner.
surv.randomForestSRC *rfsrc* Random Forest	randomForestSRC	X	X	X	X	X	featim	`na.action` has been set to `"na.impute"` by default to allow missing data support.
surv.ranger *ranger* Random Forests	ranger	X	X	X			featim	By default, internal parallelization is switched off (`num.threads = 1`), `verbose` output is disabled, `respect.unordered.factors` is set to `order` for all splitrules. All settings are changeable.
surv.rpart *rpart* Survival Tree	rpart	X	X	X	X	X	featim	`xval` has been set to `0` by default for speed.

5.2.0.4 Cluster analysis (9)

Additional learner properties:

- *prob*: Probabilities can be predicted.

Class / Short Name / Name	Packages	Num	Fac.	Ord.	NAs	Weights	Prob	Note
cluster.cmeans *cmeans* Fuzzy C-Means Clustering	e1071clue	X					prob	The `predict` method uses `cl_predict` from the `clue` package to compute the cluster memberships for new data. The default `centers = 2` is added so the method runs without setting parameters, but this must in reality of course be changed by the user.
cluster.Cobweb *cobweb* Cobweb Clustering Algorithm	RWeka	X						
cluster.dbscan *dbscan* DBScan Clustering	fpc	X						A cluster index of NA indicates noise points. Specify `method = 'dist'` if the data should be interpreted as dissimilarity matrix or object. Otherwise Euclidean distances will be used.
cluster.EM *em* Expectation-Maximization Clustering	RWeka	X						
cluster.FarthestFirst *farthestfirst* FarthestFirst Clustering Algorithm	RWeka	X						
cluster.kkmeans *kkmeans* Kernel K-Means	kernlab	X						`centers` has been set to `2L` by default. The nearest center in kernel distance determines cluster assignment of new data points. Kernel parameters have to be passed directly and not by using the `kpar` list in `kkmeans`
cluster.kmeans *kmeans* K-Means	statsclue	X					prob	The `predict` method uses `cl_predict` from the `clue` package to compute the cluster memberships for new data. The default `centers = 2` is added so the method runs without setting parameters, but this must in reality of course be changed by the user.
cluster.SimpleKMeans *simplekmeans* K-Means Clustering	RWeka	X						
cluster.XMeans *xmeans* XMeans (k-means with automatic determination of k)	RWeka	X						You may have to install the XMeans Weka package: `WPM('install-package', 'XMeans')`.

5.2.0.5 Cost-sensitive classification

For *ordinary misclassification costs* you can use all the standard classification methods listed above.

For *example-dependent costs* there are several ways to generate cost-sensitive learners from ordinary regression and classification learners. See section cost-sensitive classification and the documentation of `makeCostSensClassifWrapper()`, `makeCostSensRegrWrapper()` and `makeCostSensWeightedPairsWrapper()` for details.

5.2.0.6 Multilabel classification (3)

Class / Short Name / Name	Packages	Num	Fac.	Ord.	NAs	Weights	Props	Note
multilabel.cforest *cforest* Random forest based on conditional inference trees	party	X	X	X	X	X	prob	
multilabel.randomForestSRC *rfsrc* Random Forest	randomForestSRC	X	X		X	X	prob	`na.action` has been set to `na.impute` by default to allow missing data support.
multilabel.rFerns *rFerns* Random ferns	rFerns	X	X	X				

Moreover, you can use the binary relevance method to apply ordinary classification learners to the multilabel problem. See the documentation of function `makeMultilabelBinaryRelevanceWrapper()` and the tutorial section on multilabel classification for details.

5.3 Implemented Performance Measures

This page shows the performance measures available for the different types of learning problems as well as general performance measures in alphabetical order. (See also the documentation about `measures()` and `makeMeasure()` for available measures and their properties.)

If you find that a measure is missing, you can either open an issue or try to implement a measure yourself.

Column **Minim.** indicates if the measure is minimized during, e.g., tuning or feature selection. **Best** and **Worst** show the best and worst values the performance measure can attain. For *classification*, column **Multi** indicates if a measure is suitable for multi-class problems. If not, the measure can only be used for binary classification problems.

