

mlr Tutorial

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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    1

```

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 (`vignette("cost_sensitive_classif")`) 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 `vignette("cost_sensitive_classif")` (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 `vignette("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
## Is spatial: 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 further model 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
## Is spatial: FALSE
## Classes: 2
##      benign malignant
##         458       241
## Positive class: benign
```

In binary classification the two classes are usually referred to as *positive* and *negative* class with the positive class being the category of greater interest. This is relevant for many `vignette("performance")` like the *true positive rate* or `vignette("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
## Is spatial: 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 `makeMultilabelTaskTask()`.

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 `makeMultilabelTaskTask()`:

```
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,label13,label14
## Observations: 2417
## Features:
##      numerics      factors      ordered functionals
##          103           0           0           0
## Missings: FALSE
## Has weights: FALSE
```



```
## Has blocking: FALSE
## Is spatial: 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 `vignette("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
## Is spatial: 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
## Is spatial: FALSE
## Classes: 3
## y1, y2, y3
```

For more details see the page `vignette("cost_sensitive_classif")`.

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 `vignette("resample")`.

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 `vignette("train")` 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.feats
##      numerics      factors      ordered functionals
##           0           4           5           0
##
```

```
## $has.missings
## [1] TRUE
##
## $has.weights
## [1] FALSE
##
## $has.blocking
## [1] FALSE
##
## $is.spatial
## [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 1183.7428 1105.43087
## [2,] 0 997.1804 1502.93062
## [3,] 0 712.3112 516.14402
## [4,] 0 1857.2684 88.95549
## [5,] 0 756.9824 132.94373
## [6,] 0 601.4316 543.27986

```

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 (`vignette("create_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
## Is spatial: 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
## Is spatial: 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 (`vignette("preproc")`) 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 (`vignette("example_tasks")`).

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 (`vignette("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 (`vignette("create_learners")`). 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 (`vignette("cost_sensitive_classif")`).

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 (`vignette("integrated_learners")`).

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()
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")
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")
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)
## [[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 (`vignette("resample")`)).

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 22.23202
## 4   4  33.4 23.24985
## 6   6  28.7 22.34879
## 8   8  27.1 22.13742
## 10  10 18.9 22.13742
## 12  12 18.9 22.13742
## ... (#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          1
## 4          1
## 6          1
## 8          1
## 10         1
## 12         1
## ... (#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 22.23202
## 4     4  33.4 23.24985
## 6     6  28.7 22.34879
## 8     8  27.1 22.13742
## 10    10  18.9 22.13742
## 12    12  18.9 22.13742
### Result of predict with data passed via newdata argument
head(as.data.frame(newdata.pred))
##      response
## 2          1
## 4          1
## 6          1
## 8          1
## 10         1
## 12         1

```

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] 22.23202 23.24985 22.34879 22.13742 22.13742 22.13742
```

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")]
##           class
## 1    regr.bcart
## 2     regr.bgp
## 3  regr.bgpplm
## 4     regr.blm
## 5    regr.btgp
## 6  regr.btgpplm
##
##                                     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: 16, #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      0.020406305 0.97959369
## Mazda RX4 Wag  0.020366087 0.97963391
## Datsun 710      0.007339559 0.99266044
## Hornet 4 Drive  0.457087375 0.54291262
## Hornet Sportabout 0.981294555 0.01870544
## Valiant        0.242541057 0.75745894
```

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  54
## 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 (`vignette("roc_analysis")`).

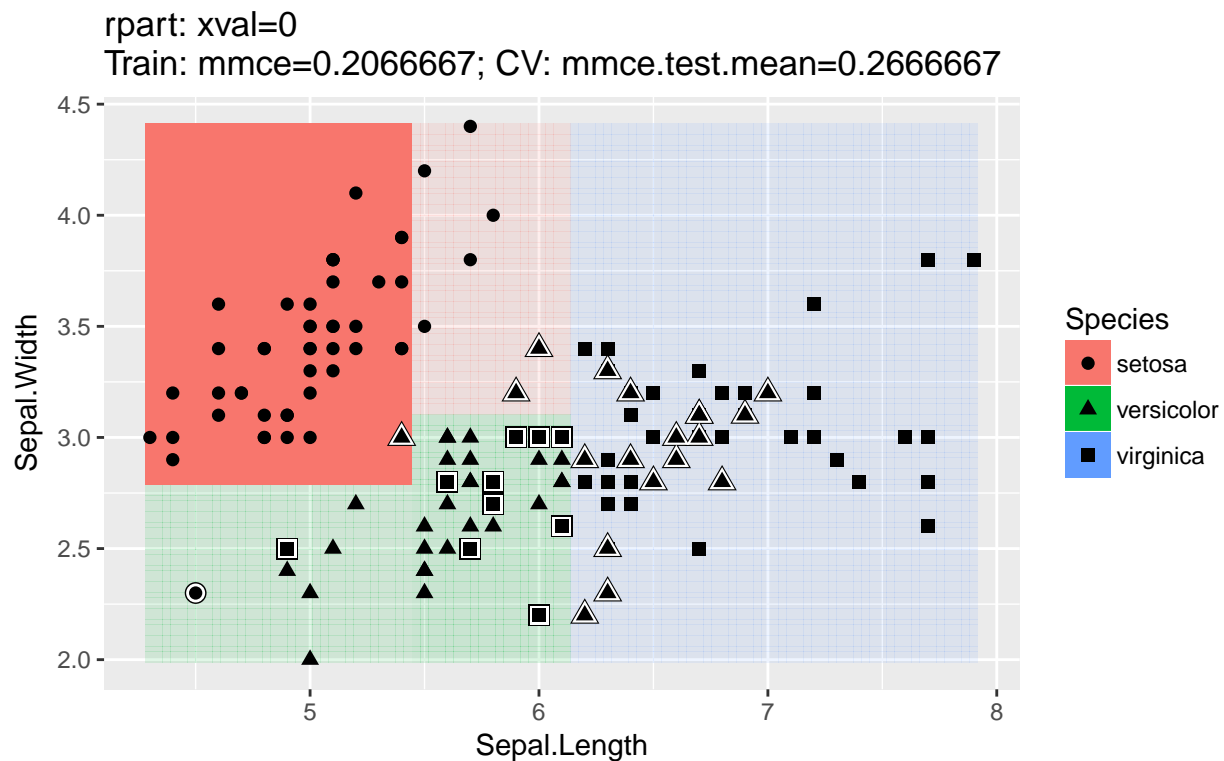
2.3.3 Visualizing the prediction

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.

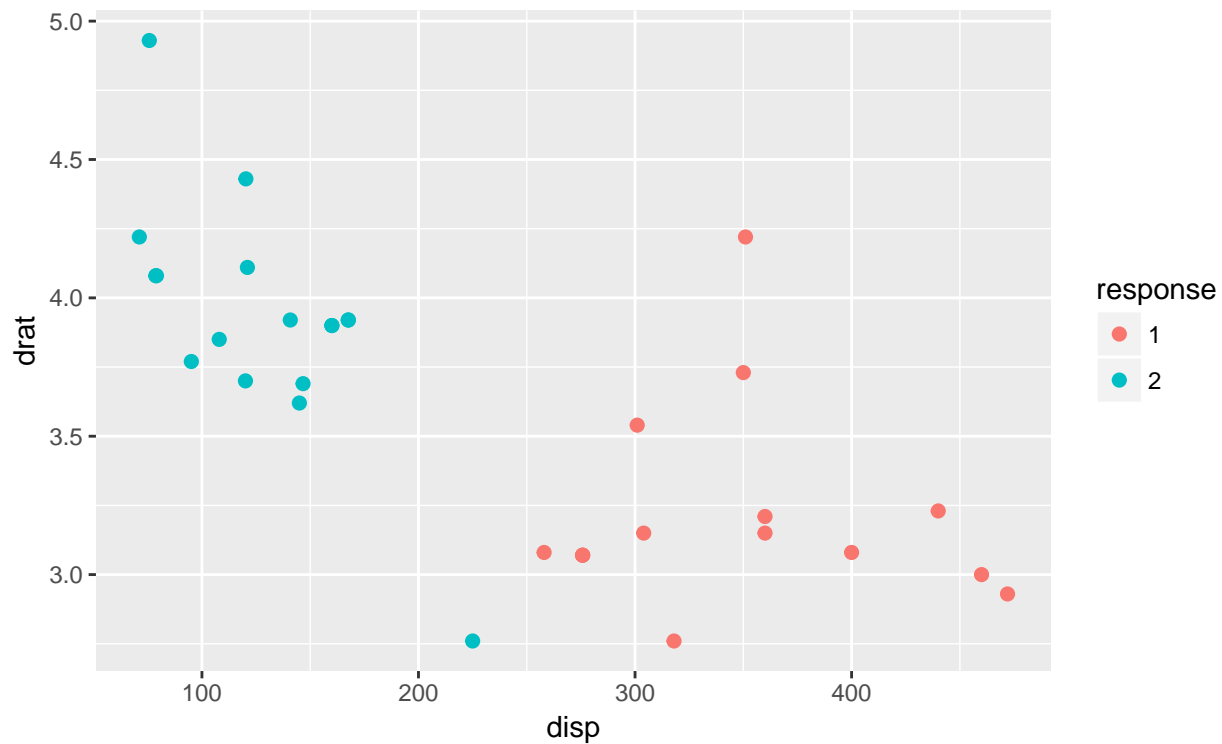
The plot title displays the ID of the Learner (`makeLearner()`) (in the following example CART), its parameters, its training performance and its cross-validation performance. `mmce` (`vignette("measures")`) stands for *mean misclassification error*, i.e., the error rate. See the sections on performance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

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



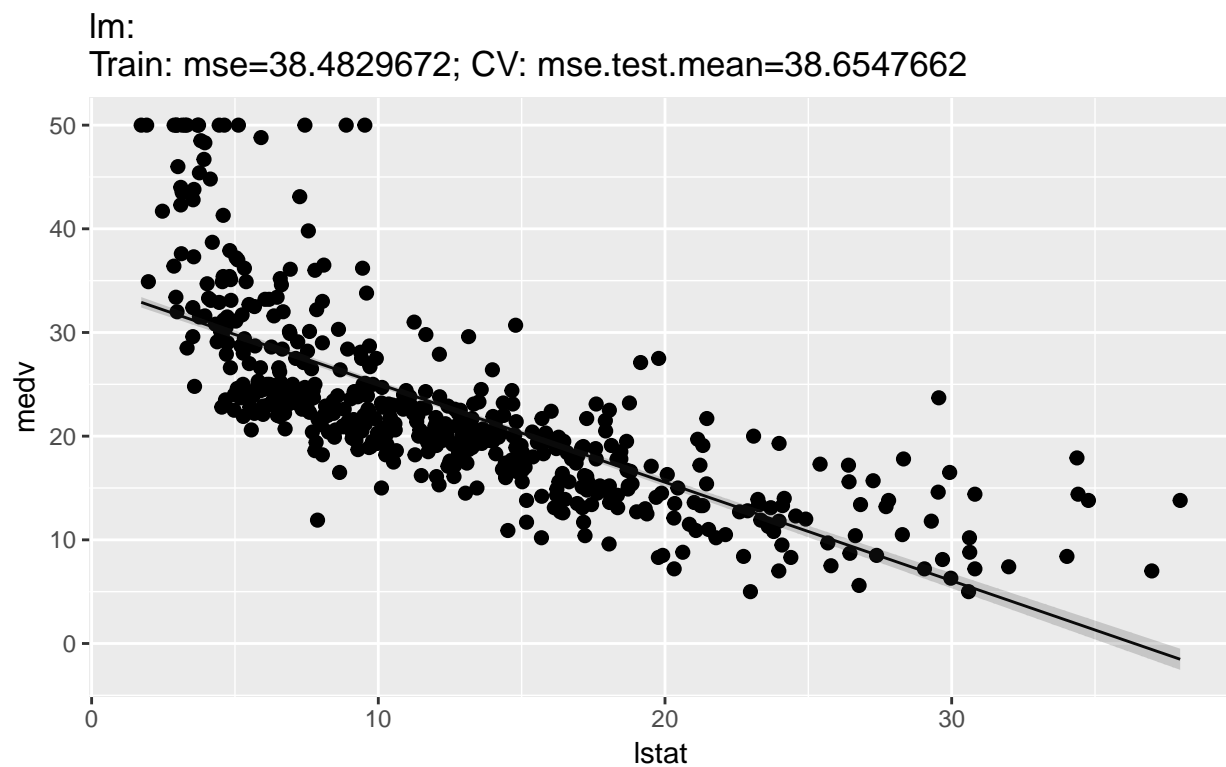
For *clustering* we also get a scatter plot of two selected features. The color of the points indicates the predicted cluster.

```
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.

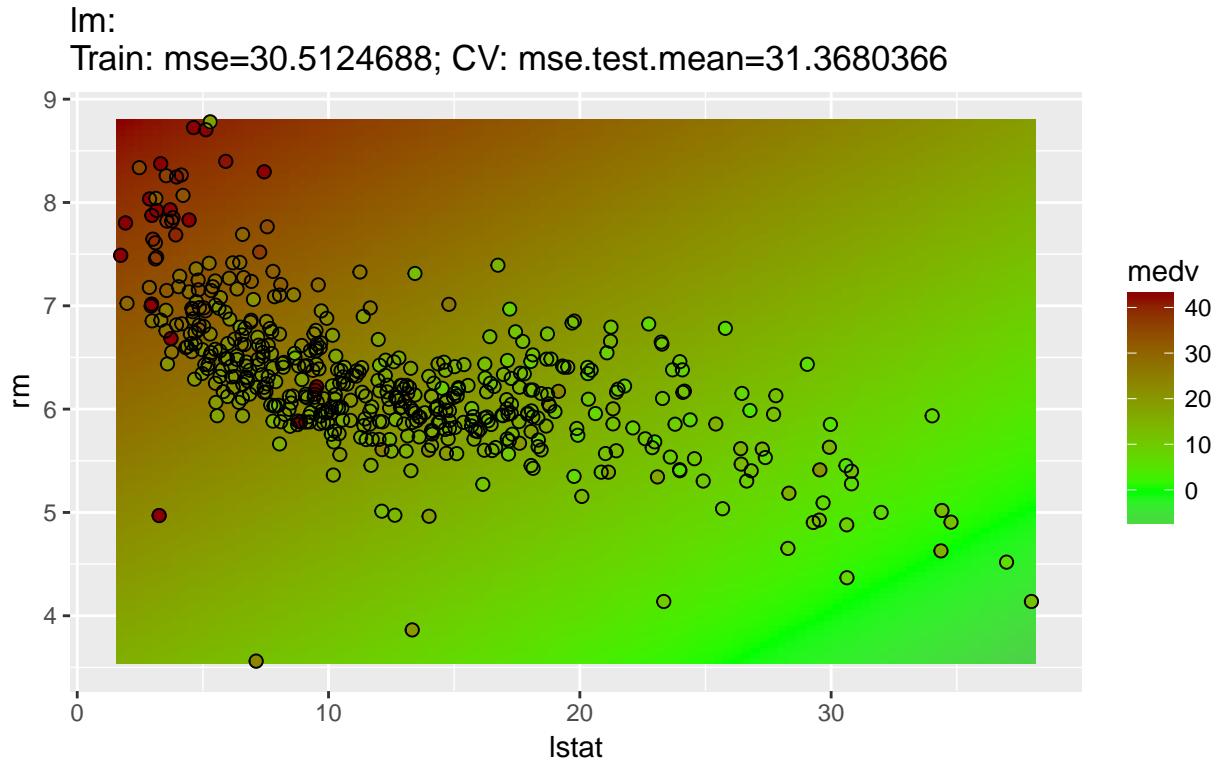
```
plotLearnerPrediction("regr.lm", features = "lstat", task = bh.task)
```



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

To see which performance measures are implemented, have a look at the table of performance measures (`vignette("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 (`vignette("create_measure")`).

2.4.2 Listing measures

The properties and requirements of the individual measures are shown in the table of performance measures (`vignette("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 (vignette("measures"))`) for regression and the misclassification rate (`mmce (vignette("measures"))`) 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` (`vignette("measures")`)) 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
## 42.81068
```

The following code computes the median of squared errors (`medse` (`vignette("measures")`)) instead.

```
performance(pred, measures = medse)
##    medse
## 8.989199
```

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 (`vignette("create_measure")`).

Calculate the mean squared error, median squared error and mean absolute error (`mae` (`vignette("measures")`)).

```
performance(pred, measures = list(mse, medse, mae))
##      mse      medse      mae
## 42.810675  8.989199  4.549951
```

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` (`vignette("measures")`)), the fitted model has to be passed.

```
performance(pred, measures = timetrain, model = mod)
## timetrain
##      0.364
```

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 (vignette("measures"))`) – 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 (`vignette("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 (vignette("measures"))`), 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

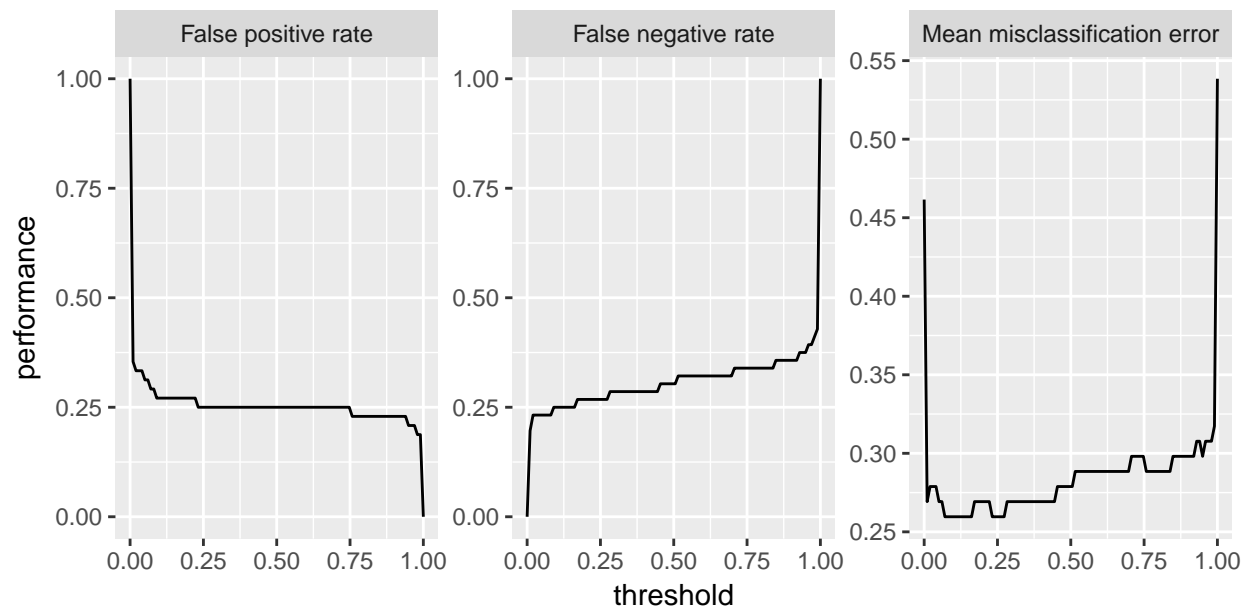
As you may recall (see the previous section on making predictions (`vignette("predict")`)) in binary classification we can adjust the threshold used to map probabilities to class labels. Helpful in this regard is are the functions `generateThreshVsPerfData()` and `plotThreshVsPerf()`, which generate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

For more performance plots and automatic threshold tuning see `vignette("roc_analysis")`.

In the following example we consider the `mlbench::Sonar()` data set and plot the false positive rate (fpr (`vignette("measures")`)), the false negative rate (fnr (`vignette("measures")`)) as well as the misclassification rate (mmce (`vignette("measures")`)) 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 faceted 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 similar table with the `calculateROCMasures()` function.

```
r = calculateROCMasures(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+)
## 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 (`vignette("predict")`), 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` (`calculateROCMasures()`) 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 $D \setminus D^{*b}$, $b = 1, \dots, B$. 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"),

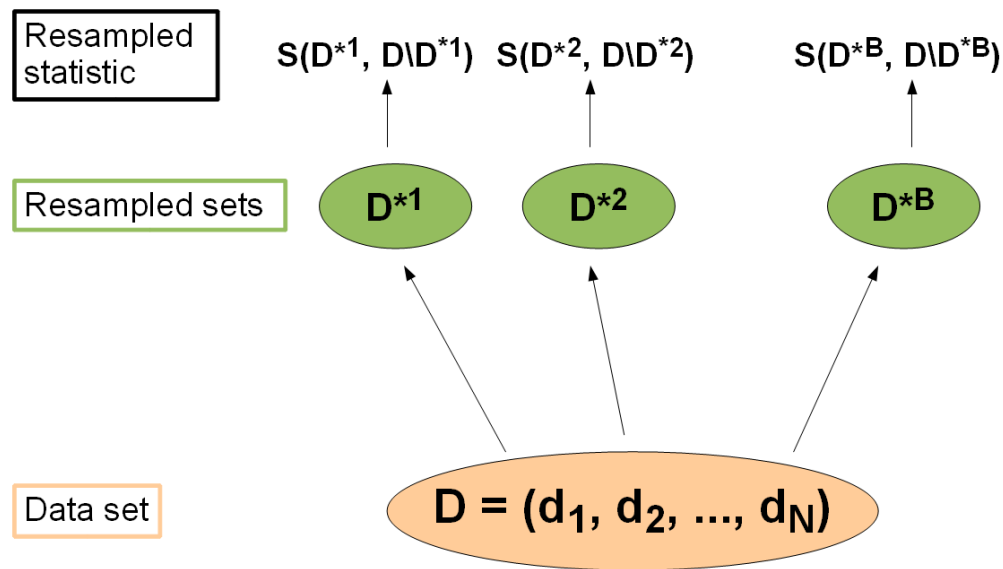


Figure 1: Resampling Figure

- 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` (`vignette("measures")`)) 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:  25.4704438
## [Resample] iter 2:  22.8413195
## [Resample] iter 3:  21.2763574
##
## Aggregated Result: mse.test.mean=23.1960402
##
r
## Resample Result
## Task: BostonHousing-example
## Learner: regr.lm
## Aggr perf: mse.test.mean=23.1960402
## Runtime: 0.045511
```

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$aggr
## mse.test.mean
##      23.19604
r$measures.test
##   iter      mse
## 1     1 25.47044
```

```
## 2    2 22.84132
## 3    3 21.27636
```

`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` (`vignette("measures")`), 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` (`vignette("measures")`)), false positive and false negative rates (`fpr` (`vignette("measures")`), `fnr` (`vignette("measures")`)), and the time it takes to train the learner (`timetrain` (`vignette("measures")`)) 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:  0.2857143  0.3500000  0.2272727  0.0200000
## [Resample] iter 2:  0.2619048  0.0588235  0.4000000  0.0200000
## [Resample] iter 3:  0.2857143  0.4000000  0.1818182  0.0190000
## [Resample] iter 4:  0.4047619  0.5357143  0.1428571  0.0200000
## [Resample] iter 5:  0.2619048  0.4000000  0.1851852  0.0200000
##
## Aggregated Result: mmce.test.mean=0.3000000,fpr.test.mean=0.3489076,fnr.test.mean=0.2274266,timetrain.test.m
##
r
## Resample Result
## Task: Sonar_example
## Learner: classif.rpart
## Aggr perf: mmce.test.mean=0.3000000,fpr.test.mean=0.3489076,fnr.test.mean=0.2274266,timetrain.test.m
## Runtime: 0.180658
```

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=0.3000000,fpr.test.mean=0.3489076,fnr.test.mean=0.2274266,timetrain.test.m
## Runtime: 0.180658
```

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 (`vignette("configureMlr")`)).

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=0.3000000,fpr.test.mean=0.3851378,fnr.test.mean=0.2248230,timetrain.test.m
## Runtime: 0.197382
```

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  50    R        M    1 test
## 2 109    M        R    1 test
## 3  71    R        R    1 test
## 4 163    M        M    1 test
## 5 158    M        M    1 test
## 6 128    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  50    R        M    1 test
## 2 109    M        R    1 test
## 3  71    R        R    1 test
## 4 163    M        M    1 test
## 5 158    M        M    1 test
## 6 128    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 (`vignette("predict")`)) 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  50    R        M    1 test
## 2 109    M        R    1 test
## 3  71    R        R    1 test
## 4 163    M        M    1 test
## 5 158    M        M    1 test
## 6 128    M        M    1 test
head(getPredictionTruth(pred))
## [1] R M R M M M
## Levels: M R
head(getPredictionResponse(pred))
## [1] M R 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=0.0200000
## Runtime: 0.0192659
r$measures.train
##   iter mmce
## 1     1 0.01
```

(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
## 74    74 versicolor versicolor
## 109  109 virginica  virginica
## 145  145 virginica  virginica
## 45    45   setosa    setosa
## 39    39   setosa    setosa
## 5     5   setosa    setosa
## ... (#rows: 100, #cols: 3)
##
##
## $test
## $test$`1`
## Prediction: 50 observations
## predict.type: response
## threshold:
## time: 0.00
##      id      truth  response
## 16    16   setosa    setosa
## 115  115 virginica  virginica
## 112  112 virginica  virginica
## 58    58 versicolor versicolor
## 132  132 virginica  virginica
## 48    48   setosa    setosa
## ... (#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 = 112; features = 8
## Hyperparameters:
##
## [[2]]
## Model for learner.id=surv.coxph; learner.class=surv.coxph
## Trained on: task.id = lung-example; obs = 111; 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
## 1 14.25714  8.000000 394.42857 212.00000 3.214286  4.245571 16.77857
## 2 28.00000  4.000000  97.42857  84.71429 4.177143  2.078286 18.58571
## 3 19.10000  6.285714 202.00000 123.00000 3.507143  3.261429 18.33429
##      vs      am    gear    carb
## 1 0.0000000 0.1428571 3.285714 3.428571
## 2 0.8571429 0.8571429 4.142857 1.571429
## 3 0.5714286 0.2857143 3.571429 3.000000
##
## [[2]]
##      mpg      cyl    disp      hp    drat      wt      qsec      vs
## 1 25.72500  4.250000 114.2000  95.1250 3.930000  2.402250 18.62250 0.7500000
## 2 17.01429  7.428571 276.0571 150.7143 2.994286  3.601429 18.11857 0.2857143
## 3 14.66667  8.000000 370.3333 246.5000 3.463333  3.903167 15.87000 0.0000000
##      am    gear    carb
## 1 0.7500000 4.375000 2.125000