The next six columns refer to information required to calculate the performance measure.

- **Pred.**: The `Prediction()` object.
- **Truth**: The true values of the response variable(s) (for supervised learning).
- **Probs**: The predicted probabilities (might be needed for classification).
- **Model**: The `WrappedModel` (`makeWrappedModel()`) (e.g., for calculating the training time).
- **Task**: The `Task()` (relevant for cost-sensitive classification).
- **Feats**: The predicted data (relevant for clustering).

Aggr. shows the default aggregation method (`aggregations()`) tied to the measure.

5.3.0.1 Classification

ID / Name	Minim.	Best	Worst	Multi	Pred.	Truth	Probs	Model	Task	Feats	Aggr.	Note
acc Accuracy		1	0	X	X	X					test.mean	Defined as: mean(response == truth)

ID / Name	Minimize	Best	Worst	Multiclass	Pred	Truth	Prob	Model	Task	Feature	Aggr.	Note
auc Area under the curve		1	0		X	X	X				test.mean	Integral over the graph that results from computing fpr and tpr for many different thresholds.
bac Balanced accuracy		1	0		X	X					test.mean	Mean of true positive rate and true negative rate.
ber Balanced error rate	X	0	1	X	X	X					test.mean	Mean of misclassification error rates on all individual classes.
brier Brier score	X	0	1		X	X	X				test.mean	The Brier score is defined as the quadratic difference between the probability and the value (1,0) for the class. That means we use the numeric representation 1 and 0 for our target classes. It is similiar to the mean squared error in regression. multiclass.brier is the sum over all one vs. all comparisons and for a binary classifcation 2 * brier.
brier.scaled Brier scaled		1	0		X	X	X				test.mean	Brier score scaled to [0,1], see http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3575184/.
f1 F1 measure		1	0		X	X					test.mean	Defined as: 2 * tp/ (sum(truth == positive) + sum(response == positive))
fdr False discovery rate	X	0	1		X	X					test.mean	Defined as: fp / (tp + fp).
fn False negatives	X	0	Inf		X	X					test.mean	Sum of misclassified observations in the negative class. Also called misses.
fnr False negative rate	X	0	1		X	X					test.mean	Percentage of misclassified observations in the negative class.
fp False positives	X	0	Inf		X	X					test.mean	Sum of misclassified observations in the positive class. Also called false alarms.
fpr False positive rate	X	0	1		X	X					test.mean	Percentage of misclassified observations in the positive class. Also called false alarm rate or fall-out.
gmean G-mean		1	0		X	X					test.mean	Geometric mean of recall and specificity.
gpr Geometric mean of precision and recall.		1	0		X	X					test.mean	Defined as: sqrt(ppv * tpr)
kappa Cohen's kappa		1	- 1	X	X	X					test.mean	Defined as: 1 - (1 - p0) / (1 - pe). With: p0 = 'observed frequency of agreement' and pe = 'expected agremeent frequency under independence
logloss Logarithmic loss	X	0	Inf	X		X	X				test.mean	Defined as: -mean(log(p_i)), where p_i is the predicted probability of the true class of observation i. Inspired by https://www.kaggle.com/wiki/MultiClassLogLoss.

ID / Name	Minimize	Best	Worst	Multiclass	Pred	Truth	Prob	Model	Task	Feature	Aggr.	Note
lsr Logarithmic Scoring Rule		0	- Inf	X		X	X				test.mean	Defined as: mean(log(p_i)), where p_i is the predicted probability of the true class of observation i. This scoring rule is the same as the negative logloss, self-information or surprisal. See: Bickel, J. E. (2007). Some comparisons among quadratic, spherical, and logarithmic scoring rules. Decision Analysis, 4(2), 49-65.
mcc Matthews correlation coefficient		1	-1		X	X					test.mean	Defined as (tp * tn - fp * fn) / sqrt((tp + fp) * (tp + fn) * (tn + fp) * (tn + fn)), denominator set to 1 if 0
mmce Mean misclassification error	X	0	1	X	X	X					test.mean	Defined as: mean(response != truth)
multiclass.au1p Weighted average 1 vs. 1 multiclass AUC		1	0.5	X	X	X	X				test.mean	Computes AUC of c(c - 1) binary classifiers while considering the a priori distribution of the classes. See Ferri et al.: https://www.math.ucdavis.edu/~saito/data/roc/ferri-class-perf-metrics.pdf.
multiclass.au1u Average 1 vs. 1 multiclass AUC		1	0.5	X	X	X	X				test.mean	Computes AUC of c(c - 1) binary classifiers (all possible pairwise combinations) while considering uniform distribution of the classes. See Ferri et al.: https://www.math.ucdavis.edu/~saito/data/roc/ferri-class-perf-metrics.pdf.
multiclass.aunp Weighted average 1 vs. rest multiclass AUC		1	0.5	X	X	X	X				test.mean	Computes the AUC treating a c-dimensional classifier as c two-dimensional classifiers, taking into account the prior probability of each class. See Ferri et al.: https://www.math.ucdavis.edu/~saito/data/roc/ferri-class-perf-metrics.pdf.
multiclass.aunu Average 1 vs. rest multiclass AUC		1	0.5	X	X	X	X				test.mean	Computes the AUC treating a c-dimensional classifier as c two-dimensional classifiers, where classes are assumed to have uniform distribution, in order to have a measure which is independent of class distribution change. See Ferri et al.: https://www.math.ucdavis.edu/~saito/data/roc/ferri-class-perf-metrics.pdf.
multiclass.brier Multiclass Brier score	X	0	2	X	X	X	X				test.mean	Defined as: (1/n) sum_i sum_j (y_ij - p_ij)^2, where y_ij = 1 if observation i has class j (else 0), and p_ij is the predicted probability of observation i for class j. From http://docs.lib.noaa.gov/rescue/mwr/078/mwr-078-01-0001.pdf.

ID / Name	Minimize	Best	Worst	Multiclass	Pred	Truth	Probs	Models	Task	Feats	Aggr.	Note
npv Negative predictive value		1	0		X	X					test.mean	Defined as: tn / (tn + fn).
ppv Positive predictive value		1	0		X	X					test.mean	Defined as: tp / (tp + fp). Also called precision. If the denominator is 0, PPV is set to be either 1 or 0 depending on whether the highest probability prediction is positive (1) or negative (0).
qsr Quadratic Scoring Rule		1	-1	X		X	X				test.mean	Defined as: 1 - (1/n) sum_i sum_j (y_ij - p_ij)^2, where y_ij = 1 if observation i has class j (else 0), and p_ij is the predicted probablity of observation i for class j. This scoring rule is the same as 1 - multiclass.brier. See: Bickel, J. E. (2007). Some comparisons among quadratic, spherical, and logarithmic scoring rules. Decision Analysis, 4(2), 49-65.
ssr Spherical Scoring Rule		1	0	X		X	X				test.mean	Defined as: mean(p_i(sum_j(p_ij))), where p_i is the predicted probability of the true class of observation i and p_ij is the predicted probablity of observation i for class j. See: Bickel, J. E. (2007). Some comparisons among quadratic, spherical, and logarithmic scoring rules. Decision Analysis, 4(2), 49-65.
tn True negatives		Inf	0		X	X					test.mean	Sum of correctly classified observations in the negative class. Also called correct rejections.
tnr True negative rate		1	0		X	X					test.mean	Percentage of correctly classified observations in the negative class. Also called specificity.
tp True positives		Inf	0		X	X					test.mean	Sum of all correctly classified observations in the positive class.
tpr True positive rate		1	0		X	X					test.mean	Percentage of correctly classified observations in the positive class. Also called hit rate or recall or sensitivity.
wkappa Mean quadratic weighted kappa		1	-1	X	X	X					test.mean	Defined as: 1 - sum(weights * conf.mat) / sum(weights * expected.mat), the weight matrix measures seriousness of disagreement with the squared euclidean metric.