```

```
## 2 0.0000000 3.000000 2.142857
## 3 0.3333333 3.666667 4.333333
##
## [[3]]
##      mpg      cyl      disp      hp      drat      wt      qsec      vs
## 1 15.57778 8.000000 353.1778 208.3333 3.216667 4.058333 16.86444 0.0000000
## 2 26.71667 4.000000 100.1000 72.5000 4.078333 2.226667 19.32333 1.0000000
## 3 20.41429 5.428571 151.7143 120.7143 3.898571 3.010714 18.24000 0.5714286
##      am      gear      carb
## 1 0.1111111 3.222222 3.555556
## 2 0.6666667 3.833333 1.333333
## 3 0.5714286 4.142857 3.714286
```

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 (`vignette("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
## 1 3847.03 1874.216 3784.2 35.92078 3481.618 17201.68 3852.807 3072.932
##      rad      tax      ptratio      b      lstat
## 1 418.9923 1158.2 3442.089 579.771 12627.36
##
## [[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 1584.566 4014.972 5711.573 276.3068 4865.633 8966.809 5489.54 2793.202
##      rad      tax      ptratio      b      lstat
## 1 593.2705 2778.539 492.5202 0 18644.28
##
## [[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 8030.12 347.0321 9403.284    0 9232.113 7703.444 7551.26 1017.188
##      rad      tax ptratio b      lstat
## 1 926.9713 7143.103 1161.508 0 16089.31
```

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=0.0201414
## Runtime: 0.0324867
```

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=22.5826012
## Runtime: 0.0496778

```

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 (`vignette("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
## Is spatial: 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 on 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] 122 40 75 112 127 41 16 115 66 29 ...
## ..$ : int [1:100] 122 54 143 136 78 10 42 102 115 66 ...
## ..$ : int [1:100] 54 40 75 143 112 136 78 10 127 41 ...
## $ test.inds :List of 3
## ..$ : int [1:50] 1 10 13 14 15 22 34 42 46 47 ...
## ..$ : int [1:50] 3 4 5 8 11 12 16 17 18 19 ...
## ..$ : int [1:50] 2 6 7 9 21 23 24 25 26 27 ...
## $ 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] 25 65 46 131 23 31 144 78 137 63 ...
## ..$ : int [1:100] 69 25 74 65 117 46 23 91 73 13 ...
## ..$ : int [1:100] 69 74 117 131 31 91 73 13 144 103 ...
## $ test.inds :List of 3
## ..$ : int [1:50] 6 13 17 21 29 34 36 44 45 47 ...
## ..$ : int [1:50] 1 4 5 10 11 12 14 15 18 19 ...
## ..$ : int [1:50] 2 3 7 8 9 16 23 24 25 26 ...
## $ group      : Factor w/ 0 levels:
## - attr(*, "class")= chr "ResampleInstance"
### Access the indices of the training observations in iteration 3
rin$train.inds[[3]]
## [1] 69 74 117 131 31 91 73 13 144 103 78 128 137 126 55 114 98
## [18] 59 107 64 12 132 149 71 18 97 127 110 81 99 4 122 5 19
## [35] 10 54 120 135 70 61 119 102 29 30 17 89 92 82 68 52 111
## [52] 15 84 22 108 88 112 123 44 11 58 139 116 106 1 14 62 95
## [69] 115 38 56 67 80 140 50 6 90 118 49 51 143 21 104 75 100
## [86] 129 45 125 86 109 36 20 136 105 34 77 47 94 40 35
```

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$aggr
## mmce.test.mean
## 0.02
r.rpart$aggr
## mmce.test.mean
## 0.08
```

- 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 $b = 1, \dots, B$ 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(vignette("measures"))`).

```

### Mean misclassification error
mmce$aggr
## Aggregation function: test.mean
mmce$aggr$fun
## function (task, perf.test, perf.train, measure, group, pred)
## mean(perf.test)
## <bytecode: 0x96e68e0>
## <environment: namespace:mlr>
### Root mean square error
rmse$aggr
## Aggregation function: test.rmse
rmse$aggr$fun
## function (task, perf.test, perf.train, measure, group, pred)
## sqrt(mean(perf.test^2))
## <bytecode: 0x12863680>
## <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 `test.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:   25.9179278 25.9179278 25.9179278 25.9179278
## [Resample] iter 2:   24.0690453 24.0690453 24.0690453 24.0690453
## [Resample] iter 3:   21.6835705 21.6835705 21.6835705 21.6835705
##
## Aggregated Result: mse.test.mean=23.8901812,mse.test.median=24.0690453,mse.test.min=21.6835705,mse.test.max=25.9179278
##
r
## Resample Result
## Task: BostonHousing-example
## Learner: regr.lm
## Aggr perf: mse.test.mean=23.8901812,mse.test.median=24.0690453,mse.test.min=21.6835705,mse.test.max=25.9179278
## Runtime: 0.0435905
r$aggr
##   mse.test.mean mse.test.median   mse.test.min   mse.test.max
##         23.89018         24.06905         21.68357         25.91793
```

2.5.6.2 Example: Calculating the training error

Below we calculate the mean misclassification error (`mmce (vignette("measures"))`) 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:    0.0400000    0.0600000
## [Resample] iter 2:    0.0300000    0.0600000
## [Resample] iter 3:    0.0400000    0.0400000
##
## Aggregated Result: mmce.test.mean=0.0533333,mmce.train.mean=0.0366667
##
r$measures.train
##   iter mmce mmce
## 1     1 0.04 0.04
## 2     2 0.03 0.03
## 3     3 0.04 0.04
r$aggr
##   mmce.test.mean mmce.train.mean
##         0.0533333         0.0366667
```

2.5.6.3 Example: Bootstrap

In *out-of-bag bootstrap estimation* B new data sets D^{*1}, \dots, 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$measures.train)
##      iter      mmce      mmce      mmce
## 1      1 0.020000000 0.020000000 0.020000000
## 2      2 0.026666667 0.026666667 0.026666667
## 3      3 0.006666667 0.006666667 0.006666667
## 4      4 0.020000000 0.020000000 0.020000000
## 5      5 0.026666667 0.026666667 0.026666667
## 6      6 0.020000000 0.020000000 0.020000000
### Compare misclassification rates for out-of-bag, b632, and b632+ bootstrap
r$aggr
## mmce.test.mean      mmce.b632 mmce.b632plus
##      0.06405639      0.04882497      0.04979022
```

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:  0.0400000 0.0423280
## [Resample] iter 2:  0.0200000 0.0185185
## [Resample] iter 3:  0.0000000 0.0000000
```

```
##
## Aggregated Result: mmce.test.mean=0.0200000,ber.test.mean=0.0202822
##
## Resample Result
## Task: iris_example
## Learner: classif.lda
## Aggr perf: mmce.test.mean=0.0200000,ber.test.mean=0.0202822
## Runtime: 0.0383365
bootstrapB632plus("regr.lm", bh.task, iters = 3, measures = list(mse, mae))
## Resampling: OOB bootstrapping
## Measures:
## [Resample] iter 1:      mse.train   mae.train   mse.test   mae.test
## [Resample] iter 2:      22.7009738  3.3051634   25.3087826  3.5818876
## [Resample] iter 3:      17.9927567  2.8369241   27.6599561  3.6510099
## [Resample] iter 3:      20.6775812  3.2669893   27.1628632  3.6956216
##
## Aggregated Result: mse.b632plus=24.4959351,mae.b632plus=3.4680055
##
## Resample Result
## Task: BostonHousing-example
## Learner: regr.lm
## Aggr perf: mse.b632plus=24.4959351,mae.b632plus=3.4680055
## Runtime: 0.069416
```

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 (`vignette("learner")`) – 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 (`vignette("performance")`) and resampling (`vignette("resample")`).

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 (`vignette("resample")`) 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=0.0466667; time: 0.0 min
## [Tune-x] 3: C=1.5; sigma=0.5
## [Tune-y] 3: mmce.test.mean=0.0400000; 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=0.0533333; time: 0.0 min
## [Tune-x] 7: C=1.5; sigma=1
## [Tune-y] 7: mmce.test.mean=0.0600000; time: 0.0 min
## [Tune-x] 8: C=2; sigma=1
## [Tune-y] 8: mmce.test.mean=0.0533333; time: 0.0 min
## [Tune-x] 9: C=0.5; sigma=1.5
## [Tune-y] 9: mmce.test.mean=0.0533333; 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=0.0466667; 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=0.0533333; 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=0.0400000
res
```

```
## Tune result:
## Op. pars: C=1.5; sigma=0.5
## mmce.test.mean=0.0400000
```

`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 (vignette("measures"))`) 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 (`vignette("advanced_tune")`).

In the example below we calculate the accuracy (`acc (vignette("measures"))`) instead of the error rate. We use function `setAggregation()`, as described on the resampling (`vignette("resample")`) 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=1.17e+03; sigma=0.000275
## 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] 1169.963
##
## $sigma
## [1] 0.0002754024
res$y
## acc.test.mean acc.test.sd
## 0.9733333 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=1.17e+03,sigma=0.000275
```

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  9.1680769  5.255698   0.2666667  0.03055050         1      0.072
## 2  5.1938345  2.344891   0.2733333  0.04163332         2      0.055
## 3  6.5843282  8.372191   0.2666667  0.03055050         3      0.054
## 4 -0.5873477 -8.473630   0.2666667  0.03055050         4      0.055
## 5  2.7339808 -4.296414   0.9400000  0.02000000         5      0.052
## 6  4.5165274 -3.857521   0.9600000  0.02000000         6      0.052
```

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:

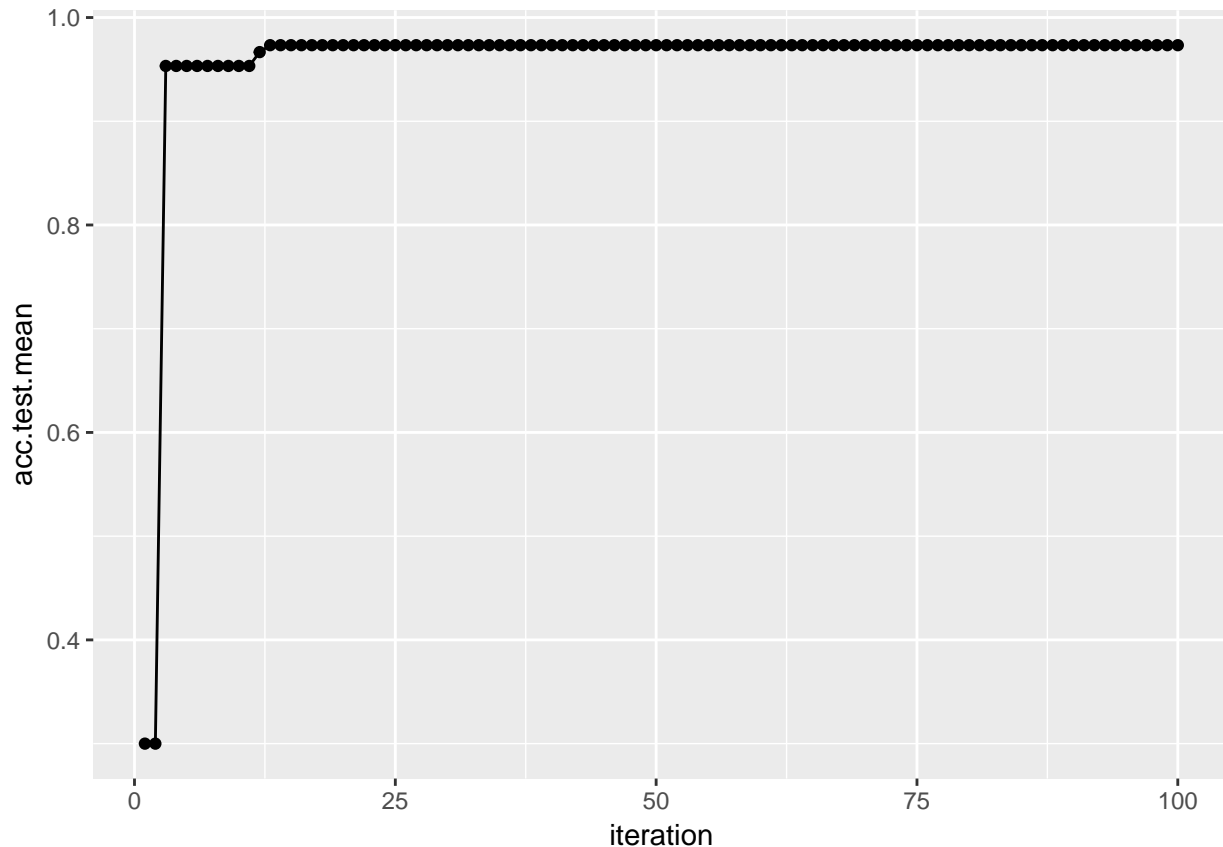
```
generateHyperParsEffectData(res, trafo = TRUE)
## HyperParsEffectData:
## Hyperparameters: C,sigma
## Measures: acc.test.mean,acc.test.sd
## Optimizer: TuneControlRandom
## Nested CV Used: FALSE
## Snapshot of data:
##           C          sigma acc.test.mean acc.test.sd iteration exec.time
## 1 1.472573e+09 1.801764e+05    0.2666667  0.03055050         1     0.072
## 2 1.562552e+05 2.212539e+02    0.2733333  0.04163332         2     0.055
## 3 3.839973e+06 2.356087e+08    0.2666667  0.03055050         3     0.054
## 4 2.586142e-01 3.360239e-09    0.2666667  0.03055050         4     0.055
## 5 5.419769e+02 5.053427e-05    0.9400000  0.02000000         5     0.052
## 6 3.284940e+04 1.388285e-04    0.9600000  0.02000000         6     0.052
```

Note that we can also generate performance on the train data along with the validation/test data, as discussed on the resampling (`vignette("resample")`) 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 -9.293791000 -3.145917      0.26          0.37         1     0.032
## 2 -1.604953841 -6.252643      0.26          0.37         2     0.032
## 3 -3.811128940  4.129502      0.26          0.37         3     0.029
## 4 -1.738500129 -2.698458      0.26          0.37         4     0.030
## 5 -4.415414161  5.211998      0.26          0.37         5     0.029
## 6 -0.008596266  2.563388      0.26          1.00         6     0.028
```

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 (`vignette("hyperpar_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` (`vignette("configureMlr")`) 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 (`vignette("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 (`vignette("measures")`), 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` (`vignette("measures")`) 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      0.0034
## 2      0.0073
## 3      0.0295
## 4      0.0081
## 5      0.0141
## 6      0.3640
## 7      0.0094
## 8      0.0141
## 9      0.4306
## 10     0.0044
## 11     0.0090
## 12     0.4302
## 13     0.0172
## 14     0.0168
## 15     0.2443
```

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      0.003
## 2 iris_example      lda      2 0.1333333 0.1666667      0.003
## 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

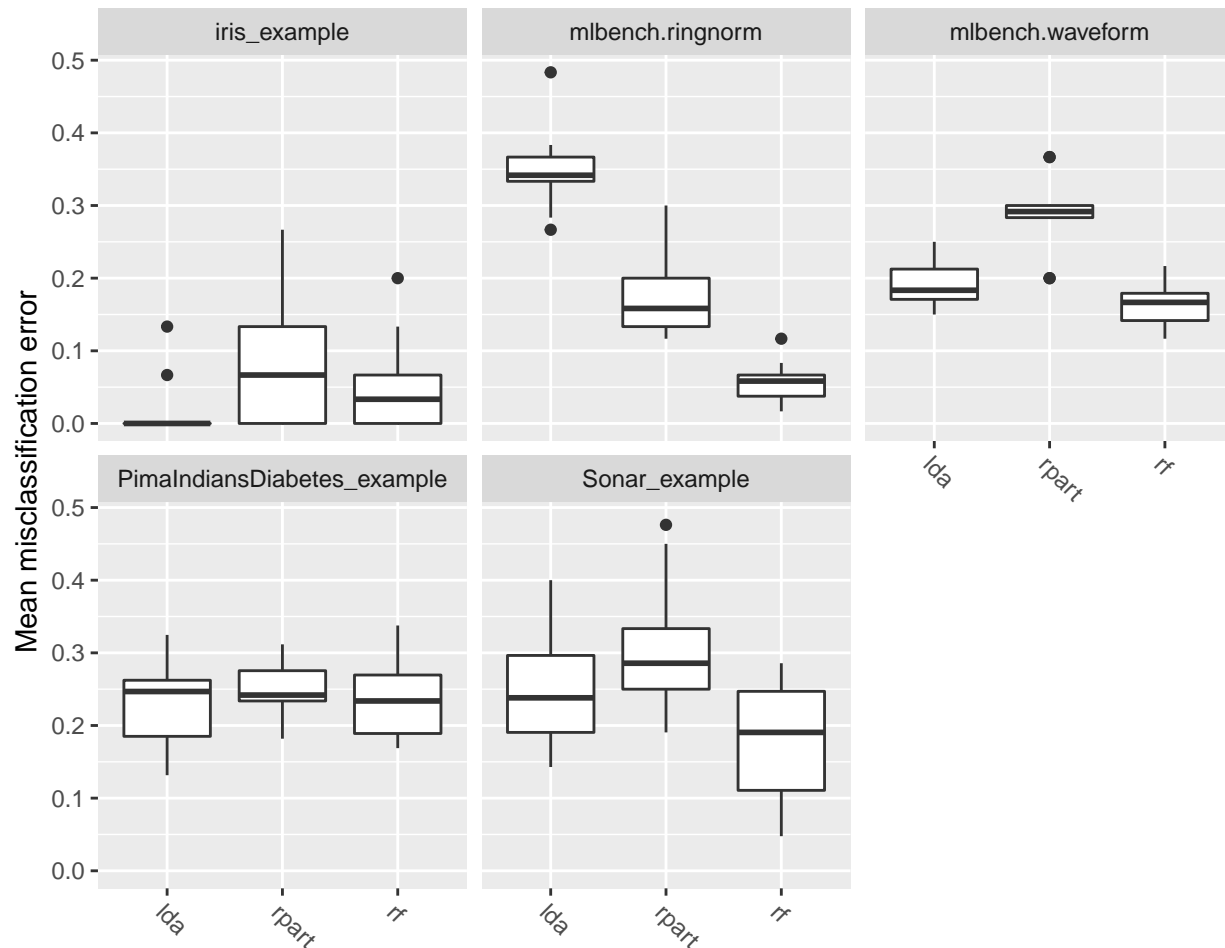
Plots are generated using `ggplot2::ggplot2()`. Further customization, such as renaming plot elements or changing colors, is easily possible.

2.7.4.2.1 Visualizing performances

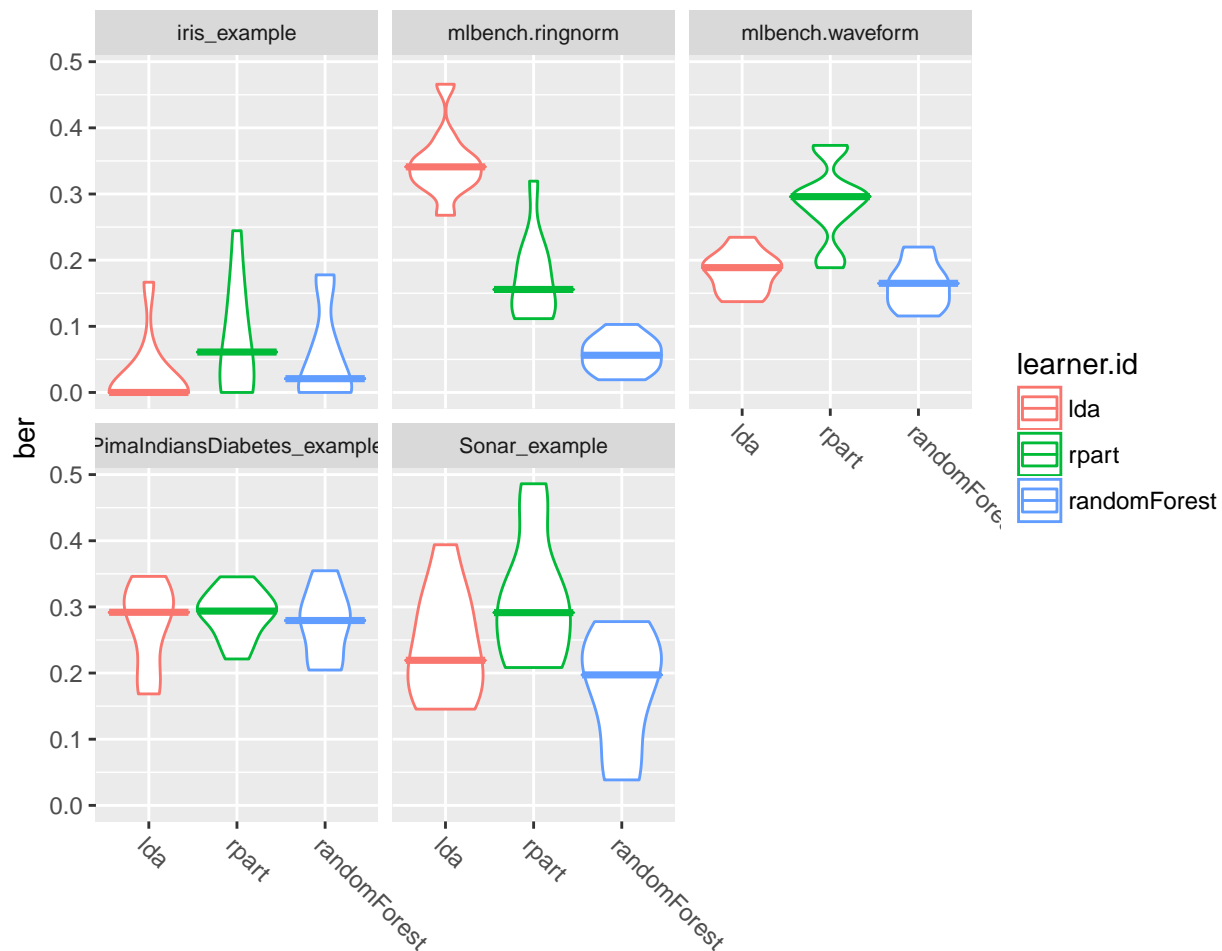
`plotBMRBoxplots()` creates box or violin plots which show the distribution of performance values across resampling iterations for one performance measure and for all learners and tasks (and thus visualize the output of `getBMRPerformances()`).

Below are both variants, box and violin plots. The first plot shows the `mmce` and the second plot the `ber` (`vignette("measures")`). Moreover, in the second plot we color the boxes according to the `learner.ids`.

```
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"
```

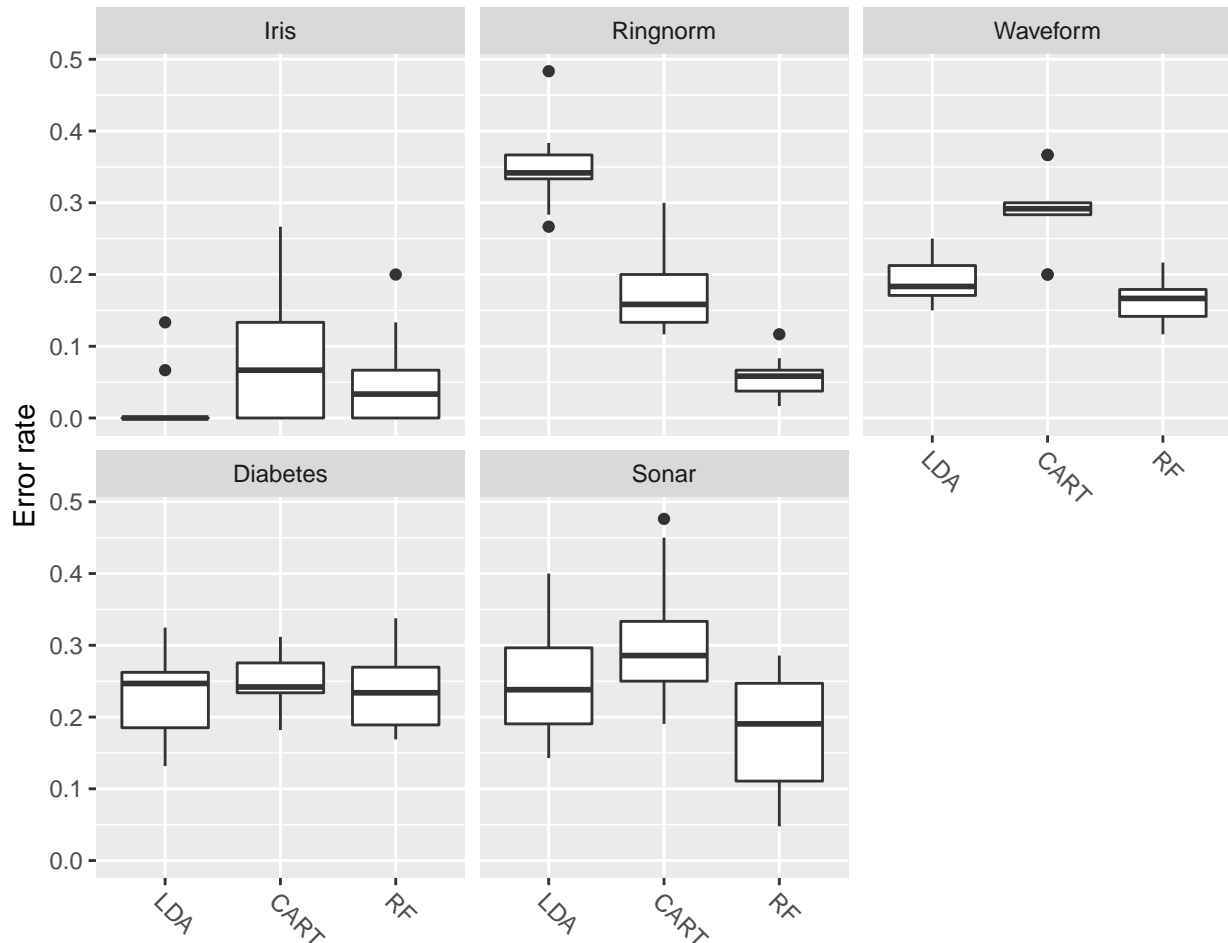
If you prefer the ids like, e.g., `mmce` and `ber` set `pretty.names = FALSE` (as done for the second plot). Of course you can also use the `ggplot2::ggplot2()` functionality like the `ggplot2::labs()` function to choose completely different labels.

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 0.003
## 2 iris_example      lda      2 0.1333333 0.1666667 0.003
## 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")

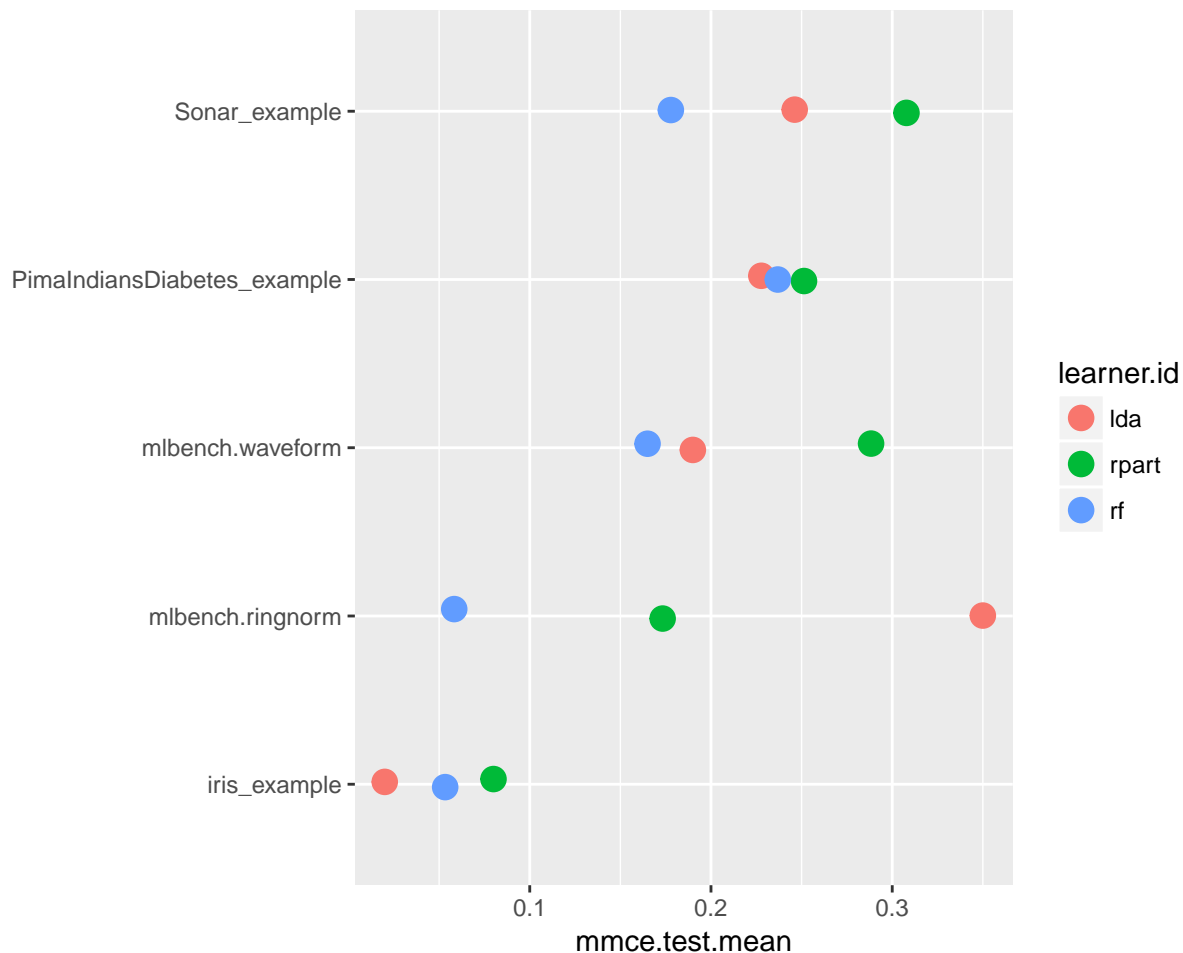
plt + ylab("Error rate")
```



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 `vignette("measures")`. 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.

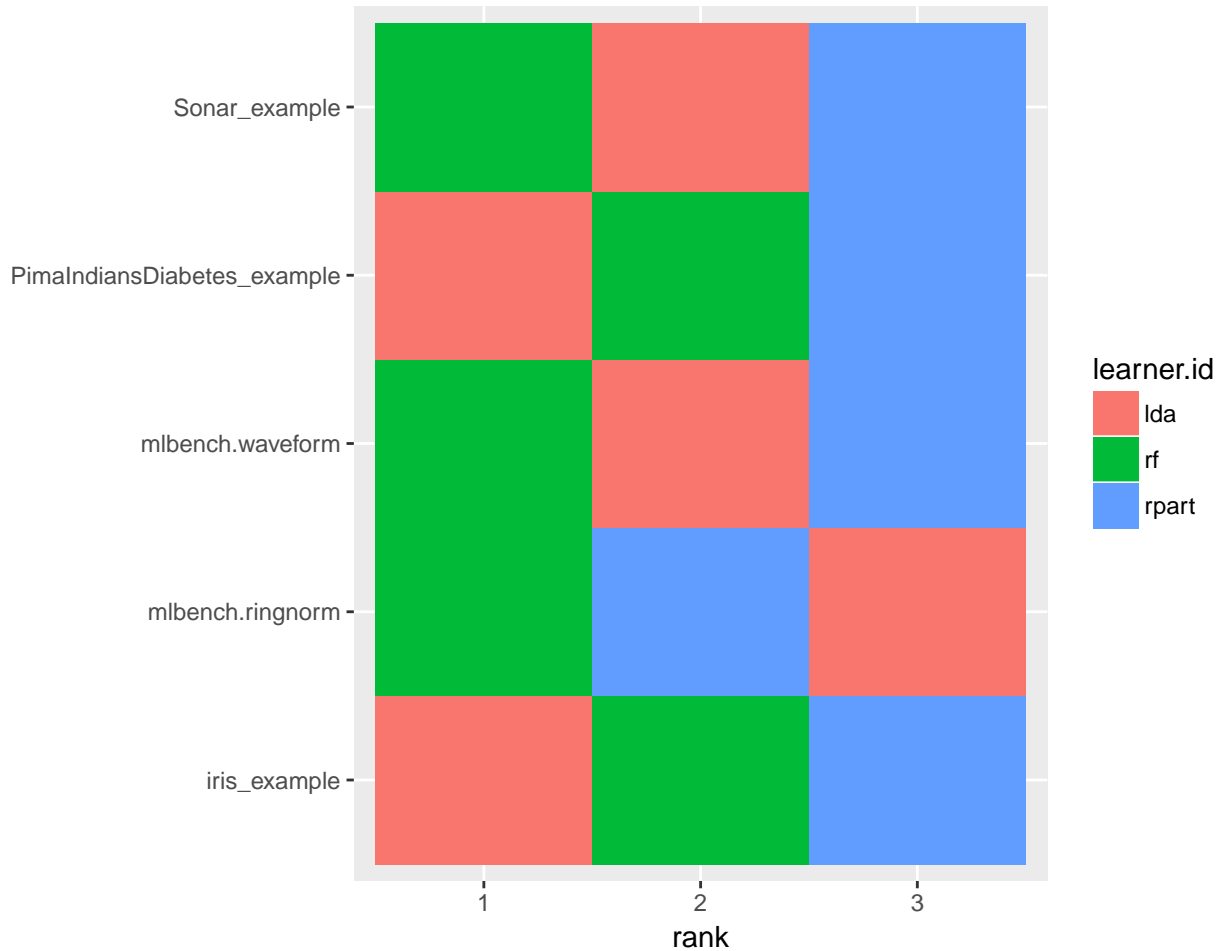
Function `convertBMRTToRankMatrix()` calculates ranks based on aggregated learner performances of one measure. We choose the mean misclassification error (`vignette("measures")`). The rank structure can be visualized by `plotBMRRanksAsBarChart()`.

```
m = convertBMRTToRankMatrix(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 `vignette("measures")`, 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.

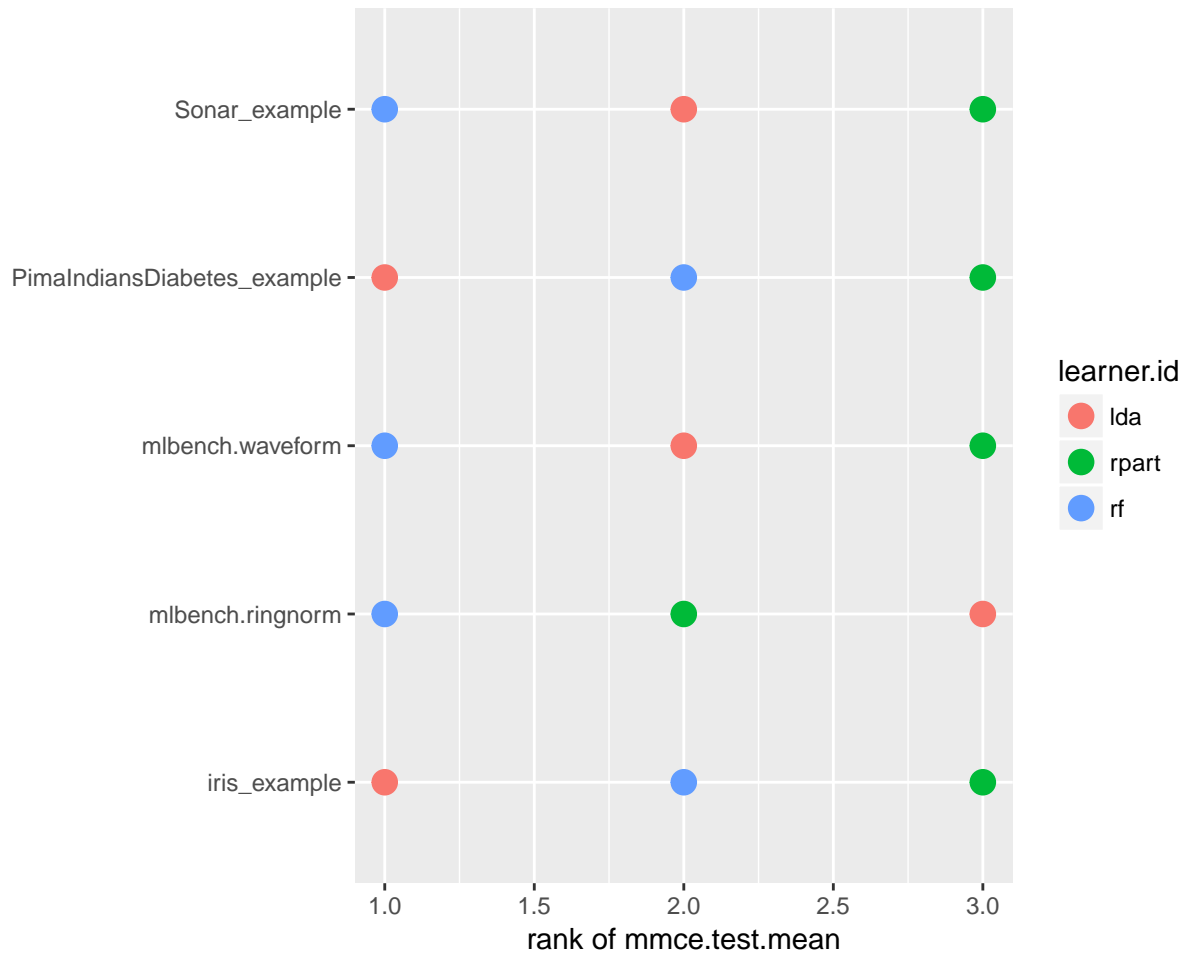
`plotBMRRanksAsBarChart()` with option `pos = "tile"` shows a corresponding heat map. The ranks are displayed on the x-axis and the learners are color-coded.

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



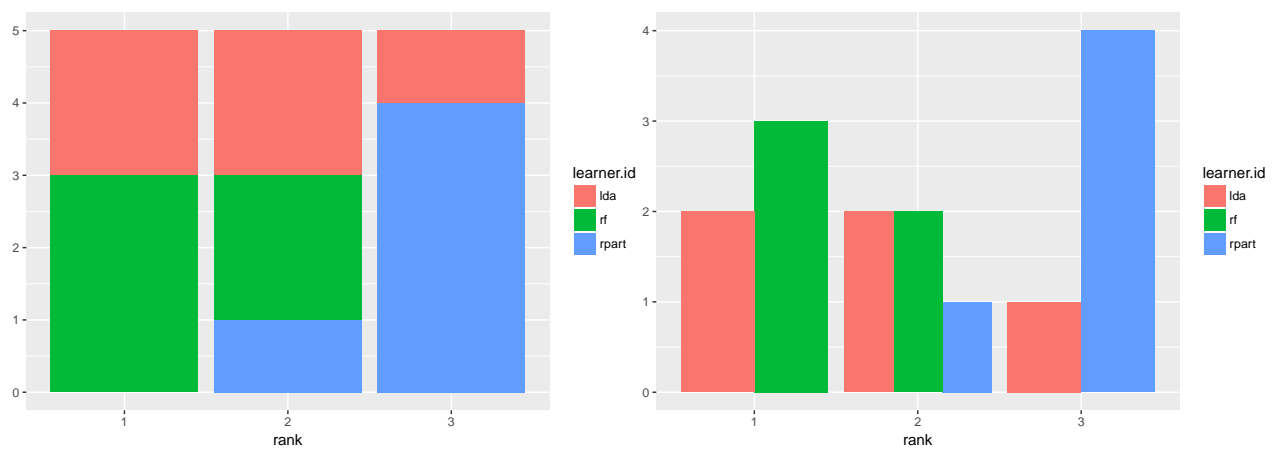
A similar plot can also be obtained via `plotBMRSummary()`. With option `trafo = "rank"` the ranks are displayed instead of the aggregated performances.

```
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 than 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 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 diagram can 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.

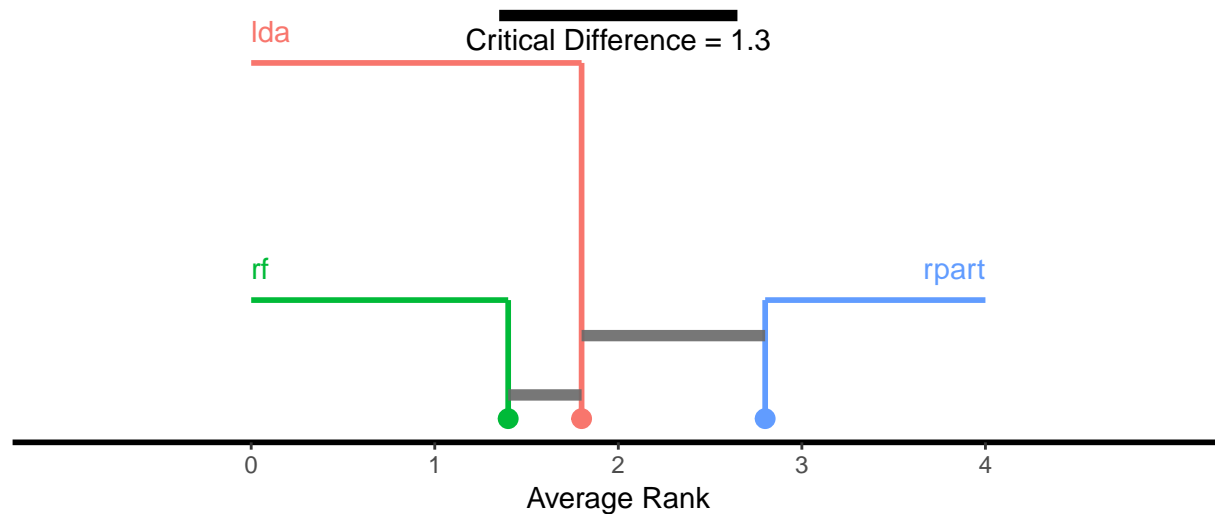
The critical difference CD is calculated by

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

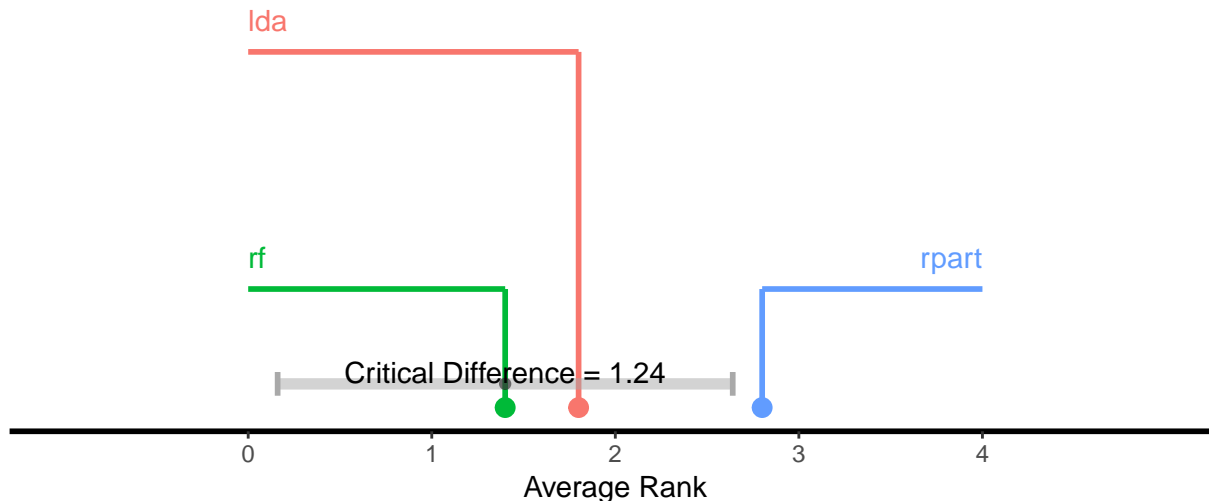
where N denotes the number of tasks, k is the number of learners, and q_{α} comes from the studentized range statistic divided by $\sqrt{2}$. For details see Demsar (2006).

Function `generateCritDifferencesData()` does all necessary calculations while function `plotCritDifferences()` draws the plot. See the tutorial page about `vignette("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))
```



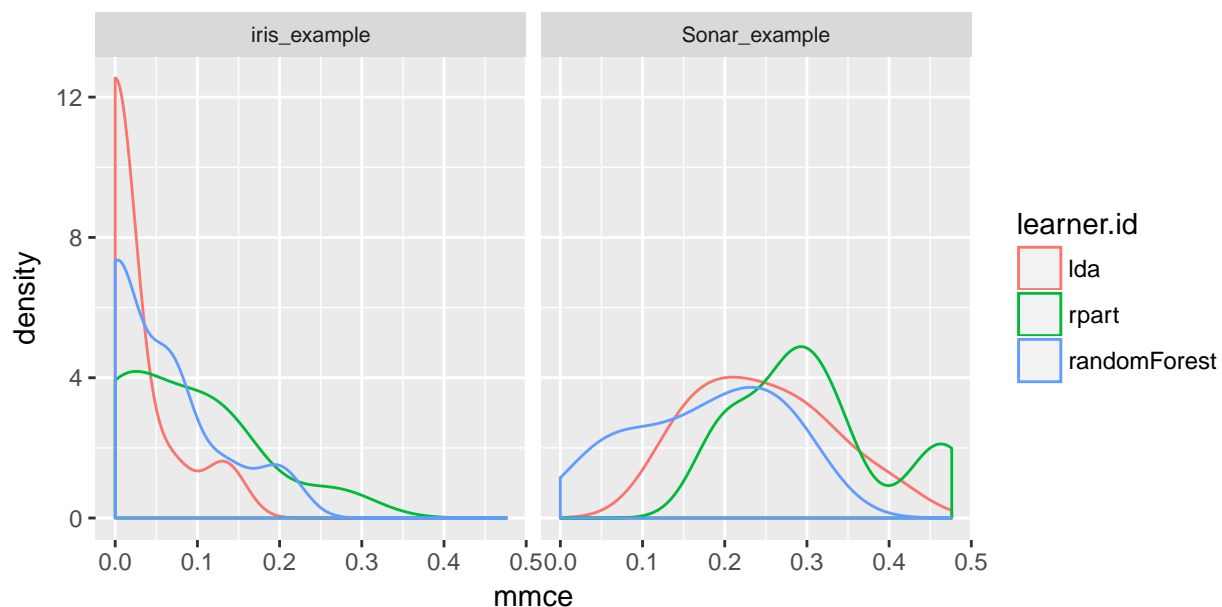
2.7.4.5 Custom plots

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))
```

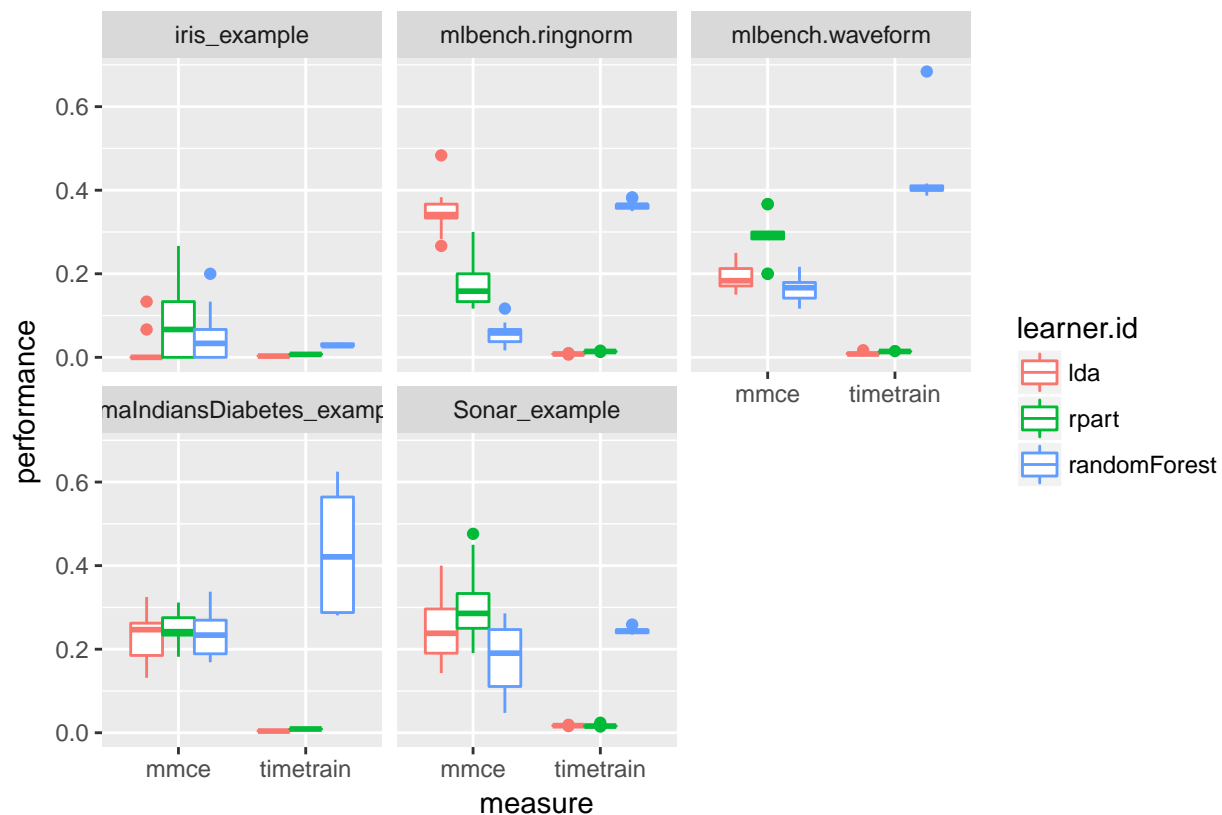


In order to plot multiple performance measures in parallel, `perf` is reshaped to long format. Below we generate grouped boxplots showing the error rate and the training time (`vignette("measures")`).

```

### 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)