5.3.0.2 Regression

ID / Name	Minimize	Best	Worst	Pred	Truth	Probs	Models	Task	Feats	Aggr.	Note
arsq Adjusted coefficient of determination		1	0	X	X					test.mean	Defined as: 1 - (1 - rsq) * (p / (n - p - 1L)). Adjusted R-squared is only defined for normal linear regression.
expvar Explained variance		1	0	X	X					test.mean	Similar to measure rsq (R-squared). Defined as explained_sum_of_squares / total_sum_of_squares.

ID / Name	Minimize	Best	Worst	Pred.	Truth	Prob	Model	Task	Feat.	Aggr.	Note
kendalltau Kendall's tau		1	-1	X	X					test.mean	Defined as: Kendall's tau correlation between truth and response. Only looks at the order. See Rosset et al.: http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.95.1398&rep=rep1&type=pdf.
mae Mean of absolute errors	X	0	Inf	X	X					test.mean	Defined as: mean(abs(response - truth))
mape Mean absolute percentage error	X	0	Inf	X	X					test.mean	Defined as the abs(truth_i - response_i) / truth_i. Won't work if any truth value is equal to zero. In this case the output will be NA.
medae Median of absolute errors	X	0	Inf	X	X					test.mean	Defined as: median(abs(response - truth)).
medse Median of squared errors	X	0	Inf	X	X					test.mean	Defined as: median((response - truth)^2).
mse Mean of squared errors	X	0	Inf	X	X					test.mean	Defined as: mean((response - truth)^2)
msle Mean squared logarithmic error	X	0	Inf	X	X					test.mean	Defined as: mean((log(response + 1, exp(1)) - log(truth + 1, exp(1)))^2). This measure is mostly used for count data, note that all predicted and actual target values must be greater or equal '-1' to compute the measure.
rae Relative absolute error	X	0	Inf	X	X					test.mean	Defined as sum_of_absolute_errors / mean_absolute_deviation. Undefined for single instances and when every truth value is identical. In this case the output will be NA.
rmse Root mean squared error	X	0	Inf	X	X					test.rmse	The RMSE is aggregated as sqrt(mean(rmse.vals.on.test.sets^2)). If you don't want that, you could also use `test.mean`.
rmsle Root mean squared logarithmic error	X	0	Inf	X	X					test.mean	Defined as: sqrt(msle). Definition taken from: Definition taken from: https: / /www.kaggle.com / wiki / RootMeanSquaredLogarithmicError. This measure is mostly used for count data, note that all predicted and actual target values must be greater or equal '-1' to compute the measure.
rrse Root relative squared error	X	0	Inf	X	X					test.mean	Defined as sqrt (sum_of_squared_errors / total_sum_of_squares). Undefined for single instances and when every truth value is identical. In this case the output will be NA.
rsq Coefficient of determination		1	-Inf	X	X					test.mean	Also called R-squared, which is 1 - residual_sum_of_squares / total_sum_of_squares.

ID / Name	Minimize	Best	Worst	Pred.	Truth	Prob.	Model	Task	Feature	Aggr.	Note
sae Sum of absolute errors	X	0	Inf	X	X					test.mean	Defined as: sum(abs(response - truth))
spearmanrho Spearman's rho		1	-1	X	X					test.mean	Defined as: Spearman's rho correlation between truth and response. Only looks at the order. See Rosset et al.: http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.95.1398&rep=rep1&type=pdf.
sse Sum of squared errors	X	0	Inf	X	X					test.mean	Defined as: sum((response - truth)^2)

5.3.0.3 Survival analysis

ID / Name	Minimize	Best	Worst	Pred.	Truth	Prob.	Model	Task	Feature	Aggr.	Note
cindex Harrell's Concordance index		1	0	X	X					test.mean	Fraction of all pairs of subjects whose predicted survival times are correctly ordered among all subjects that can actually be ordered. In other words, it is the probability of concordance between the predicted and the observed survival.
cindex.uno Uno's Concordance index		1	0	X	X		X			test.mean	Fraction of all pairs of subjects whose predicted survival times are correctly ordered among all subjects that can actually be ordered. In other words, it is the probability of concordance between the predicted and the observed survival. Corrected by weighting with IPCW as suggested by Uno. Implemented in survAUC::UnoC.
iauc.uno Uno's estimator of cumulative AUC for right censored time-to-event data		1	0	X	X		X	X		test.mean	To set an upper time limit, set argument max.time (defaults to max time in complete task). Implemented in survAUC::AUC.uno.
ibrier Integrated brier score using Kaplan-Meier estimator for weighting	X	0	1		X		X	X		test.mean	To set an upper time limit, set argument max.time (defaults to max time in test data). Implemented in pec::pec