```



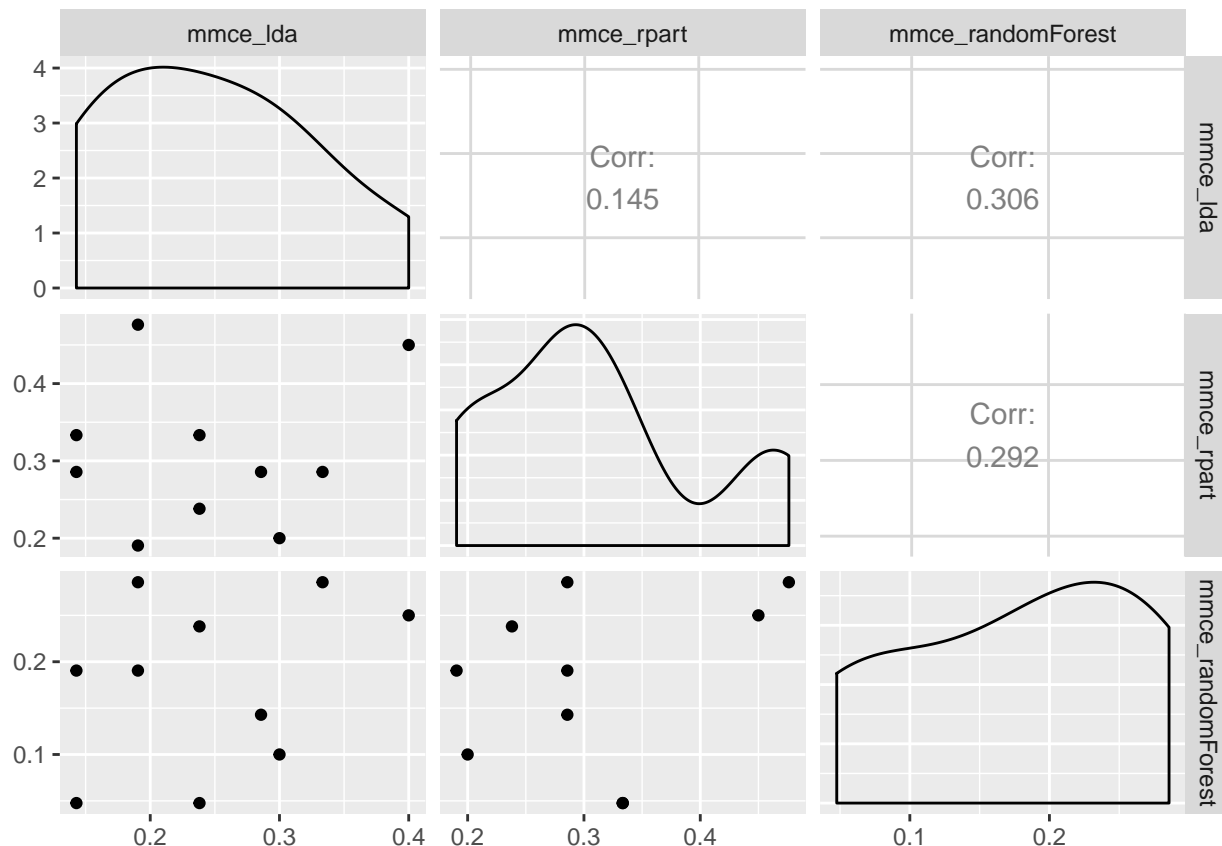
It might also be useful to assess if learner performances in single resampling iterations, i.e., in one fold, are related. This might help to gain further insight, for example by having a closer look at train and test sets from iterations where one learner performs exceptionally well while another one 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 (`vignette("measures")`) 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 `vignette("roc_analysis")` and functions `generateThreshVsPerfData()`, `plotROCCurves()`, and `plotViperCharts()` as well as the page about `vignette("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 `vignette("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 `vignette("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 `vignette("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 (`vignette("create_learner")`), 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

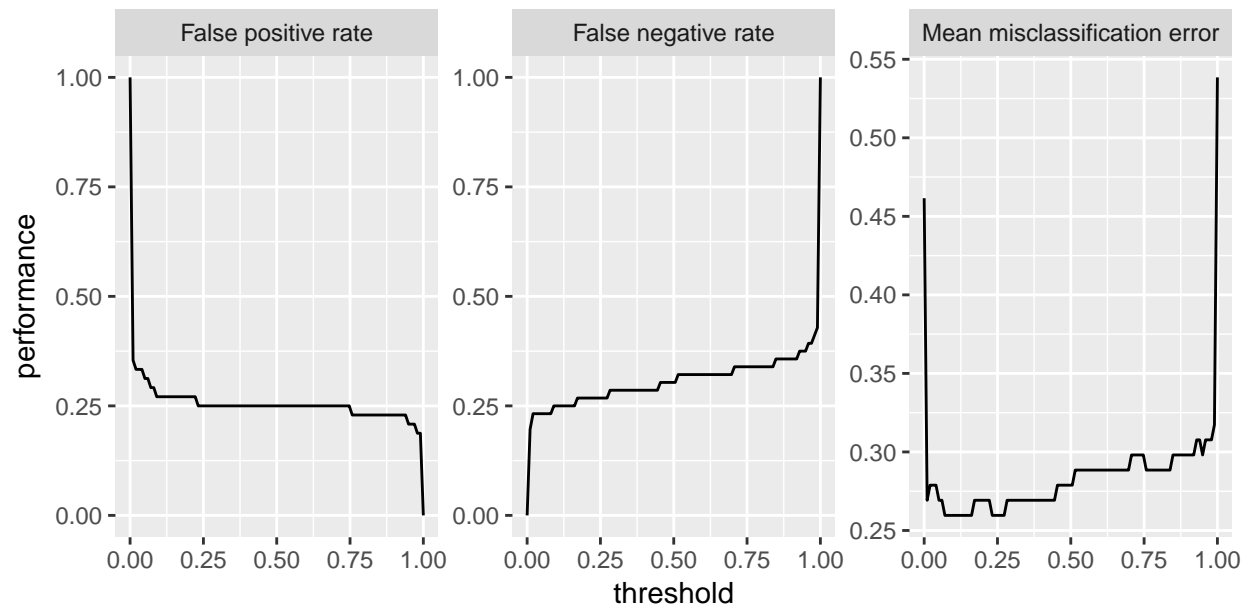
In the example below we create a plot of classifier performance as function of the decision threshold for the binary classification problem `sonar.task`. The generation function `generateThreshVsPerfData()` creates an object of class `ThreshVsPerfData` which contains the data for the plot in slot `$data`.

```
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 0.0000000
## 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` names 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 `ids` 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.

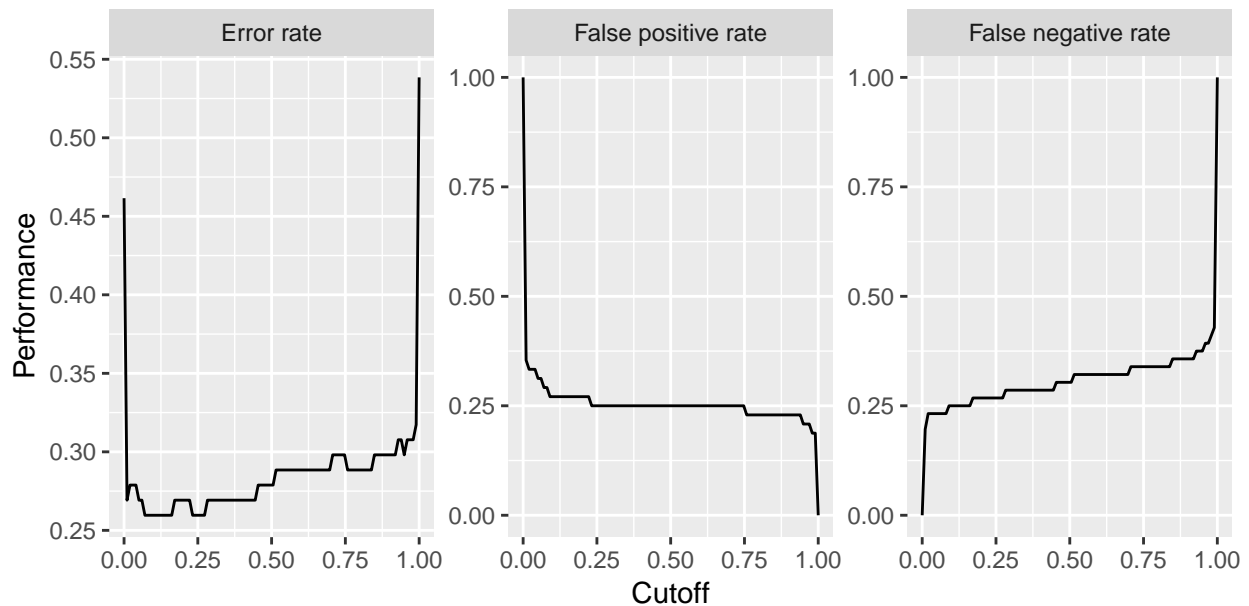
What will probably come up most often is changing labels and annotations. Generally, this can be done by manipulating the `ggplot2::ggplot()` object, in this example the object returned by `plotThreshVsPerf()`, using the usual `ggplot2::ggplot2()` functions like `ggplot2::labs()` or `ggplot2::labeller()`. 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
```



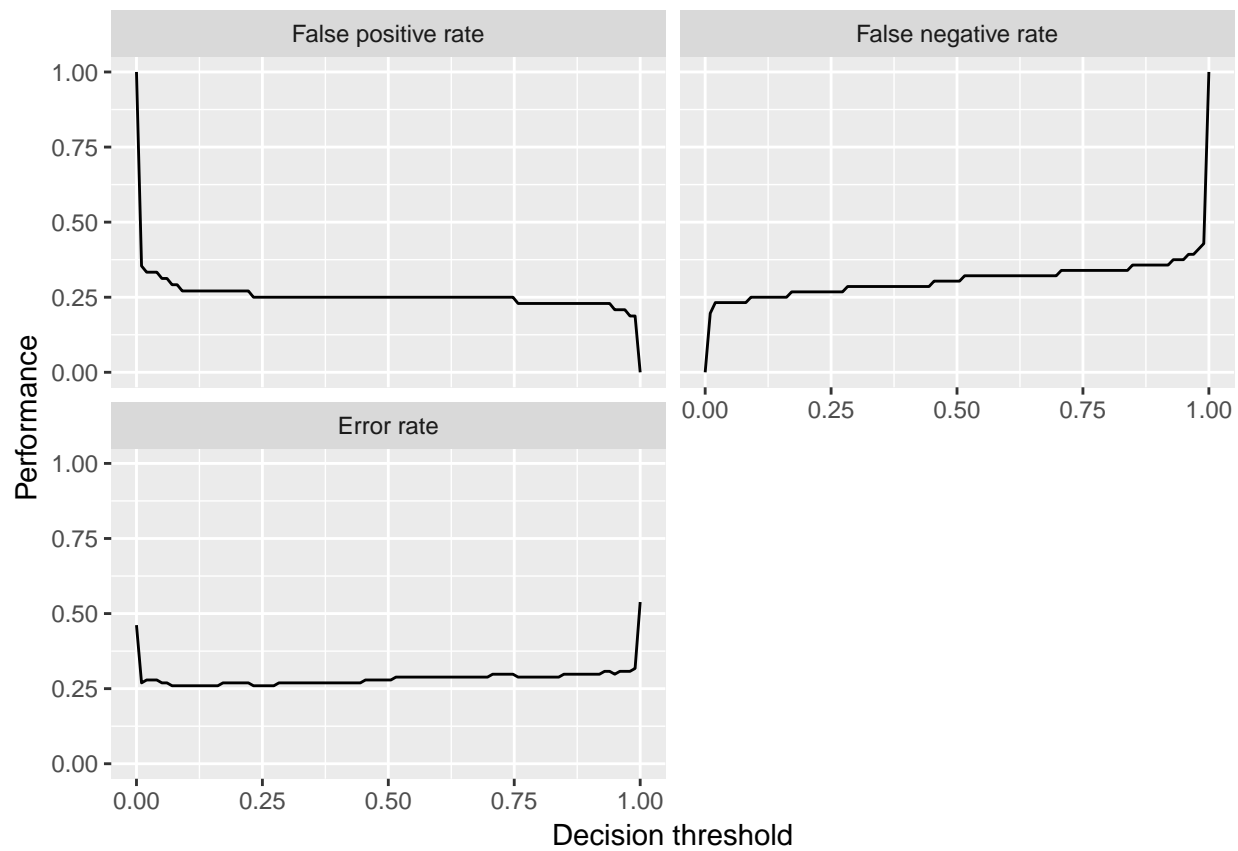
Using the `ggplot2::labeller()` function requires calling `ggplot2::facet_wrap()` (or `ggplot2::facet_grid()`), which can be useful if you want to change how the panels are positioned (number of rows and columns) or influence the axis limits.

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

measure_names = c(
  fpr = "False positive rate",
  fnr = "False negative rate",
  mmce = "Error rate"
)

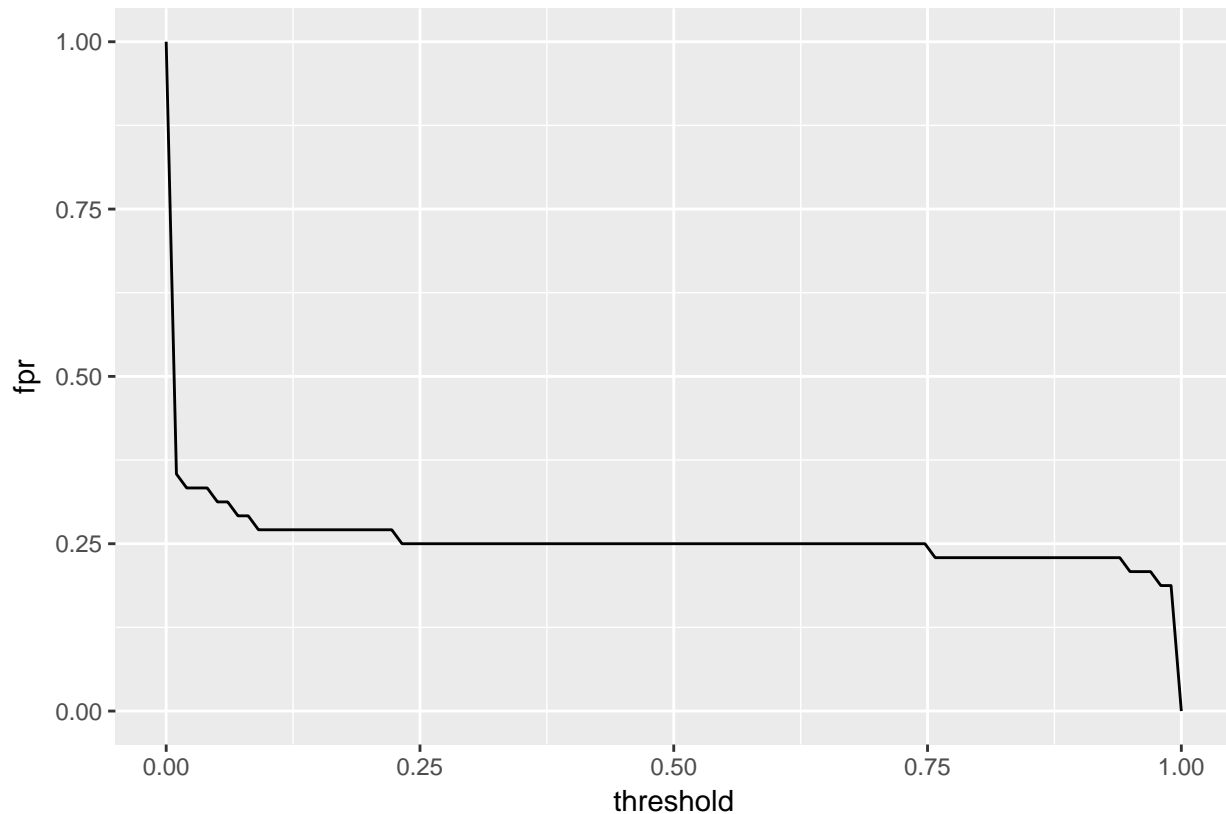
### Manipulate the measure names via the labeller function and
### arrange the panels in two columns and choose common axis limits for all panels
plt = plt + facet_wrap(~ measure, labeller = labeller(measure = measure_names), ncol = 2)
plt = plt + xlab("Decision threshold") + ylab("Performance")
```

```
plt
```



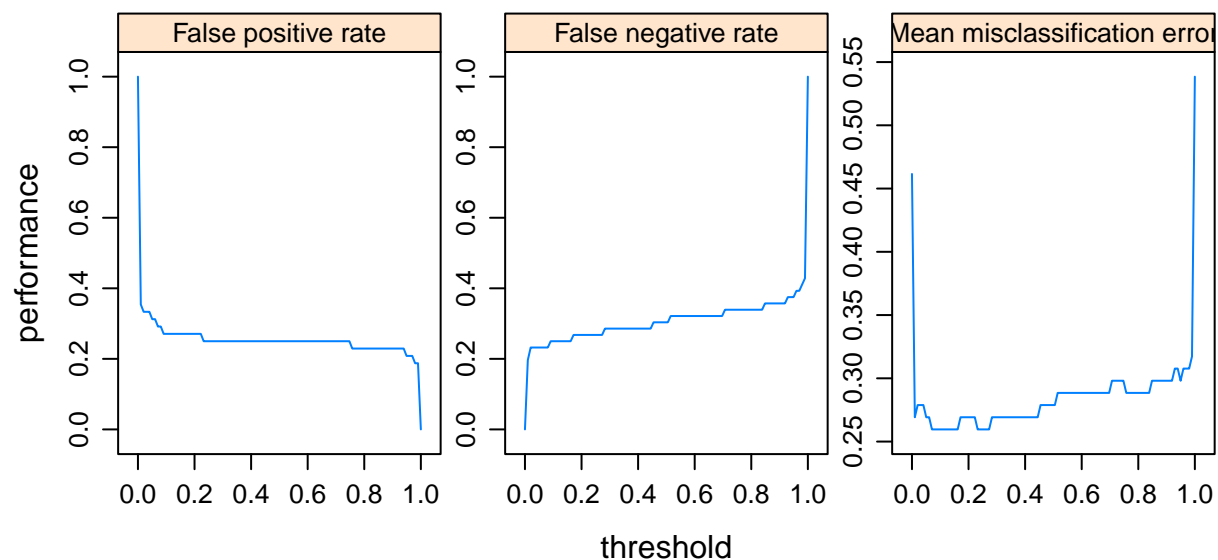
Instead of using the built-in function `plotThreshVsPerf()` we could also manually create the plot based on the output of `generateThreshVsPerfData()`: In this case to plot only one measure.

```
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()`.

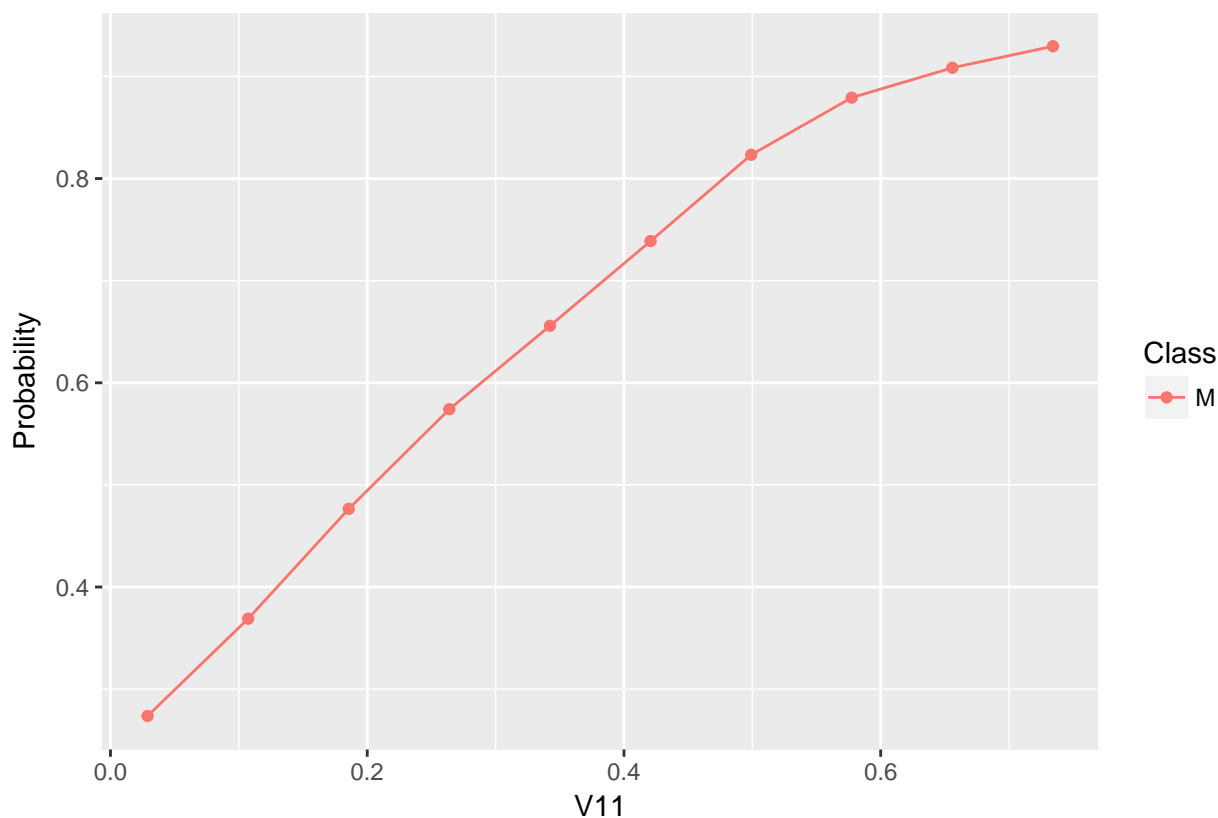
```
lattice::xyplot(fpr + fnr + mmce ~ threshold, data = d$data, type = "l", ylab = "performance",
  outer = TRUE, scales = list(relation = "free"),
  strip = strip.custom(factor.levels = sapply(d$measures, function(x) x$name),
    par.strip.text = list(cex = 0.8)))
```



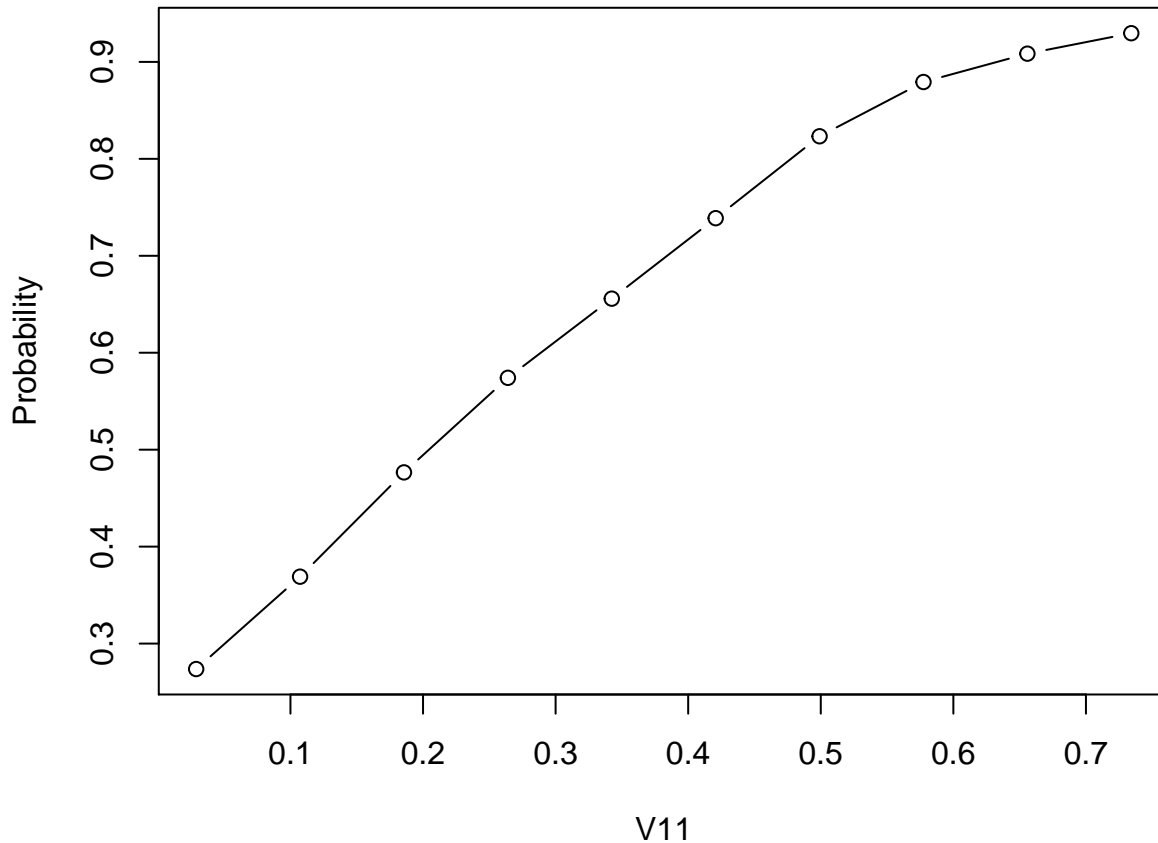
Let's conclude with a brief look on a second example. Here we use `plotPartialDependence()` but extract

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")
plt = plotPartialDependence(pd)
head(plt$data)
##   Class Probability Feature      Value
## 1     M   0.2737158    V11 0.0289000
## 2     M   0.3689970    V11 0.1072667
## 3     M   0.4765742    V11 0.1856333
## 4     M   0.5741233    V11 0.2640000
## 5     M   0.6557857    V11 0.3423667
## 6     M   0.7387962    V11 0.4207333
plt
```



```
plot(Probability ~ 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
<code>generateThreshVsPerfData()</code>	<code>plotThreshVsPerf()</code>	<code>plotThreshVsPerfGGVIS()</code>
	<code>plotROCCurves()</code>	—
<code>generateCritDifferencesData()</code>	<code>plotCritDifferences()</code>	—
<code>generateHyperParsEffectData()</code>	<code>plotHyperParsEffect()</code>	
<code>generateFilterValuesData()</code>	<code>plotFilterValues()</code>	<code>plotFilterValuesGGVIS()</code>
<code>generateLearningCurveData()</code>	<code>plotLearningCurve()</code>	<code>plotLearningCurveGGVIS()</code>
<code>generatePartialDependenceData()</code>	<code>plotPartialDependence()</code>	<code>plotPartialDependenceGGVIS()</code>
<code>generateFunctionalANOVAData()</code>		
<code>generateCalibrationData()</code>	<code>plotCalibration()</code>	—

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 11.279525
## iter 20 value 5.430138
## iter 30 value 5.311668
## iter 40 value 5.306693
## iter 50 value 5.304200
## iter 60 value 5.304086
## final value 5.304084
## 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 new
## 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 k
## 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 n
## 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 vignette("benchmark_experiments") 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 (`vignette("preproc")`)
- Imputation (`vignette("impute")`)
- Bagging (`vignette("bagging")`)
- Tuning (`vignette("tune")`)
- Feature selection (`vignette("feature_selection")`)
- Cost-sensitive classification (`vignette("cost_sensitive_classif")`)
- Over- and undersampling (`vignette("imbalanced_classification_problems")`) for imbalanced classification problems
- Multiclass extension (`makeMulticlassWrapper()`) for binary-class learners
- Multilabel classification (`vignette("multilabel")`)

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 exemplarily 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: 0.0000000
## [Resample] iter 2: 0.1333333
## [Resample] iter 3: 0.0666667
## [Resample] iter 4: 0.0666667
```

```
## [Resample] iter 5:    0.0666667
## [Resample] iter 6:    0.0000000
## [Resample] iter 7:    0.0000000
## [Resample] iter 8:    0.1333333
## [Resample] iter 9:    0.1333333
## [Resample] iter 10:   0.0666667
##
## Aggregated Result: mmce.test.mean=0.0666667
##
## Task: iris, Learner: classif.rpart.bagged
## Resampling: cross-validation
## Measures:          mmce
## [Resample] iter 1:    0.0000000
## [Resample] iter 2:    0.1333333
## [Resample] iter 3:    0.0666667
## [Resample] iter 4:    0.0000000
## [Resample] iter 5:    0.0000000
## [Resample] iter 6:    0.0000000
## [Resample] iter 7:    0.0000000
## [Resample] iter 8:    0.1333333
## [Resample] iter 9:    0.1333333
## [Resample] iter 10:   0.0666667
##
## Aggregated Result: mmce.test.mean=0.0533333
##
##   task.id          learner.id mmce.test.mean
## 1   iris          classif.rpart    0.0666667
## 2   iris classif.rpart.bagged    0.0533333
```

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` (`vignette("measures")`) 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` (`vignette("measures")`) (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=7; bw.feats=0.883
## [Tune-y] 1: mmce.test.mean=0.0533333; time: 0.1 min
## [Tune-x] 2: minsplit=2; bw.feats=0.972
## [Tune-y] 2: mmce.test.mean=0.0666667; time: 0.1 min
## [Tune-x] 3: minsplit=4; bw.feats=0.886
## [Tune-y] 3: mmce.test.mean=0.0666667; time: 0.1 min
## [Tune-x] 4: minsplit=5; bw.feats=0.402
## [Tune-y] 4: mmce.test.mean=0.0600000; time: 0.1 min
## [Tune-x] 5: minsplit=2; bw.feats=0.43
## [Tune-y] 5: mmce.test.mean=0.0533333; time: 0.1 min
## [Tune-x] 6: minsplit=9; bw.feats=0.733
## [Tune-y] 6: mmce.test.mean=0.0533333; time: 0.1 min
## [Tune-x] 7: minsplit=6; bw.feats=0.928
## [Tune-y] 7: mmce.test.mean=0.0533333; time: 0.1 min
## [Tune-x] 8: minsplit=9; bw.feats=0.324
## [Tune-y] 8: mmce.test.mean=0.0666667; time: 0.1 min
## [Tune-x] 9: minsplit=10; bw.feats=0.918
## [Tune-y] 9: mmce.test.mean=0.0533333; time: 0.1 min
## [Tune-x] 10: minsplit=10; bw.feats=0.729

```

```
## [Tune-y] 10: mmce.test.mean=0.0533333; time: 0.1 min
## [Tune] Result: minsplit=10; bw.feats=0.918 : mmce.test.mean=0.0533333
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 (`vignette("task")`):

- `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 (`vignette("feature_selection")`) and
- Imputation of missing values (`vignette("impute")`).

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 (`vignette("wrapper")`):

- `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 (`vignette("tune")`) 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
## Is spatial: 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 (`vignette("benchmark_experiments")`). 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      0.3752933
## 2 Sonar_example classif.qda.preproc 0.2068323
```

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 (`vignette("tune")`) 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=8; predict.method=plug-in
## mmce.test.mean=0.1828157
as.data.frame(res$opt.path)[1:3]
##      ppc.pcaComp predict.method mmce.test.mean
## 1             1      plug-in      0.5144928
## 2             8      plug-in      0.1828157
## 3            14      plug-in      0.1877847
## 4            21      plug-in      0.2117322
## 5            27      plug-in      0.2790890
## 6            34      plug-in      0.2646653
## 7            40      plug-in      0.2548654
## 8            47      plug-in      0.2356108
## 9            53      plug-in      0.2887509
## 10           60      plug-in      0.3752933
## 11             1      debiased      0.4664596
## 12             8      debiased      0.2213251
## 13            14      debiased      0.2358178
## 14            21      debiased      0.2310559
## 15            27      debiased      0.2887509
## 16            34      debiased      0.2885438
## 17            40      debiased      0.2884748
## 18            47      debiased      0.3124224
## 19            53      debiased      0.3271222
## 20            60      debiased      0.3601794
```

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 (`vignette("wrapper")`) 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(vignette("measures"))`) 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=27.5336255
## Runtime: 0.183388
```

```

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=43.0790850
## Runtime: 0.136821

```

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 (`vignette("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=0.1; center=FALSE; scale=TRUE
## mse.test.mean=9.8440543
as.data.frame(res$opt.path)
##      decay center scale mse.test.mean dob eol error.message exec.time
## 1      0    TRUE  TRUE      17.113844  1  NA          <NA>      0.055
## 2     0.05    TRUE  TRUE      14.220106  2  NA          <NA>      0.051
## 3     0.1    TRUE  TRUE      10.657447  3  NA          <NA>      0.052
## 4      0   FALSE  TRUE      14.908486  4  NA          <NA>      0.040
## 5     0.05   FALSE  TRUE      13.093784  5  NA          <NA>      0.048
## 6     0.1   FALSE  TRUE       9.844054  6  NA          <NA>      0.066
## 7      0    TRUE FALSE      60.223553  7  NA          <NA>      0.040
## 8     0.05    TRUE FALSE      39.393784  8  NA          <NA>      0.063
## 9     0.1    TRUE FALSE      46.145350  9  NA          <NA>      0.051
## 10     0   FALSE FALSE      79.225348 10  NA          <NA>      0.031
## 11    0.05   FALSE FALSE      44.610436 11  NA          <NA>      0.060
## 12    0.1   FALSE FALSE      40.470000 12  NA          <NA>      0.053
```

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[apply(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 (`vignette("create_imputation")`).

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")]
##           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 (`vignette("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] :50    Min.   :56.00
## 1st Qu.: 18.00    1st Qu.:115.8    (8,16]:87    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	(16,24]	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$data)
##      Ozone      Solar.R      Wind      Temp
## Min.   : 1.00   Min.   : 7.0   (0,8] :35   Min.   :56.00
## 1st Qu.: 16.00  1st Qu.:113.8   (8,16]:60  1st Qu.:69.00
## Median : 34.00  Median :224.0   (16,24]: 5   Median :79.50
## Mean   : 41.59   Mean   :194.5           Mean :76.87
## 3rd Qu.: 63.00  3rd Qu.:274.0           3rd Qu.:84.00
## Max.   :135.00  Max.   :334.0           Max.   :93.00
## NA's   :31
## Solar.R.dummy Wind.dummy
## FALSE:93      FALSE:90
## TRUE : 7       TRUE :10
##
##
##
##
imp$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 (`vignette("measures")`) is calculated.

```
rdesc = makeResampleDesc("CV", iters = 3)
r = resample(lrn, task, resampling = rdesc, show.info = FALSE, models = TRUE)
r$aggr
## mse.test.mean
##      520.1596
lapply(r$models, getLearnerModel, more.unwrap = TRUE)
## [[1]]
##
## Call:
## stats::lm(formula = f, data = d)
##
```

```
## Coefficients:
##      (Intercept)          Solar.R          Wind(8,16]
##      -61.92877          0.06847          -26.32834
##      Wind(16,24]          Temp    Solar.R.dummyTRUE
##      -24.70946          1.40012          -25.23600
##      Wind.dummyTRUE
##      -8.86861
##
##
## [[2]]
##
## Call:
## stats::lm(formula = f, data = d)
##
## Coefficients:
##      (Intercept)          Solar.R          Wind(8,16]
##      -116.97606          0.02231          -14.46570
##      Wind(16,24]          Temp    Solar.R.dummyTRUE
##      -18.69823          2.11034          -5.09015
##      Wind.dummyTRUE
##      -1.91083
##
##
## [[3]]
##
## Call:
## stats::lm(formula = f, data = d)
##
## Coefficients:
##      (Intercept)          Solar.R          Wind(8,16]
##      -88.31383          0.08974          -27.77765
##      Wind(16,24]          Temp    Solar.R.dummyTRUE
##      -7.78686          1.69506          -13.49901
##      Wind.dummyTRUE
##      2.63137
```

A second possibility to fuse a learner with imputation is provided by `makePreprocWrapperCaret()`, which is an interface to `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.itsers = 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
## 0.25
```

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
## 0.2161905
```

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
```

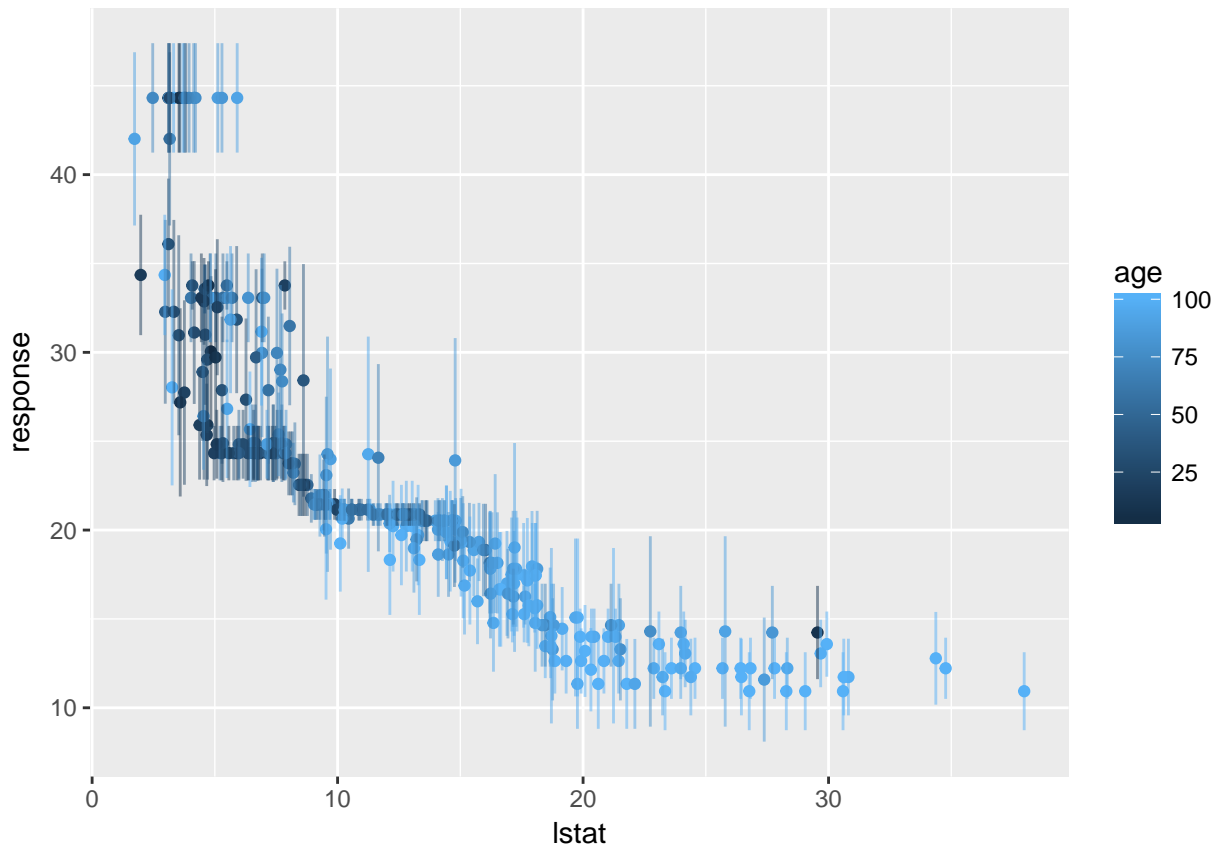
Predict the response and calculate the standard deviation:

```
pred = predict(mod, task = bh.task, subset = test.inds)
head(as.data.frame(pred))
##   id truth response      se
## 2  2  21.6 21.44537 0.8641988
## 3  3  34.7 33.06789 2.4965680
## 5  5  36.2 33.06789 2.4965680
## 6  6  28.7 24.33055 1.5321721
## 8  8  27.1 14.44748 2.3458197
## 9  9  16.5 13.58193 1.8335539
```

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	-2.8865944	vanilladot	NA	NA	0.04	1	NA
## 2	1.5514434	polydot	NA	4	0.08	1	NA
## 3	1.4195381	polydot	NA	2	0.04	1	NA
## 4	0.1502372	polydot	NA	4	0.08	1	NA
## 5	2.5552287	rbfdot	5.078769	NA	0.44	1	NA
## 6	-2.2188679	polydot	NA	4	0.06	1	NA

```
## error.message exec.time
## 1          <NA>      0.054
## 2          <NA>      0.122
## 3          <NA>      0.062
## 4          <NA>      0.025
## 5          <NA>      0.030
## 6          <NA>      0.027
```

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	-4.904589	NA
## 2	classif.ksvm	3.227199	NA
## 3	classif.randomForest	NA	209


```
## 4 classif.randomForest      NA      322
## 5 classif.randomForest      NA      178
## 6 classif.randomForest      NA      211
## mmce.test.mean dob eol error.message exec.time
## 1      0.04666667      1 NA      <NA>      0.086
## 2      0.18000000      1 NA      <NA>      0.075
## 3      0.04666667      1 NA      <NA>      0.058
## 4      0.04666667      1 NA      <NA>      0.077
## 5      0.04666667      1 NA      <NA>      0.060
## 6      0.04000000      1 NA      <NA>      0.061
```

3.6.2 Multi-criteria evaluation and optimization

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

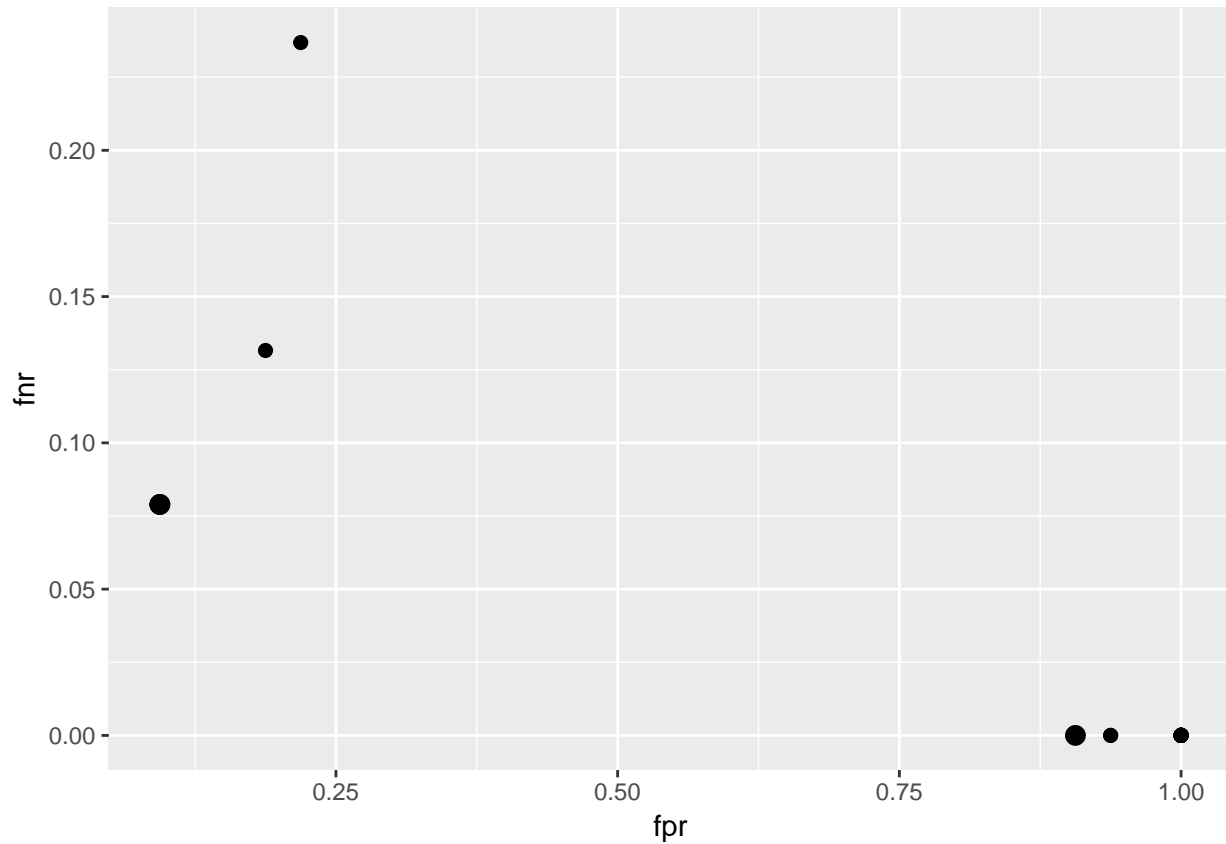
In the following example we aim to minimize both, the false positive and the false negative rates (`fpr` and `fnr`). We again tune the hyperparameters of an SVM (function `kernlab::ksvm()`) with a radial basis kernel and use `sonar.task()` for illustration. As search strategy we choose a random search.

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: 3
head(as.data.frame(trafoOptPath(res$opt.path)))
##           C          sigma fpr.test.mean fnr.test.mean dob eol
## 1 4.660981e+02 9.048434e+02      1.000000      0.00000000      1 NA
## 2 1.204990e+02 3.422372e-04      0.21875      0.23684211      2 NA
## 3 3.136853e+02 2.081896e-02      0.09375      0.07894737      3 NA
## 4 1.607247e+03 2.970328e+03      1.000000      0.00000000      4 NA
## 5 3.345867e-04 7.439081e+02      1.000000      0.00000000      5 NA
## 6 6.109190e+02 2.563639e+03      1.000000      0.00000000      6 NA
## error.message exec.time
## 1      <NA>      0.044
## 2      <NA>      0.043
## 3      <NA>      0.045
## 4      <NA>      0.051
## 5      <NA>      0.042
## 6      <NA>      0.045
```

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 `vignette("filter_methods")`.

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

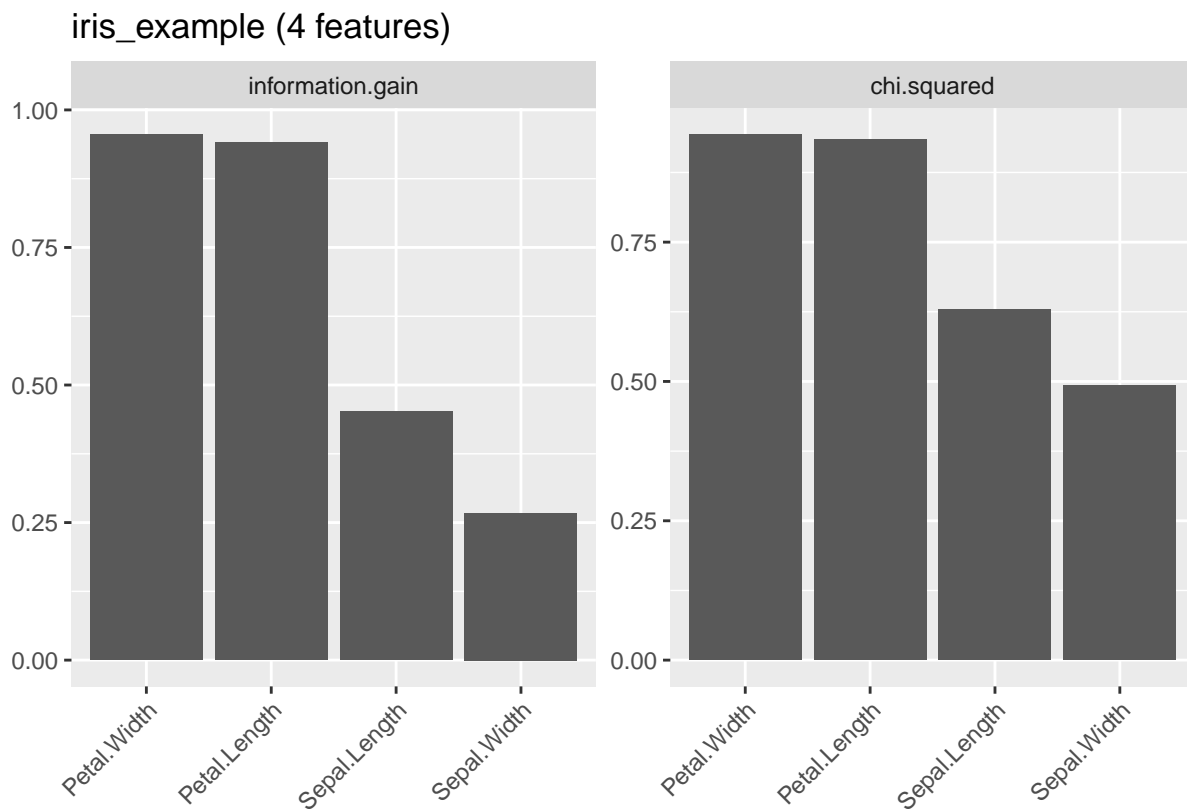
```
fv = generateFilterValuesData(iris.task, method = "information.gain")
fv
## FilterValues:
## Task: iris_example
##      name      type information.gain
## 1 Sepal.Length numeric      0.4521286
## 2 Sepal.Width  numeric      0.2672750
## 3 Petal.Length numeric      0.9402853
## 4 Petal.Width  numeric      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 faceted 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
## Is spatial: 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` (`vignette("measures")`) 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
##      0.05333333
```

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 (`vignette("tune")`).

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=46.9108563; time: 0.0 min
```

```
## [Tune-x] 2: fw.perc=0.25
## [Tune-y] 2: mse.test.mean=46.9108563; time: 0.0 min
## [Tune-x] 3: fw.perc=0.3
## [Tune-y] 3: mse.test.mean=47.0886751; time: 0.0 min
## [Tune-x] 4: fw.perc=0.35
## [Tune-y] 4: mse.test.mean=35.6293077; time: 0.0 min
## [Tune-x] 5: fw.perc=0.4
## [Tune-y] 5: mse.test.mean=35.6293077; time: 0.0 min
## [Tune-x] 6: fw.perc=0.45
## [Tune-y] 6: mse.test.mean=30.9353931; time: 0.0 min
## [Tune-x] 7: fw.perc=0.5
## [Tune-y] 7: mse.test.mean=30.9353931; time: 0.0 min
## [Tune] Result: fw.perc=0.5 : mse.test.mean=30.9353931
res
## Tune result:
## Op. pars: fw.perc=0.5
## mse.test.mean=30.9353931
```