5.3.0.4 Cluster analysis

ID / Name	Minimize	Best	Worst	Pred.	Truth	Probs	Model	Task	Feats	Aggr.	Note

ID / Name	Minimize	Best	Worst	Pred.	Truth	Probs	Model	Task	Feats	Aggr.	Note
db Davies-Bouldin cluster separation measure	X	0	Inf	X					X	test.mean	Ratio of the within cluster scatter, to the between cluster separation, averaged over the clusters. See `?clusterSim::index.DB`.
dunn Dunn index		Inf	0	X					X	test.mean	Defined as the ratio of the smallest distance between observations not in the same cluster to the largest intra-cluster distance. See `?clValid::dunn`.
G1 Calinski-Harabasz pseudo F statistic		Inf	0	X					X	test.mean	Defined as ratio of between-cluster variance to within cluster variance. See `?clusterSim::index.G1`.
G2 Baker and Hubert adaptation of Goodman-Kruskal's gamma statistic		1	0	X					X	test.mean	Defined as: (number of concordant comparisons - number of discordant comparisons) / (number of concordant comparisons + number of discordant comparisons). See `?clusterSim::index.G2`.
silhouette Rousseeuw's silhouette internal cluster quality index		Inf	0	X					X	test.mean	Silhouette value of an observation is a measure of how similar an object is to its own cluster compared to other clusters. The measure is calculated as the average of all silhouette values. See `?clusterSim::index.S`.

5.3.0.5 Cost-sensitive classification

ID / Name	Minimize	Best	Worst	Pred.	Truth	Probs	Model	Task	Feats	Aggr.	Note
mcp Misclassification penalty	X	0	Inf	X				X		test.mean	Average difference between costs of oracle and model prediction.
meancosts Mean costs of the predicted choices	X	0	Inf	X				X		test.mean	Defined as: mean(y), where y is the vector of costs for the predicted classes.

Note that in case of *ordinary misclassification costs* you can also generate performance measures from cost

matrices by function `makeCostMeasure()`. For details see the tutorial page on cost-sensitive classification and also the page on custom performance measures.

5.3.0.6 Multilabel classification

ID / Name	Minimize	Best	Worst	Pred.	Truth	Prob.	Model	Task	Feats	Aggr.	Note
multilabel.acc Accuracy (multilabel)		1	0	X	X					test.mean	Averaged proportion of correctly predicted labels with respect to the total number of labels for each instance, following the definition by Charte and Charte: https: / /journal.r-project.org / archive / 2015 - 2 / charte-charte.pdf. Fractions where the denominator becomes 0 are replaced with 1 before computing the average across all instances.
multilabel.f1 F1 measure (multilabel)		1	0	X	X					test.mean	Harmonic mean of precision and recall on a per instance basis (Micro-F1), following the definition by Montanes et al.: http: / /www.sciencedirect.com / science / article / pii / S0031320313004019. Fractions where the denominator becomes 0 are replaced with 1 before computing the average across all instances.
multilabel.hamloss Hamming loss	X	0	1	X	X					test.mean	Proportion of labels that are predicted incorrectly, following the definition by Charte and Charte: https://journal.r-project.org/archive/2015-2/charte-charte.pdf.
multilabel.ppv Positive predictive value (multilabel)		1	0	X	X					test.mean	Also called precision. Averaged ratio of correctly predicted labels for each instance, following the definition by Charte and Charte: https: / /journal.r-project.org / archive / 2015 - 2 / charte-charte.pdf. Fractions where the denominator becomes 0 are ignored in the average calculation.
multilabel.subset01 Subset-0-1 loss	X	0	1	X	X					test.mean	Proportion of observations where the complete multilabel set (all 0-1-labels) is predicted incorrectly, following the definition by Charte and Charte: https://journal.r-project.org/archive/2015-2/charte-charte.pdf.
multilabel.tpr TPR (multilabel)		1	0	X	X					test.mean	Also called recall. Averaged proportion of predicted labels which are relevant for each instance, following the definition by Charte and Charte: https: / /journal.r-project.org / archive / 2015 - 2 / charte-charte.pdf. Fractions where the denominator becomes 0 are ignored in the average calculation.