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    46.91086    1  NA          <NA>      0.402
## 2    0.25   46.91086    2  NA          <NA>      0.282
## 3    0.3    47.08868    3  NA          <NA>      0.280
## 4    0.35   35.62931    4  NA          <NA>      0.324
## 5    0.4    35.62931    5  NA          <NA>      0.357
## 6    0.45   30.93539    6  NA          <NA>      0.355
## 7    0.5    30.93539    7  NA          <NA>      0.369
```

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

```
res$x
## $fw.perc
## [1] 0.5
res$y
## mse.test.mean
##      30.93539
```

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=0.5
getFilteredFeatures(mod)
## [1] "crim" "zn" "rm" "dis" "rad" "lstat"
```

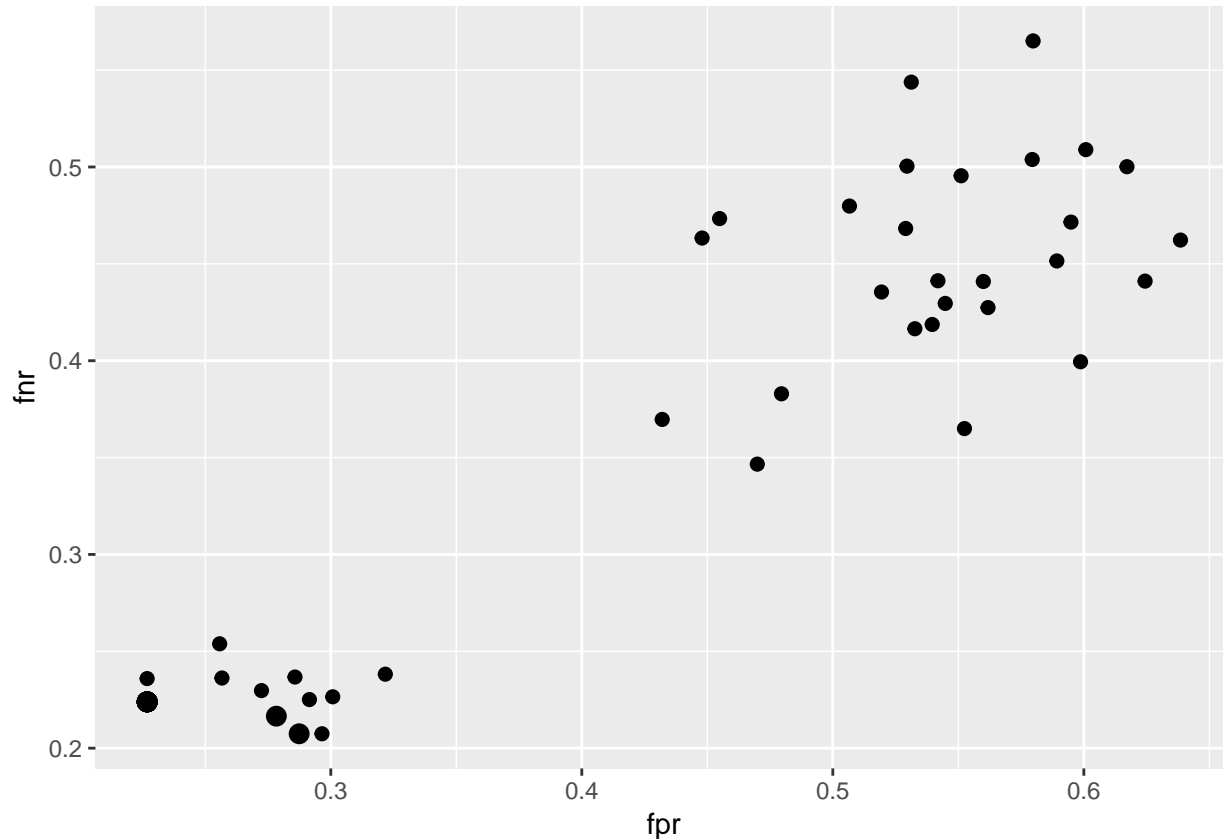
Here is another example using multi-criteria tuning (`vignette("tune")`). We consider linear discriminant analysis (`MASS::lda()`) with precedent feature selection based on the Chi-squared statistic of

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` (`vignette("measures")`) and `fnr` (`vignette("measures")`), 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: 14
head(as.data.frame(res$opt.path))
##   fw.threshold fpr.test.mean fnr.test.mean dob eol error.message exec.time
## 1    0.2634261    0.2268398    0.2238972   1  NA          <NA>         3.024
## 2    0.4110662    0.2857359    0.2367244   2  NA          <NA>         3.307
## 3    0.6250347    0.5524459    0.3649684   3  NA          <NA>         3.086
## 4    0.8627359    0.5290260    0.4682606   4  NA          <NA>         3.157
## 5    0.7135354    0.5948701    0.4715518   5  NA          <NA>         3.617
## 6    0.6123250    0.5794372    0.5038584   6  NA          <NA>         2.532
```

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 (vignette("measures"))).

```
### 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 (18): mean_perimeter, mean_smoothness, mean_concavepoints, mean_fractaldim, SE_radius, SE_t
## cindex.test.mean=0.8431373
```

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

```
sfeats$x
## [1] "mean_perimeter"      "mean_smoothness"    "mean_concavepoints"
## [4] "mean_fractaldim"     "SE_radius"          "SE_texture"
## [7] "SE_perimeter"        "SE_area"            "SE_smoothness"
## [10] "SE_compactness"      "SE_concavity"       "worst_radius"
## [13] "worst_compactness"   "worst_concavity"    "worst_concavepoints"
## [16] "worst_symmetry"      "worst_fractaldim"   "pnodes"
sfeats$y
## cindex.test.mean
##      0.8431373
```

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` (`vignette("measures")`). `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=23.3961169

```

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

```

analyzeFeatSelResult(sfeats)
## Features          : 11
## Performance       : mse.test.mean=23.3961169
## crim, zn, chas, nox, rm, dis, rad, tax, ptratio, b, lstat
##
## Path to optimum:
## - Features:      0  Init   :                      Perf = 84.933  Diff: NA   *
## - Features:      1  Add    : lstat                 Perf = 38.899  Diff: 46.034 *
## - Features:      2  Add    : rm                    Perf = 31.219  Diff: 7.68   *
## - Features:      3  Add    : ptratio                Perf = 27.84   Diff: 3.3787 *
## - Features:      4  Add    : dis                    Perf = 26.963  Diff: 0.87749 *
## - Features:      5  Add    : nox                    Perf = 25.55   Diff: 1.4128 *
## - Features:      6  Add    : b                      Perf = 24.93   Diff: 0.61993 *
## - Features:      7  Add    : zn                     Perf = 24.639  Diff: 0.29142 *
## - Features:      8  Add    : chas                    Perf = 24.445  Diff: 0.19423 *
## - Features:      9  Add    : rad                     Perf = 24.307  Diff: 0.13795 *
## - Features:     10  Add    : tax                     Perf = 23.821  Diff: 0.48592 *
## - Features:     11  Add    : crim                    Perf = 23.396  Diff: 0.42461 *
##
## 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 (17): mean_perimeter, mean_smoothness, mean_compactness, mean_fractaldim, SE_perimeter, SE_
## cindex.test.mean=0.6659149
```

The selected features are:

```
sfeats$x
## [1] "mean_perimeter" "mean_smoothness" "mean_compactness"
## [4] "mean_fractaldim" "SE_perimeter" "SE_area"
## [7] "SE_smoothness" "SE_compactness" "SE_concavity"
## [10] "SE_concavepoints" "SE_symmetry" "worst_radius"
## [13] "worst_texture" "worst_area" "worst_smoothness"
## [16] "worst_symmetry" "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
## 0.5710864
```

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

```
lapply(r$models, getFeatSelResult)
## [[1]]
## FeatSel result:
## Features (18): mean_radius, mean_smoothness, mean_compactness, mean_concavepoints, mean_symmetry, me
## cindex.test.mean=0.6987273
##
## [[2]]
## FeatSel result:
## Features (21): mean_radius, mean_smoothness, mean_concavity, mean_symmetry, mean_fractaldim, SE_radi
## cindex.test.mean=0.6990393
##
## [[3]]
## FeatSel result:
## Features (13): mean_radius, mean_area, mean_concavity, SE_texture, SE_smoothness, SE_compactness, SE
## cindex.test.mean=0.6634901
##
## [[4]]
## FeatSel result:
## Features (17): mean_radius, mean_smoothness, mean_fractaldim, SE_radius, SE_perimeter, SE_area, SE_c
## cindex.test.mean=0.6701509
##
## [[5]]
## FeatSel result:
## Features (11): mean_radius, mean_compactness, mean_concavepoints, mean_symmetry, SE_texture, SE_conc
## cindex.test.mean=0.6086901
```

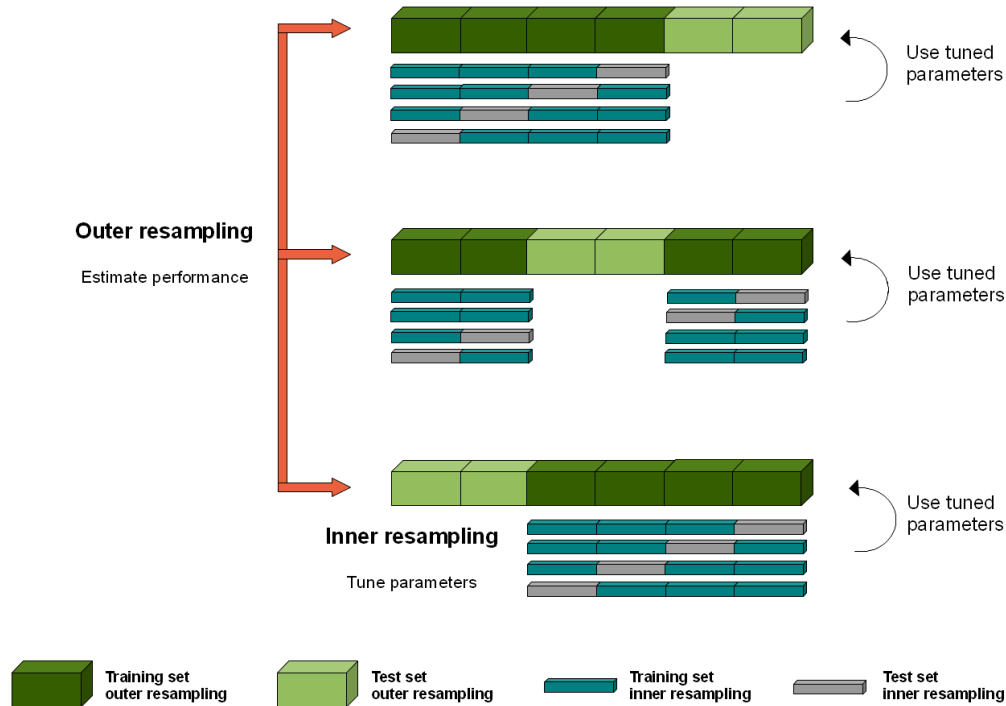


Figure 2: Nested Resampling Figure

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 (`vignette("tune")`) or feature selection (`vignette("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 (`vignette("wrapper")`). 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 (`vignette("resample")`)) 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 (`vignette("parallelization")`).

3.8.1 Tuning

As you might recall from the tutorial page about tuning (`vignette("tune")`), 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 tuning a grid search is used to find the hyperparameters with lowest error rate (`mmce` (`vignette("measures")`) 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 = FALSE)

### 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=0.0333333
## Runtime: 6.21612
```

You can obtain the error rates on the 3 outer test sets by:

```
r$measures.test
##   iter mmce
## 1    1 0.06
## 2    2 0.00
## 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$extract
## [[1]]
## Tune result:
## Op. pars: C=2; sigma=0.25
## mmce.test.mean=0.0294118
##
## [[2]]
## Tune result:
## Op. pars: C=1; sigma=0.25
## mmce.test.mean=0.0147059
##
## [[3]]
## Tune result:
## Op. pars: C=2; sigma=0.25
## mmce.test.mean=0.0441176
names(r$extract[[1]])
## [1] "learner" "control" "x" "y" "threshold" "opt.path"
```

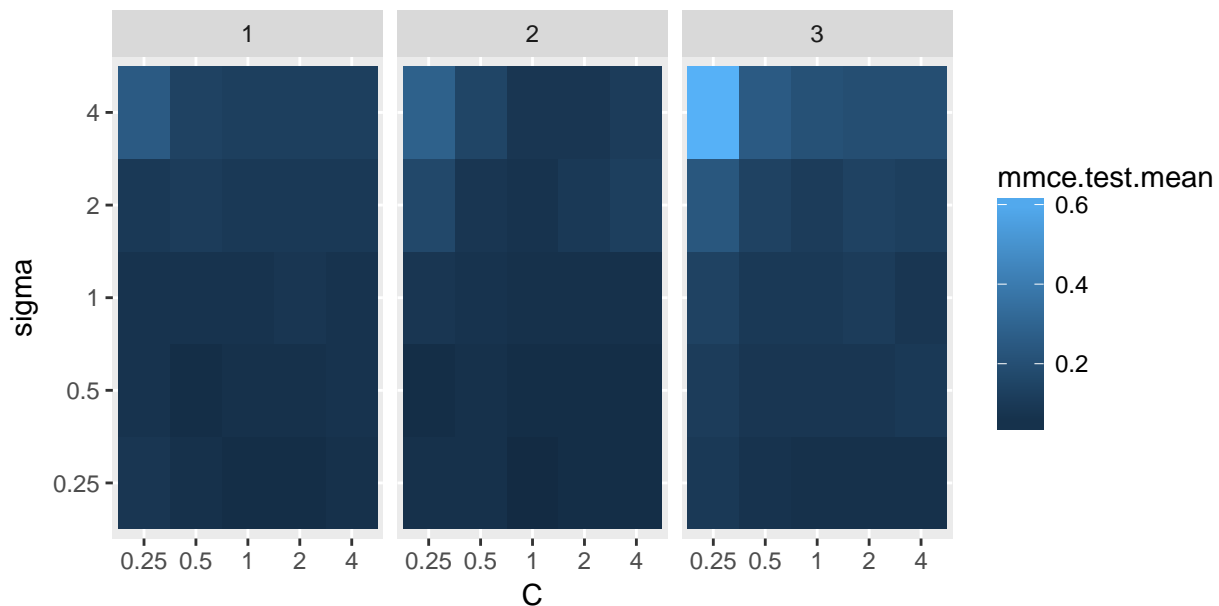
We can compare the optimal parameter settings obtained in the 3 resampling iterations. As you can see, the optimal configuration usually depends on the data. You may be able to identify a *range* of parameter settings that achieve good performance though, e.g., the values for `C` should be at least 1 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   0.07352941    1  NA          <NA>    0.070    1
## 2  0.5   0.25   0.04411765    2  NA          <NA>    0.068    1
## 3  1     0.25   0.02941176    3  NA          <NA>    0.081    1
## 4  2     0.25   0.02941176    4  NA          <NA>    0.071    1
## 5  4     0.25   0.04411765    5  NA          <NA>    0.069    1
## 6  0.25  0.5   0.05882353    6  NA          <NA>    0.065    1
## 7  0.5   0.5   0.02941176    7  NA          <NA>    0.067    1
## 8  1     0.5   0.04411765    8  NA          <NA>    0.070    1
## 9  2     0.5   0.04411765    9  NA          <NA>    0.068    1
## 10 4     0.5   0.05882353   10  NA          <NA>    0.069    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 0.25
## 3 2 0.25
```

3.8.2 Feature selection

As you might recall from the section about feature selection (`vignette("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=30.4363012
## Runtime: 14.2263
r$measures.test
##   iter    mse
## 1     1 38.2561
## 2     2 22.6165

```

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$extract
## [[1]]
## FeatSel result:
## Features (10): crim, indus, chas, nox, rm, age, dis, ptratio, b, lstat
## mse.test.mean=19.4211656
##
## [[2]]
## FeatSel result:
## Features (10): zn, chas, nox, rm, dis, rad, tax, ptratio, b, lstat
## mse.test.mean=25.6812830
### Selected features in the first outer resampling iteration
r$extract[[1]]$x
## [1] "crim"    "indus"   "chas"    "nox"     "rm"      "age"     "dis"
## [8] "ptratio" "b"       "lstat"
### Resampled performance of the selected feature subset on the first inner training set
r$extract[[1]]$y
## mse.test.mean
##      19.42117

```

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.

```

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 72.81755
## 2    1 0     0    0 0 0 0 0 0 0 0 0 0 75.50339
## 3    0 1     0    0 0 0 0 0 0 0 0 0 0 64.86120
## 4    0 0     1    0 0 0 0 0 0 0 0 0 0 53.44312
## 5    0 0     0    1 0 0 0 0 0 0 0 0 0 72.70370

```



```
## 6    0 0    0 0 1 0 0 0 0 0    0 0    0    59.89298
##   dob eol error.message exec.time
## 1    1 2      <NA>      0.043
## 2    2 2      <NA>      0.058
## 3    2 2      <NA>      0.066
## 4    2 2      <NA>      0.062
## 5    2 2      <NA>      0.067
## 6    2 2      <NA>      0.061
```

An easy-to-read version of the optimization path for sequential feature selection can be obtained with function `analyzeFeatSelResult()`.

```
analyzeFeatSelResult(r$extract[[1]])
## Features          : 10
## Performance       : mse.test.mean=19.4211656
## crim, indus, chas, nox, rm, age, dis, ptratio, b, lstat
##
## Path to optimum:
## - Features:    0  Init    :                Perf = 72.818  Diff: NA    *
## - Features:    1  Add     : lstat          Perf = 35.032  Diff: 37.786  *
## - Features:    2  Add     : rm             Perf = 26.895  Diff: 8.1371  *
## - Features:    3  Add     : ptratio         Perf = 22.348  Diff: 4.5465  *
## - Features:    4  Add     : crim           Perf = 21.629  Diff: 0.71946  *
## - Features:    5  Add     : b              Perf = 21.163  Diff: 0.46538  *
## - Features:    6  Add     : dis            Perf = 20.799  Diff: 0.36418  *
## - Features:    7  Add     : nox            Perf = 19.713  Diff: 1.0863  *
## - Features:    8  Add     : indus          Perf = 19.645  Diff: 0.068117  *
## - Features:    9  Add     : chas           Perf = 19.543  Diff: 0.10187  *
## - Features:   10  Add     : age            Perf = 19.421  Diff: 0.1218  *
##
## 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 threshold 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=24.2278416
## Runtime: 6.9819

```

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 = 338; 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 = 337; 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"   "chas"    "nox"     "rm"      "age"
## [8] "dis"     "rad"     "tax"     "ptratio" "b"        "lstat"
##
## [[2]]
## [1] "crim"    "zn"      "indus"   "nox"     "rm"      "age"     "dis"
## [8] "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

```

```
## mse.test.mean=25.8771054
##
## [[2]]
## Tune result:
## Op. pars: fw.threshold=0.4
## mse.test.mean=28.3932273
##
## [[3]]
## Tune result:
## Op. pars: fw.threshold=0
## mse.test.mean=24.3237275
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    25.87711    1  NA          <NA>      0.367
## 2          0.2    26.11571    2  NA          <NA>      0.373
## 3          0.4    26.71688    3  NA          <NA>      0.382
## 4          0.6    33.19461    4  NA          <NA>      0.394
## 5          0.8    82.78797    5  NA          <NA>      0.315
## 6           1    82.78797    6  NA          <NA>      0.311
```

3.8.3 Benchmark experiments

In a benchmark experiment multiple learners are compared on one or several tasks (see also the section about benchmarking (`vignette("benchmark_experiments")`)). 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 (`vignette("parallelization")`).

As mentioned in the section about benchmark experiments (`vignette("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 `kknns::kknns()`. 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` (`vignette("measures")`)), which is used as tuning criterion, and also calculate the balanced error rate (`ber` (`vignette("measures")`)).

```
### 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      0.9800000    0.02083333
## 2  iris_example classif.kknn.tuned      0.9600000    0.04166667
## 3 Sonar_example classif.ksvm.tuned      0.4456098    0.50000000
## 4 Sonar_example classif.kknn.tuned      0.8224390    0.16963554
```

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 (`vignette("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 0.9800000 0.02083333
## 2  iris_example classif.kknn.tuned      1 0.9600000 0.04166667
## 3 Sonar_example classif.ksvm.tuned      1 0.4400000 0.50000000
## 4 Sonar_example classif.ksvm.tuned      2 0.4512195 0.50000000
```

```
## 5 Sonar_example classif.kknn.tuned      1 0.8400000 0.15909091
## 6 Sonar_example classif.kknn.tuned      2 0.8048780 0.18018018
```

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=0.5; sigma=0.5
## mmce.test.mean=0.1176471
##
##
## $iris_example$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=0.5; sigma=1
## mmce.test.mean=0.3285714
##
## $Sonar_example$classif.ksvm.tuned[[2]]
## Tune result:
## Op. pars: C=2; sigma=1
## mmce.test.mean=0.2142857
##
##
## $Sonar_example$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=3
## mmce.test.mean=0.0476190
```

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 0.5   0.5    0.11764706 NA
## 2  iris_example classif.kknn.tuned    1 NA     NA    0.04901961  3
```

```
## 3 Sonar_example classif.ksvm.tuned 1 0.5 1.0 0.32857143 NA
## 4 Sonar_example classif.ksvm.tuned 2 2.0 1.0 0.21428571 NA
## 5 Sonar_example classif.kknn.tuned 1 NA NA 0.08571429 5
## 6 Sonar_example classif.kknn.tuned 2 NA NA 0.04761905 3
```

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 0.5 1 0.3285714
## 2 Sonar_example classif.ksvm.tuned 2 2.0 1 0.2142857
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 (`vignette("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 25.72184
## 2 BostonHousing-example regr.lm.featsel 25.40691
```

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 (9): zn, nox, rm, dis, rad, tax, ptratio, b, lstat
## mse.test.mean=17.7096055
##
```

```
## `$BostonHousing-example`$regr.lm.featsel[[2]]
## FeatSel result:
## Features (5): chas, rm, ptratio, b, lstat
## mse.test.mean=32.1006980
getBMRFeatSelResults(res, drop = TRUE)
## $regr.rpart
## NULL
##
## $regr.lm.featsel
## $regr.lm.featsel[[1]]
## FeatSel result:
## Features (9): zn, nox, rm, dis, rad, tax, ptratio, b, lstat
## mse.test.mean=17.7096055
##
## $regr.lm.featsel[[2]]
## FeatSel result:
## Features (5): chas, rm, ptratio, b, lstat
## mse.test.mean=32.1006980
```

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]]$x
## [1] "zn"      "nox"      "rm"      "dis"      "rad"      "tax"      "ptratio"
## [8] "b"       "lstat"
#### Resampled performance of the selected feature subset on the first inner training set
feats[[1]]$y
## mse.test.mean
##      17.70961
```

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  60.48810
## 2    1  0    0    0  0  0  0  0  0  0  0  0  0  51.86075
## 3    0  1    0    0  0  0  0  0  0  0  0  0  0  49.56972
## 4    0  0    1    0  0  0  0  0  0  0  0  0  0  48.42359
## 5    0  0    0    1  0  0  0  0  0  0  0  0  0  58.27987
## 6    0  0    0    0  1  0  0  0  0  0  0  0  0  48.74020
##   dob eol error.message exec.time
## 1    1    2          <NA>    0.026
## 2    2    2          <NA>    0.037
## 3    2    2          <NA>    0.038
## 4    2    2          <NA>    0.036
## 5    2    2          <NA>    0.034
## 6    2    2          <NA>    0.039
analyzeFeatSelResult(feats[[1]])
```

```

## Features          : 9
## Performance      : mse.test.mean=17.7096055
## zn, nox, rm, dis, rad, tax, ptratio, b, lstat
##
## Path to optimum:
## - Features:    0  Init    :                Perf = 60.488  Diff: NA    *
## - Features:    1  Add     : lstat          Perf = 27.917  Diff: 32.572 *
## - Features:    2  Add     : rm             Perf = 23.25   Diff: 4.6668  *
## - Features:    3  Add     : ptratio        Perf = 20.399  Diff: 2.8512  *
## - Features:    4  Add     : b             Perf = 20.146  Diff: 0.2525  *
## - Features:    5  Add     : dis            Perf = 19.943  Diff: 0.20316 *
## - Features:    6  Add     : nox           Perf = 18.307  Diff: 1.636   *
## - Features:    7  Add     : zn            Perf = 17.912  Diff: 0.39474 *
## - Features:    8  Add     : tax           Perf = 17.872  Diff: 0.04027 *
## - Features:    9  Add     : rad           Perf = 17.71   Diff: 0.16231 *
##
## 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      24.83978
## 2 BostonHousing-example regr.lm.filtered.tuned      23.24207
### Performances on individual outer test data sets
getBMRPerformances(res, as.df = TRUE)
##           task.id           learner.id iter      mse
## 1 BostonHousing-example      regr.rpart     1 20.13399
## 2 BostonHousing-example      regr.rpart     2 24.56381
## 3 BostonHousing-example      regr.rpart     3 29.82154
## 4 BostonHousing-example regr.lm.filtered.tuned     1 22.01168
## 5 BostonHousing-example regr.lm.filtered.tuned     2 21.94481
## 6 BostonHousing-example regr.lm.filtered.tuned     3 25.76973

```


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 $k = 1, \dots, K$).

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
## Is spatial: 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: 0.03
##   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: 0.03
##   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 (vignette("measures"))`) 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=0.5571230,mmce.test.mean=0.3530387
## Runtime: 0.367241
```

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`.

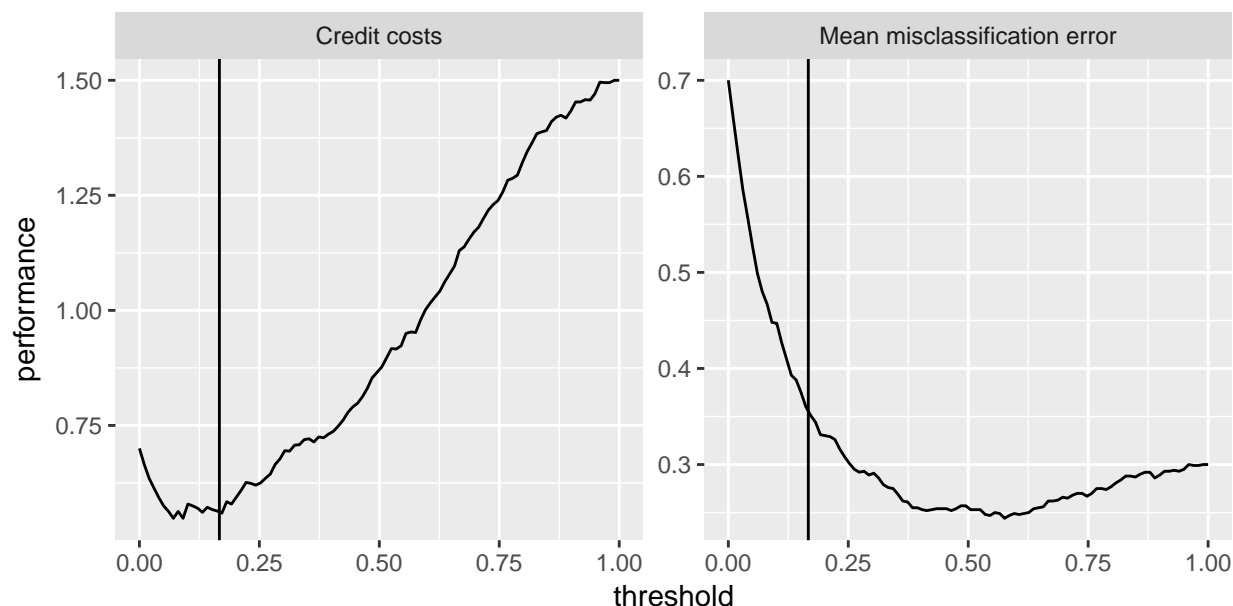
```
### Cross-validated performance with default thresholds
performance(setThreshold(r$pred, 0.5), measures = list(credit.costs, mmce))
## credit.costs      mmce
##      0.8769788      0.2570055
```

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 (vignette("measures"))`). 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=0.8769788,mmce.test.mean=0.2570055
## Runtime: 0.442516
### 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] 0.07399897
##
## $perf
## credit.costs
##      0.542078
```

`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 (`vignette("integrated_learners")`) in the Appendix or use `listLearners()`.

```
### Learners that accept observation weights
listLearners("classif", properties = "weights")[c("class", "package")]
##           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")]
##           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=0.5590860,mmce.test.mean=0.3590177
## Runtime: 0.415488
```

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=0.6191041,mmce.test.mean=0.3350236
## Runtime: 0.592427

```

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=6
## credit.costs.test.mean=0.5450630,mmce.test.mean=0.3730107
as.data.frame(tune.res$opt.path)[1:3]
##      wcw.weight credit.costs.test.mean mmce.test.mean
## 1           4           0.5840931           0.3320206
## 2          4.5           0.5720841           0.3480157
## 3           5           0.5590860           0.3590177
## 4          5.5           0.5500800           0.3660157
## 5           6           0.5450630           0.3730107
## 6          6.5           0.5470620           0.3830058
## 7           7           0.5450660           0.3890058
## 8          7.5           0.5460610           0.3940048
## 9           8           0.5480421           0.4039938
## 10          8.5           0.5520521           0.4119958
## 11          9           0.5540660           0.4180018
## 12         9.5           0.5520640           0.4200038
## 13         10           0.5600571           0.4279969
## 14        10.5           0.5540660           0.4300019
## 15         11           0.5530590           0.4329989
## 16        11.5           0.5520491           0.4359929
## 17         12           0.5580491           0.4419929

```

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()`).

```

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
##          0.422      0.322

```

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=0.5610850,mmce.test.mean=0.3570007
## Runtime: 0.410548

```

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=6.75
## credit.costs.test.mean=0.5250670,mmce.test.mean=0.3730107

```

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 $k, l = 1, \dots, K$, $k \neq l$. 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=8.2393045,mmce.test.mean=0.2779742
## Runtime: 0.122278
### 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
## 6.1657168 0.3899791
```

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
## -1.436863e-09  8.431295e-01  1.568705e-01
##
## $perf
## [1] 4.889558
```

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=0.386,0.116,...
## wf.costs.test.mean=2.5676358,mmce.test.mean=0.1619773
```

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
## Is spatial: FALSE
## Classes: 3
## setosa, versicolor, virginica

```

mlr provides several wrappers (`vignette("wrapper")`) 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` (`vignette("measures")`)) and the misclassification penalty (`mcp` (`vignette("measures")`)). The latter measure is the average difference between the costs caused by the predicted class labels, i.e., `meancosts` (`vignette("measures")`), 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: 0.26
##   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
## 156.2028 151.3589
```

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 *preprocessing* 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 (`vignette("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 (`vignette("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
## 0.0372549 0.5090000 0.6339000
performance(predict(mod.under, newdata = data.imbal.test), measures = list(mmce, ber, auc))
##      mmce      ber      auc
## 0.06666667 0.52400000 0.71190000
```

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 (`vignette("wrapper")`). This way over- and undersampling can be applied to already existing learners (`vignette("learner")`) 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
## 0.02941176 0.50500000 0.62610000
performance(predict(mod.under, newdata = data.imbal.test), measures = list(mmce, ber, auc))
##      mmce      ber      auc
## 0.05882353 0.52000000 0.66010000
```

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
## 0.01960784 0.50000000 0.50000000
```

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 (`vignette("bagging")`). 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.maxc1 = "all"`) or bootstrapped with replacement to increase variability between training data sets during iterations (`obw.maxc1 = "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
##      0.03372549      0.47409704      0.53566890
```

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$aggr
## mmce.test.mean  ber.test.mean  auc.test.mean
##      0.03666667      0.46622952      0.56951834
obw.lrn = setPredictType(obw.lrn, "prob")
r2 = resample(learner = obw.lrn, task = task, resampling = rdesc, show.info = FALSE,
  measures = list(mmce, ber, auc))
r2$aggr
## mmce.test.mean  ber.test.mean  auc.test.mean
##      0.04431373      0.47618935      0.54403530
```

While *overbagging* slightly 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 (`vignette("cost_sensitive_classif")`)).

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 (`vignette("wrapper")`). 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 (`vignette("cost_sensitive_classif")`) and imbalanced classification problems (`vignette("over_and_undersampling")`) 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(vignette("measures"))`) and also several generalizations of the AUC to the multi-class case (e.g., `multiclass.aulp(vignette("measures"))`, `multiclass.aulu(vignette("measures"))`) 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 (`vignette("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 (`vignette("learner")`)] that are capable of predicting probabilities. Have a look at the learner table in the Appendix (`vignette("integrated_learners")`) 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)
```

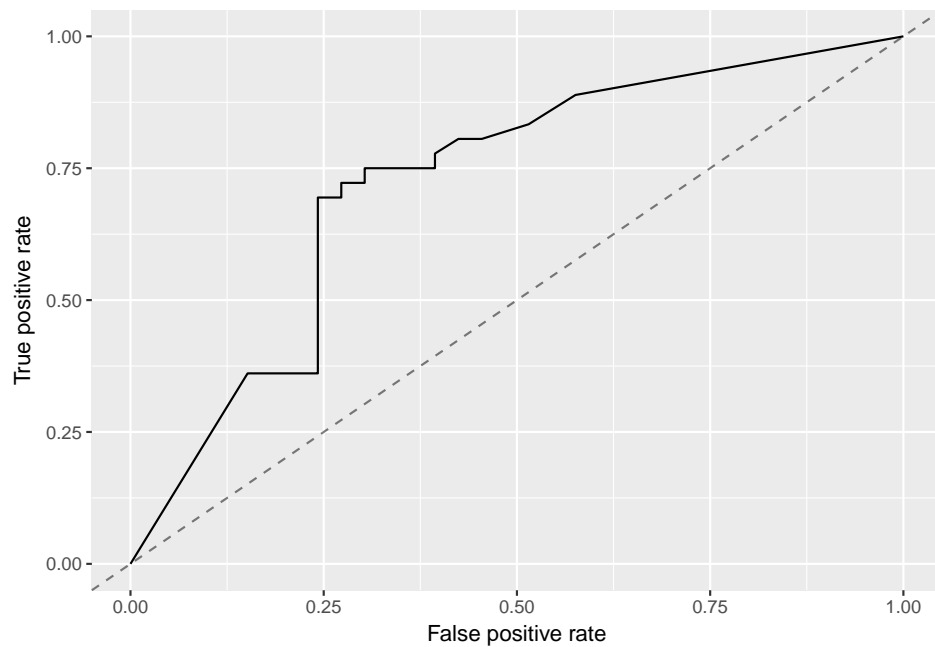
Since we want to plot ROC curves we calculate the false and true positive rates (`fpr` (`vignette("measures")`) and `tpr` (`vignette("measures")`)). Additionally, we also compute error rates (`mmce` (`vignette("measures")`)).

```
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)
```

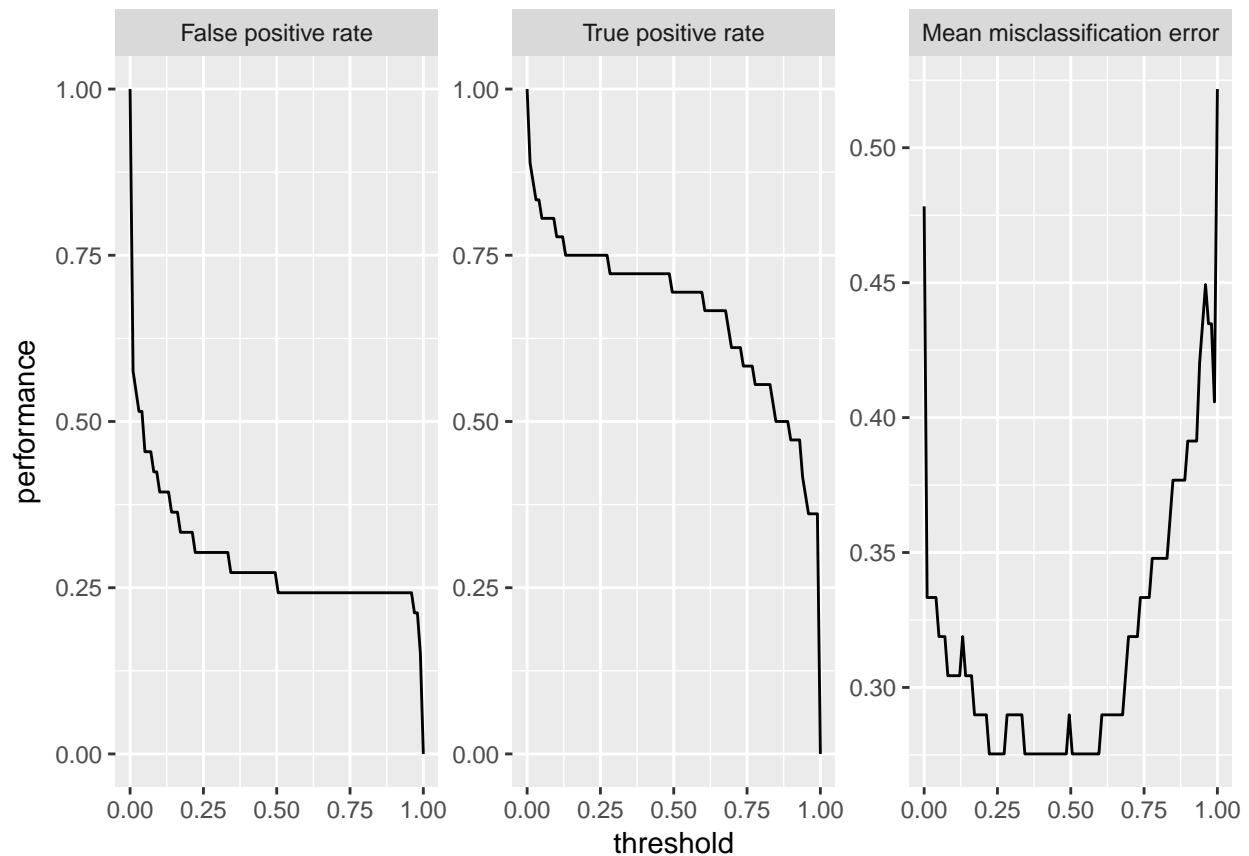


The corresponding area under curve (`auc (vignette("measures"))`) can be calculated as usual by calling `performance()`.

```
performance(pred1, auc)
##      auc
## 0.7340067
```

`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)
```

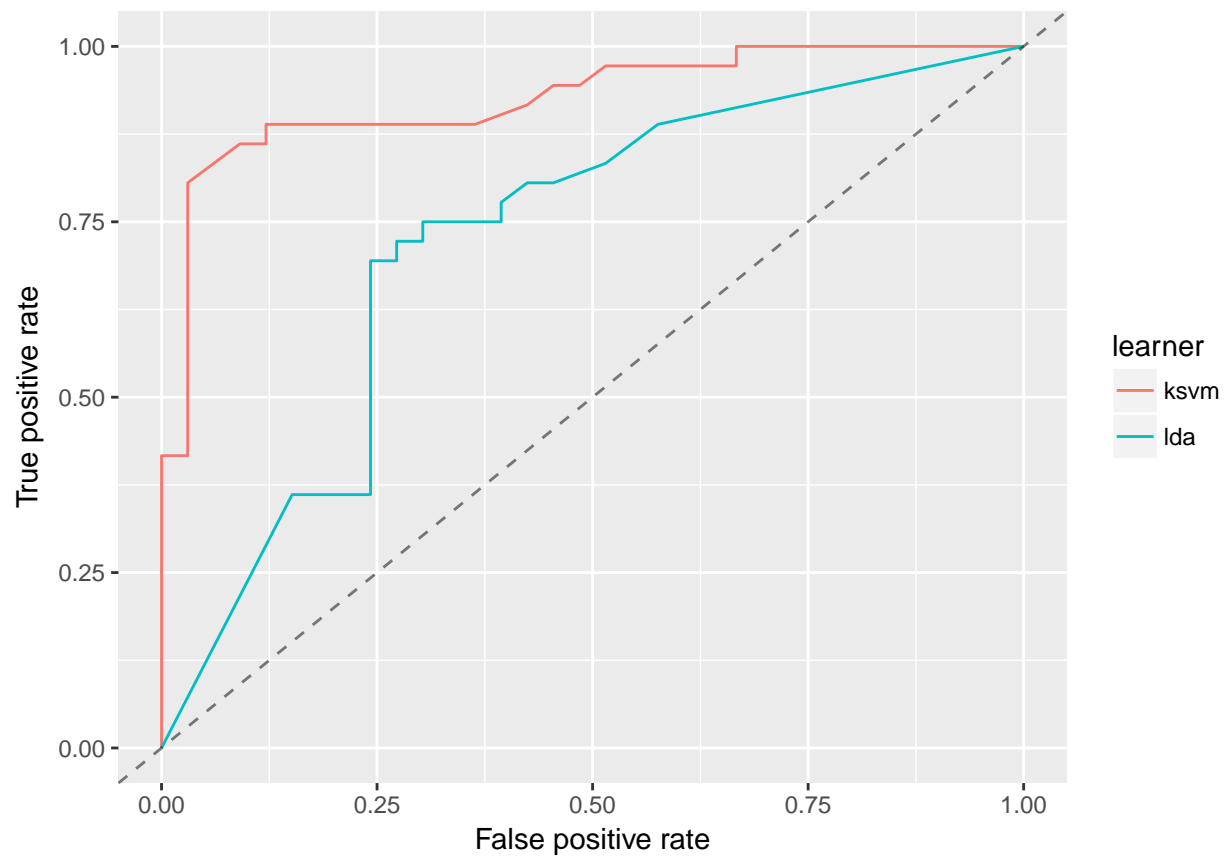


Additional to linear discriminant analysis (`MASS::lda()`) we try a support vector machine with RBF kernel (`kernlab::ksvm()`).

```
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)
```

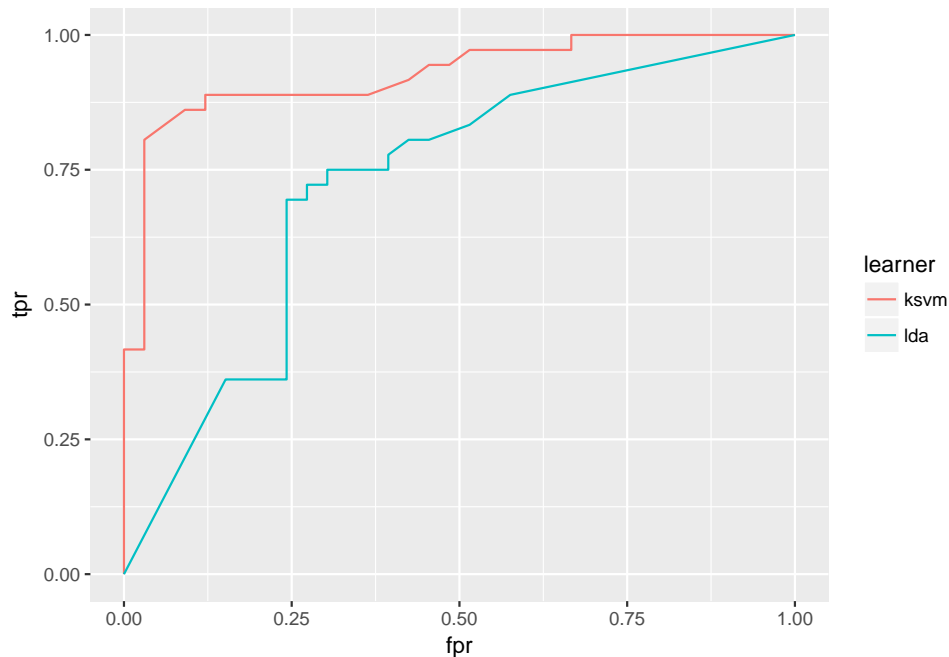


It's clear from the plot above that `kernlab::ksvm()` has a slightly higher AUC than `lda (MASS::lda())`.

```
performance(pred2, auc)
##          auc
## 0.9250842
```

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")
```

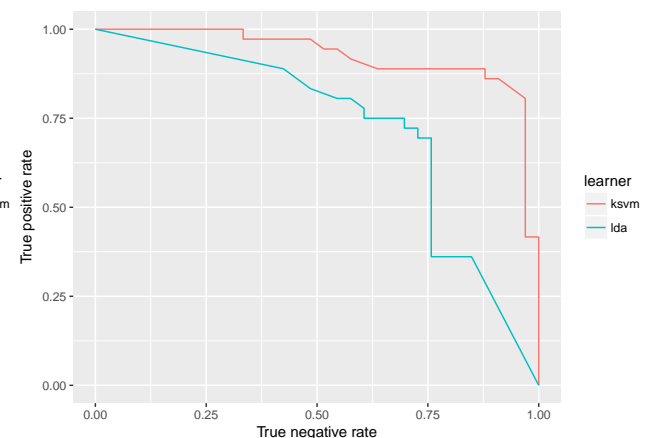
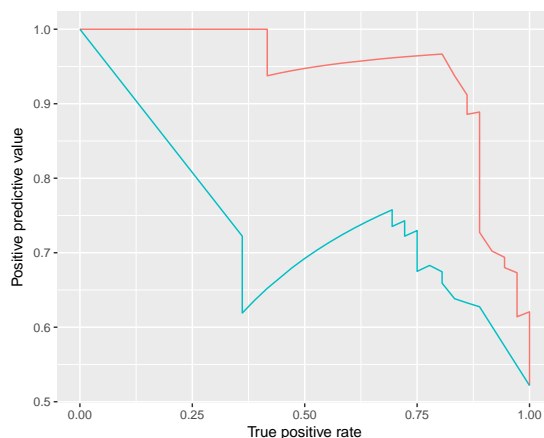


It is easily possible to generate other performance plots by passing the appropriate performance measures to `generateThreshVsPerfData()` and `plotROCCurves()`. Below, we generate a *precision/recall graph* (precision = positive predictive value = ppv, recall = tpr) and a *sensitivity/specificity plot* (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 (`vignette("benchmark_experiments")`)) and, ideally, the support vector machine should have been tuned (`vignette("tune")`).

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` (`vignette("measures")`). The error rate (`mmce` (`vignette("measures")`)) 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` (`vignette("measures")`) as well as the error rate (for a threshold/cutoff value of 0.5).

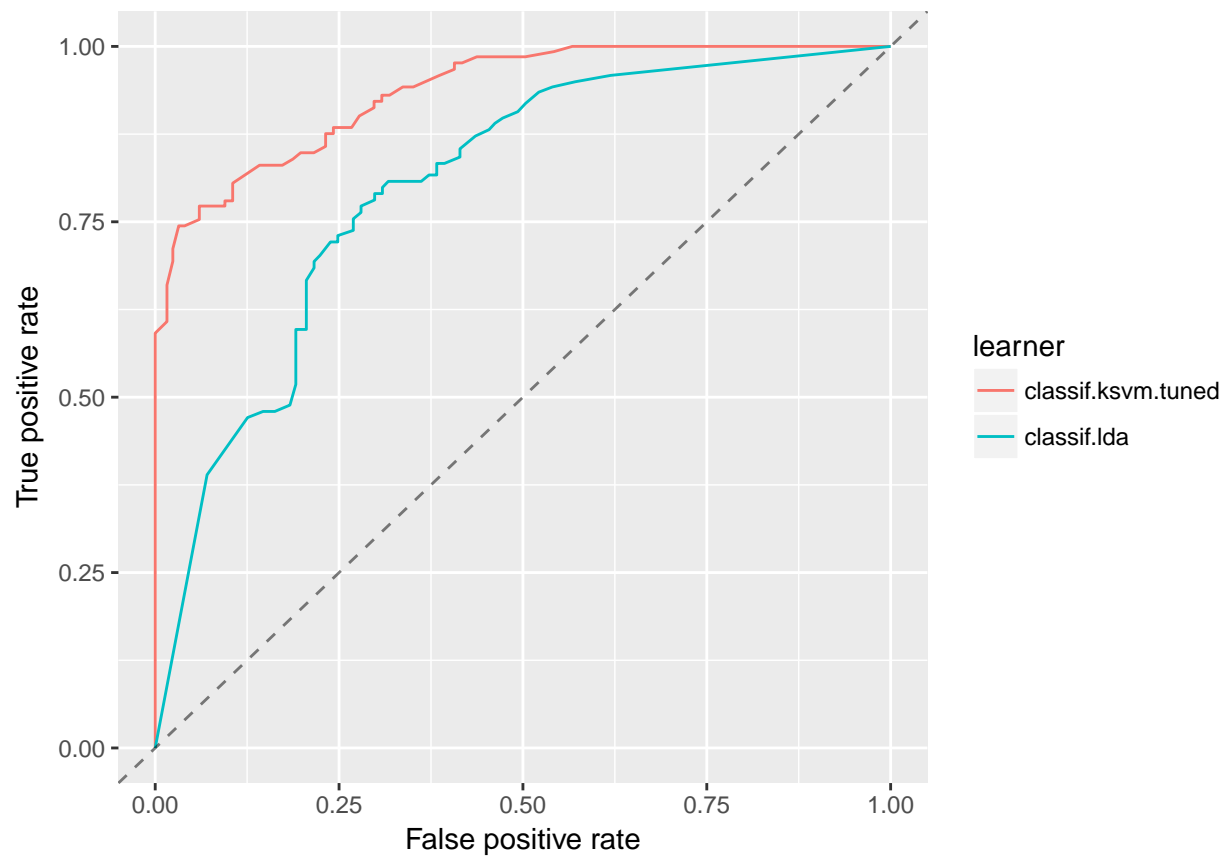
```
### Benchmark experiment
lrns = list(lrn1, lrn2)
rdesc.outer = makeResampleDesc("CV", iters = 5)

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	0.8135470	0.2644599
## 2	Sonar_example	classif.ksvm.tuned	0.9329499	0.1868757

Calling `generateThreshVsPerfData()` and `plotROCCurves()` on the benchmark result (`BenchmarkResult()`) produces a plot with ROC curves for all learners in the experiment.