5.3.0.7 General performance measures

ID / Name	Minim	Best	Worst	Pred.	Truth	Probs	Model	Task	Feats	Aggr.	Note
featperc Percentage of original features used for model	X	0	1	X			X			test.mean	Useful for feature selection.
timeboth timetrain + timepredict	X	0	Inf	X			X			test.mean	
timepredict Time of predicting test set	X	0	Inf	X						test.mean	
timetrain Time of fitting the model	X	0	Inf				X			test.mean	

5.4 Integrated Filter Methods

The following table shows the available methods for calculating the feature importance. Columns **Classif**, **Regr** and **Surv** indicate if classification, regression or survival analysis problems are supported. Columns **Fac.**, **Num.** and **Ord.** show if a particular method can deal with `factor`, `numeric` and `ordered factor` features.

5.4.1 Current methods

Method	Package	Description	Classif	Regr	Surv	Fac.	Num.	Ord.
anova.test	Rfast	ANOVA Test for binary and multiclass classification tasks	X				X	
auc		AUC filter for binary classification tasks	X				X	
carscore	care	CAR scores		X			X	
cforest.importance	party	Permutation importance of random forest fitted in package 'party'	X	X	X	X	X	X
chi.squared	FSelector	Chi-squared statistic of independence between feature and target	X	X		X	X	
gain.ratio	FSelector	Entropy-based gain ratio between feature and target	X	X		X	X	
information.gain	FSelector	Entropy-based information gain between feature and target	X	X		X	X	
kruskal.test		Kruskal Test for binary and multiclass classification tasks	X			X	X	
linear.correlation	Rfast	Pearson correlation between feature and target		X			X	
mrmr	mRMRe	Minimum redundancy, maximum relevance filter		X	X		X	X
oneR	FSelector	oneR association rule	X	X		X	X	
permutation.importance		Aggregated difference between feature permuted and unpermuted predictions	X	X	X	X	X	X
randomForest.importance	randomForest	Importance based on OOB-accuracy or node inpurity of random forest fitted in package 'randomForest'.	X	X		X	X	
randomForestSRC.importance	randomForestSRC	Importance of random forests fitted in package 'randomForestSRC'. Importance is calculated using argument 'permute'.	X	X	X	X	X	X

Method	Package	Description	Class.	Regr.	Surv.	Fac.	Num.	Ord.
randomForestSRC.var.select	randomForestSRC	Minimal depth of / variable hunting via method var.select on random forests fitted in package 'randomForestSRC'.	X	X	X	X	X	X
rank.correlation	Rfast	Spearman's correlation between feature and target		X			X	
relief	FSelector	RELIEF algorithm	X	X		X	X	
symmetrical.uncertainty	FSelector	Entropy-based symmetrical uncertainty between feature and target	X	X		X	X	
univariate.model.score		Resamples an mlr learner for each input feature individually. The resampling performance is used as filter score, with rpart as default learner.	X	X	X	X	X	X
variance		A simple variance filter	X	X	X		X	

5.4.2 Deprecated methods

Method	Package	Description	Class.	Regr.	Surv.	Fac.	Num.	Ord.
rf.importance	randomForestSRC	Importance of random forests fitted in package 'randomForestSRC'. Importance is calculated using argument 'permute'. (DEPRECATED)	X	X	X	X	X	X
rf.min.depth	randomForestSRC	Minimal depth of random forest fitted in package 'randomForestSRC. (DEPRECATED)	X	X	X	X	X	X
univariate		Resamples an mlr learner for each input feature individually. The resampling performance is used as filter score, with rpart as default learner. (DEPRECATED)	X	X	X	X	X	X