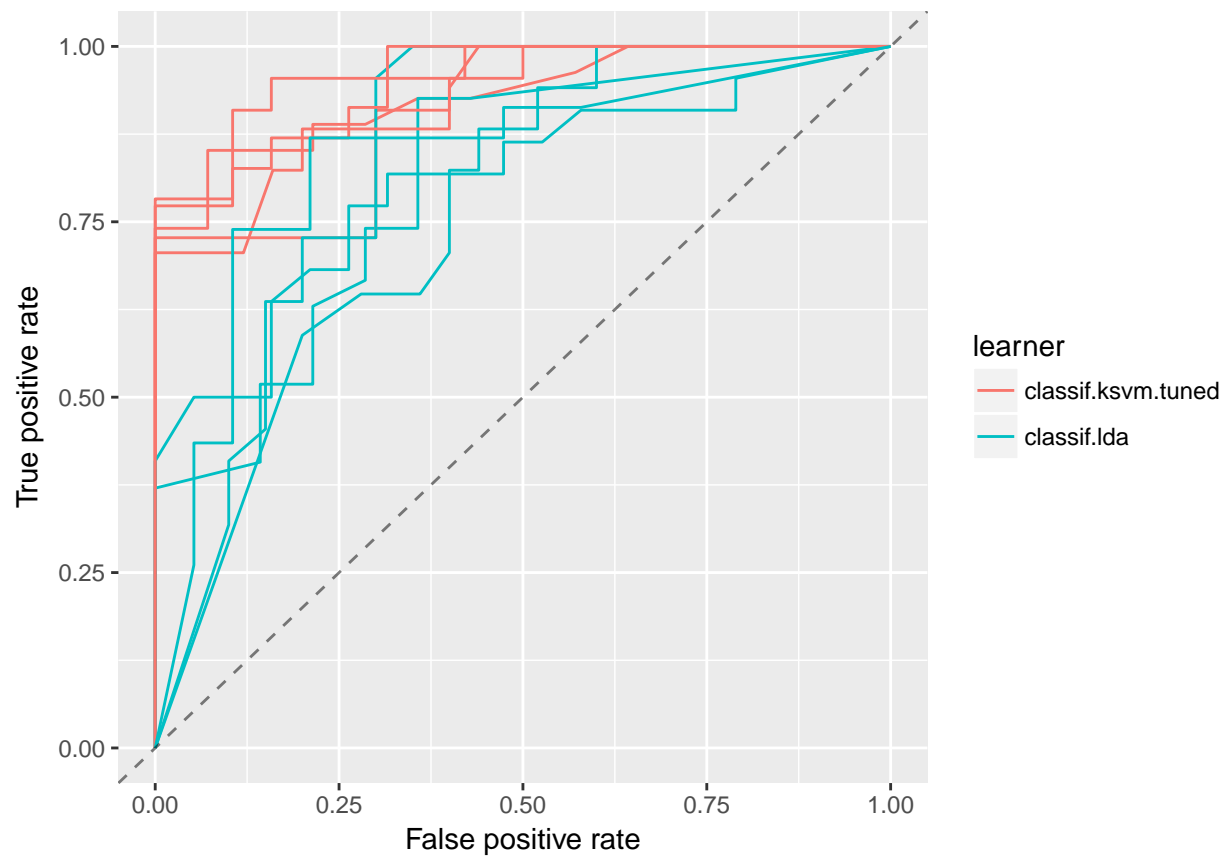
```
df = generateThreshVsPerfData(bmr, measures = list(fpr, tpr, mmce))
plotROCCurves(df)
```

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.

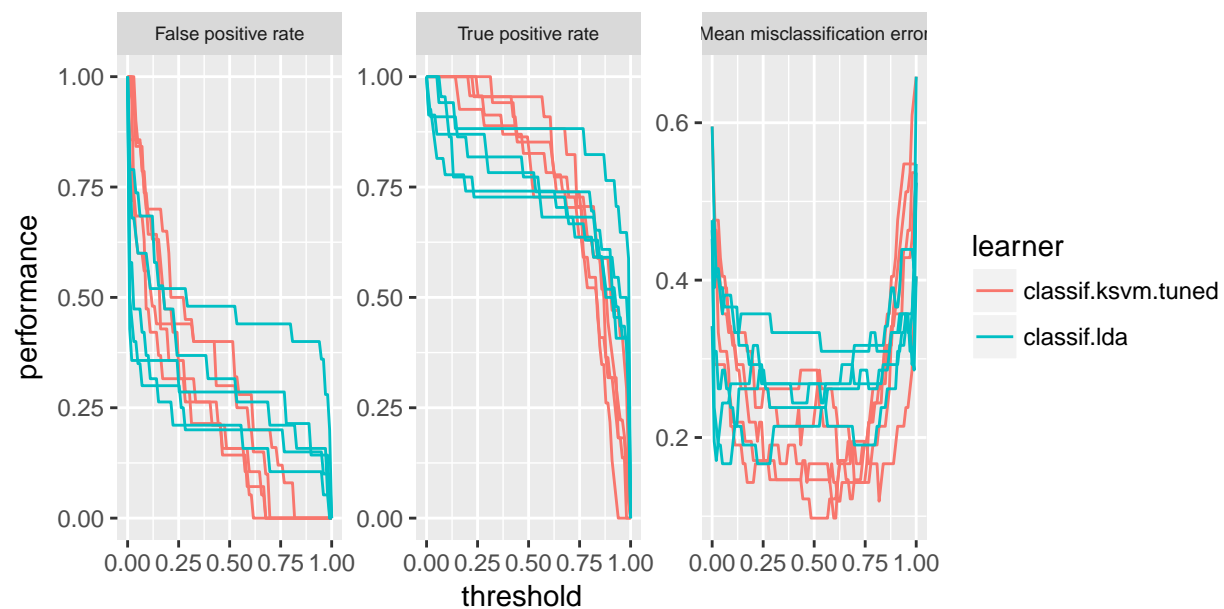
If you want to plot the individual ROC curves for each resample iteration set `aggregate = FALSE`.

```
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()`.

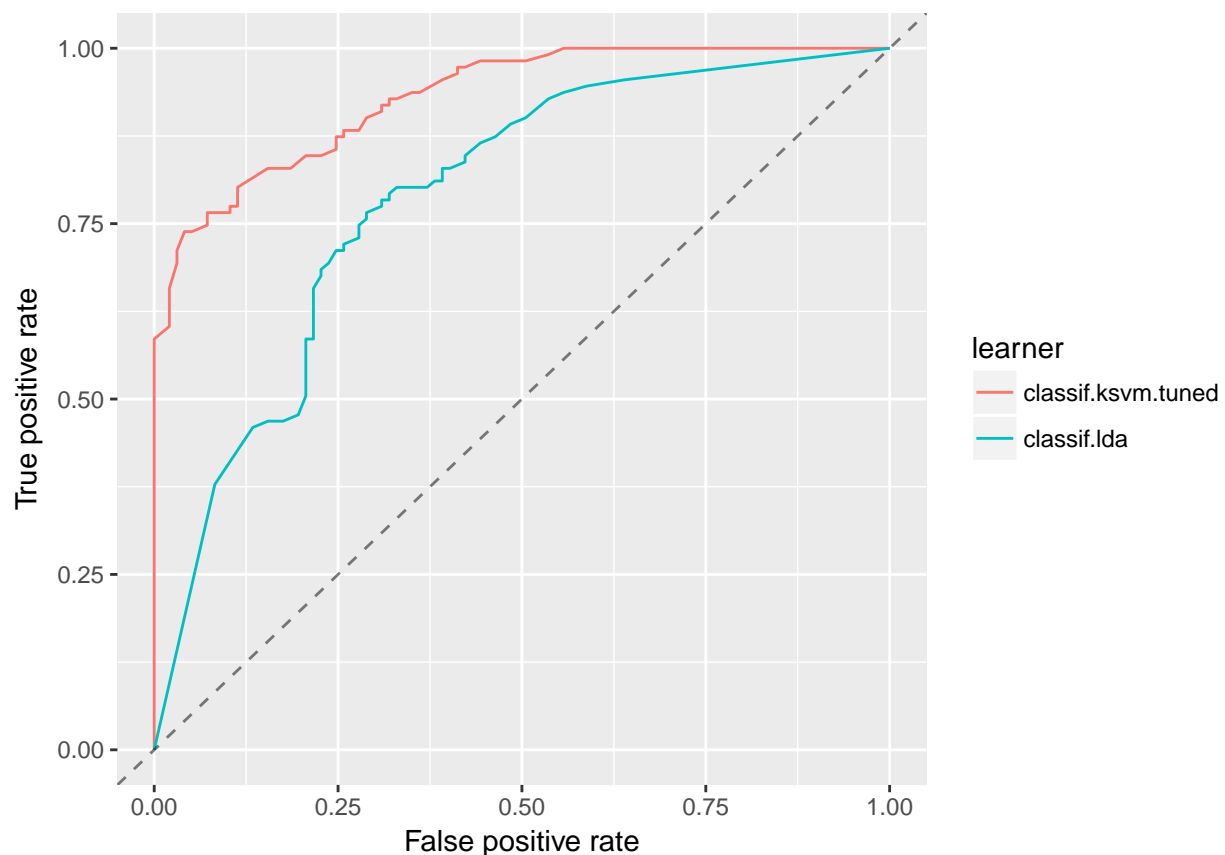
Below, the predictions are extracted from the `BenchmarkResult()` via function `getBMRPredictions()`, the class is changed and the ROC curves are created.

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 our 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)

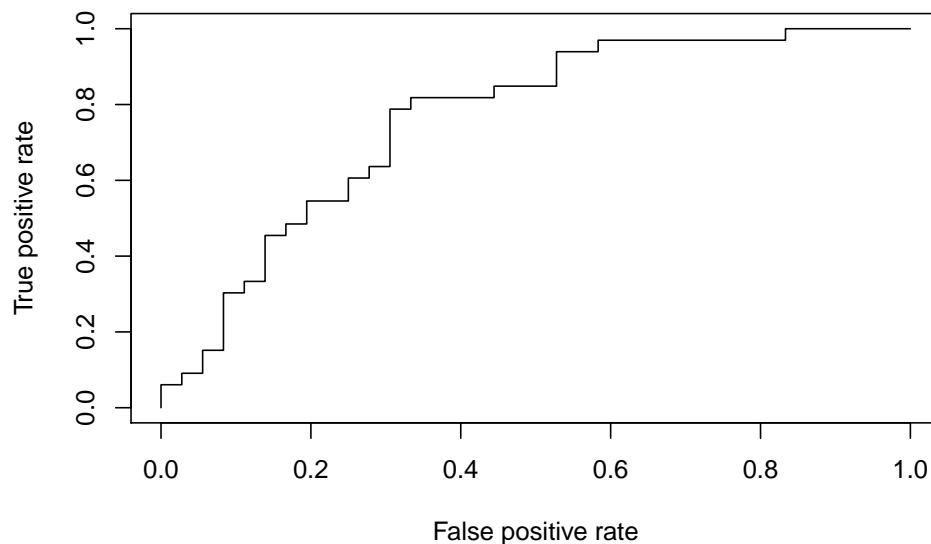
### Train and predict linear discriminant analysis
lrn1 = makeLearner("classif.lda", predict.type = "prob")
mod1 = train(lrn1, sonar.task, subset = train.set)
pred1 = predict(mod1, task = sonar.task, subset = test.set)
```

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")

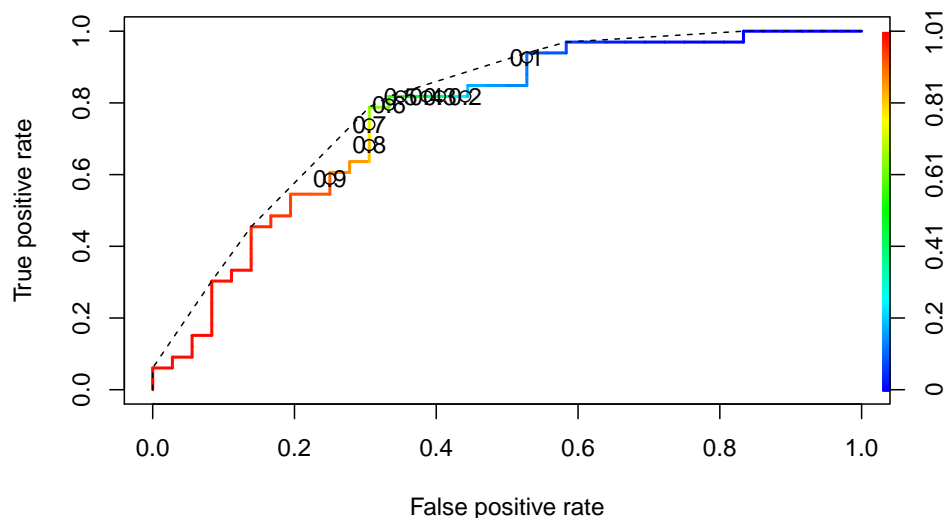
### Draw ROC curve
ROCR::plot(ROCRperf1)
```



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)

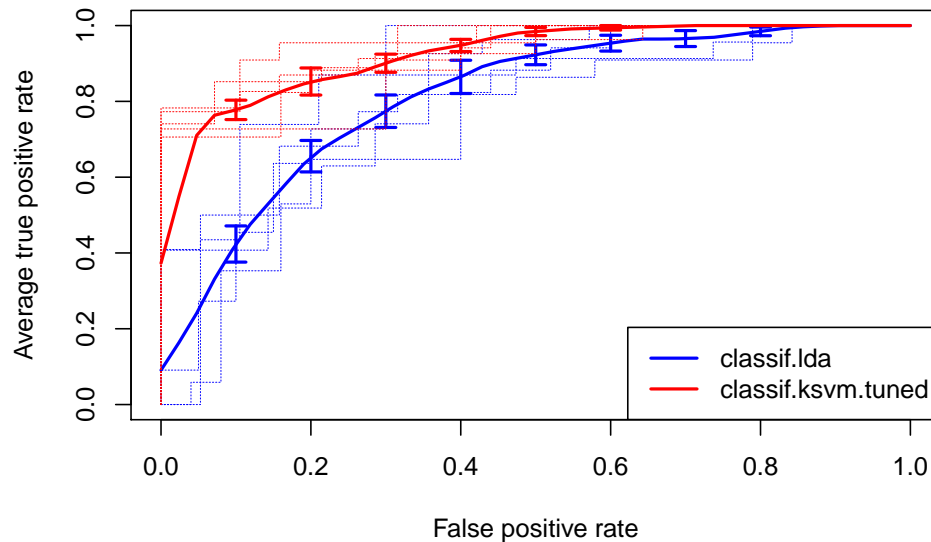
### Calculate true and false positive rate
ROCRperfs = lapply(ROCRpreds, function(x) ROCR::performance(x, "tpr", "fpr"))
```

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"))
```

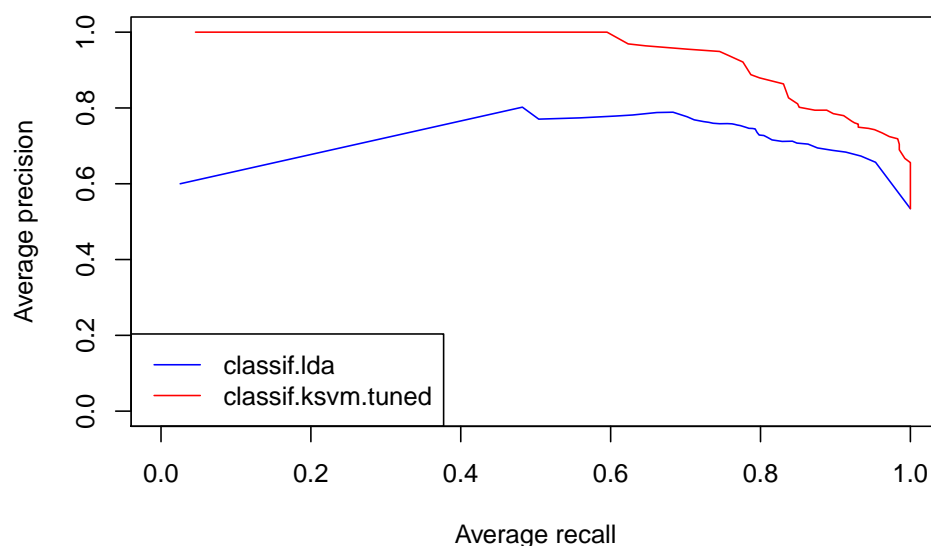


In order to create other evaluation plots like *precision/recall graphs* you just have to change the performance measures when calling `ROCR::performance()`. (Note that you have to use the measures provided by ROCR listed in `ROCR::performance()` and not `mlr`'s performance measures.)

```
### 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"))
```

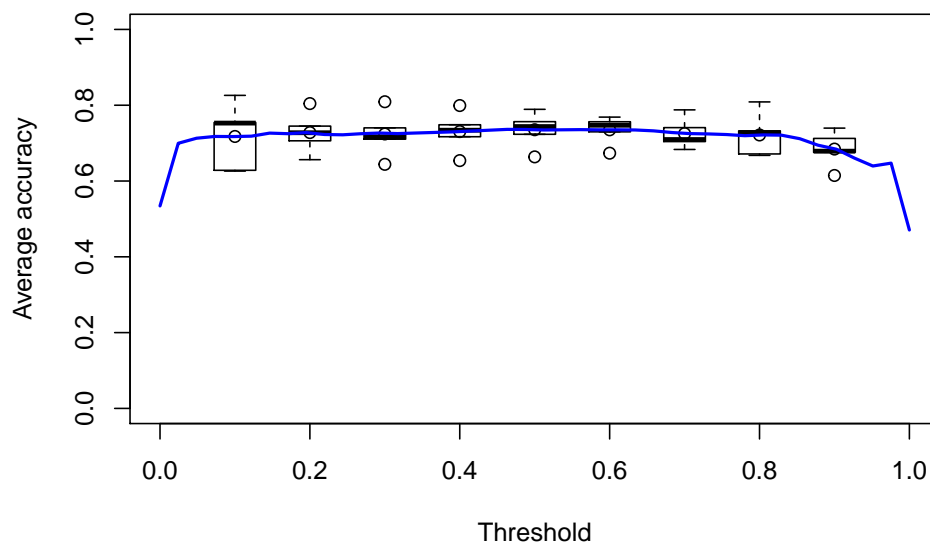


If you want to plot a performance measure versus the threshold, specify only one measure when calling `ROCR::performance()`. Below the average accuracy over the 5 cross-validation iterations is plotted against the threshold. Moreover, boxplots for certain threshold values (0.1, 0.2, ..., 0.9) are drawn.

```
### 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,label13,label14
## Observations: 2417
## Features:
##      numerics      factors    ordered functionals
##          103           0           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Is spatial: 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 classifier 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=MultilabelBinaryRelevance
## 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) (`vignette("measures")`) to calculate. The default measure for multilabel classification is the Hamming loss `multilabel.hamloss` (`vignette("measures")`). All available measures for multilabel classification can be shown by `listMeasures()` and found in the table of performance measures (`vignette("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
## 0.8696731 0.2052131 0.4615852
## multilabel.f1 timepredict
## 0.5709344 2.3530000
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 (`vignette("resample")`). 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=0.2214963
## Runtime: 9.12273
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=0.4734905
## Runtime: 1.20892
```

3.12.7 Binary performance

If you want to calculate a binary performance measure like, e.g., the accuracy (`vignette("measures")`), the mmce (`vignette("measures")`) or the auc (`vignette("measures")`) 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 (`vignette("measures")`) 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    0.69921390    0.3007861
## label2    0.58378155    0.4162185
## label3    0.70004137    0.2999586
## label4    0.70831609    0.2916839
## label5    0.70459247    0.2954075
## label6    0.59453868    0.4054613
## label7    0.54902772    0.4509723
## label8    0.53496070    0.4650393
## label9    0.31237071    0.6876293
## label10   0.44724866    0.5527513
## label11   0.46007447    0.5399255
## label12   0.52875465    0.4712453
## label13   0.53413322    0.4658668
## label14   0.01406703    0.9859330
```

3.13 Learning Curve Analysis

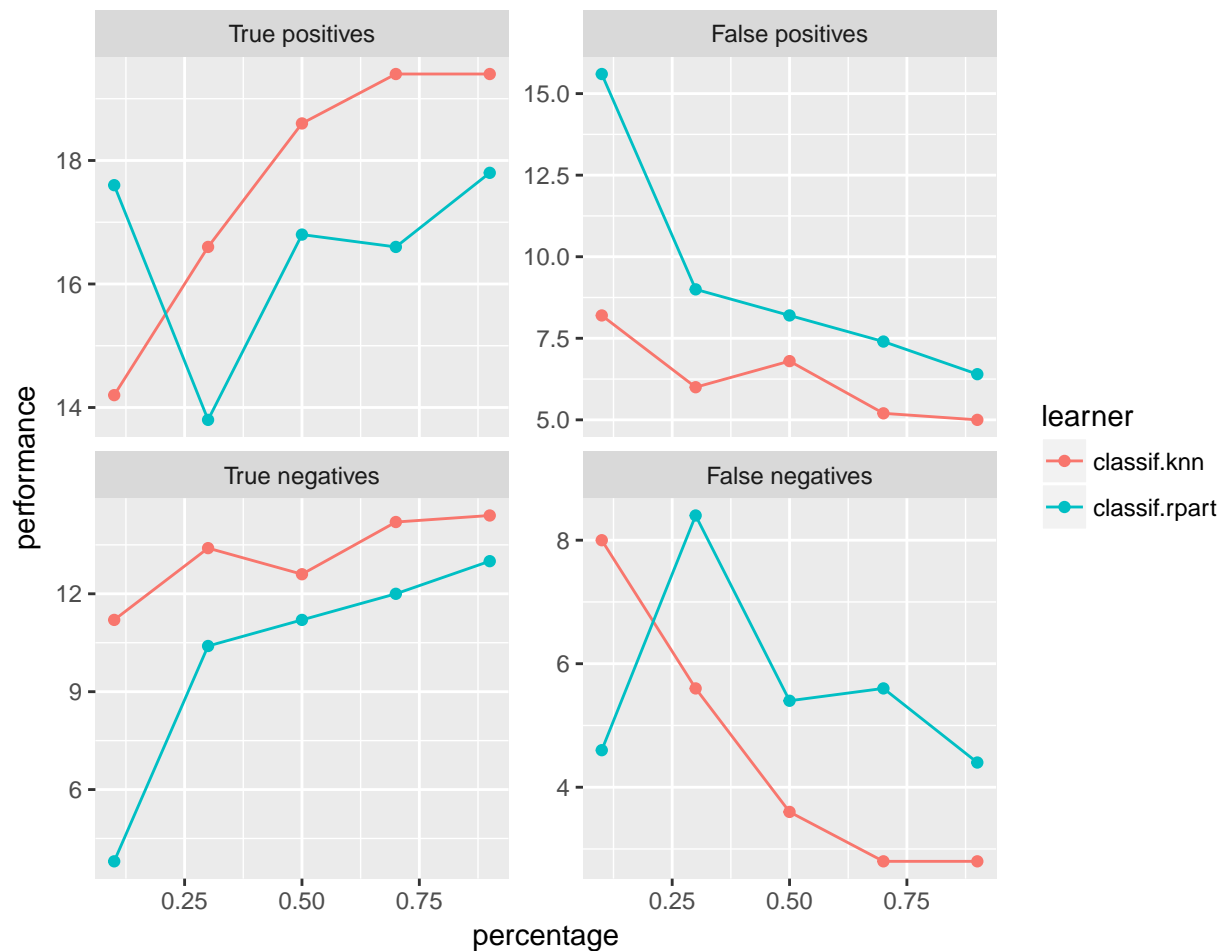
To analyze how the increase of observations in the training set improves the performance of a learner the *learning curve* is an appropriate visual tool. The experiment is conducted with an increasing subsample size and the performance is measured. In the plot the x-axis represents the relative subsample 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 (`vignette("integrated_learners")`) and multiple performance measures (`vignette("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 faceted subplots are created for each measure input to `generateLearningCurveData()`. If `facet = "measure"` learners are mapped to color, and vice versa.

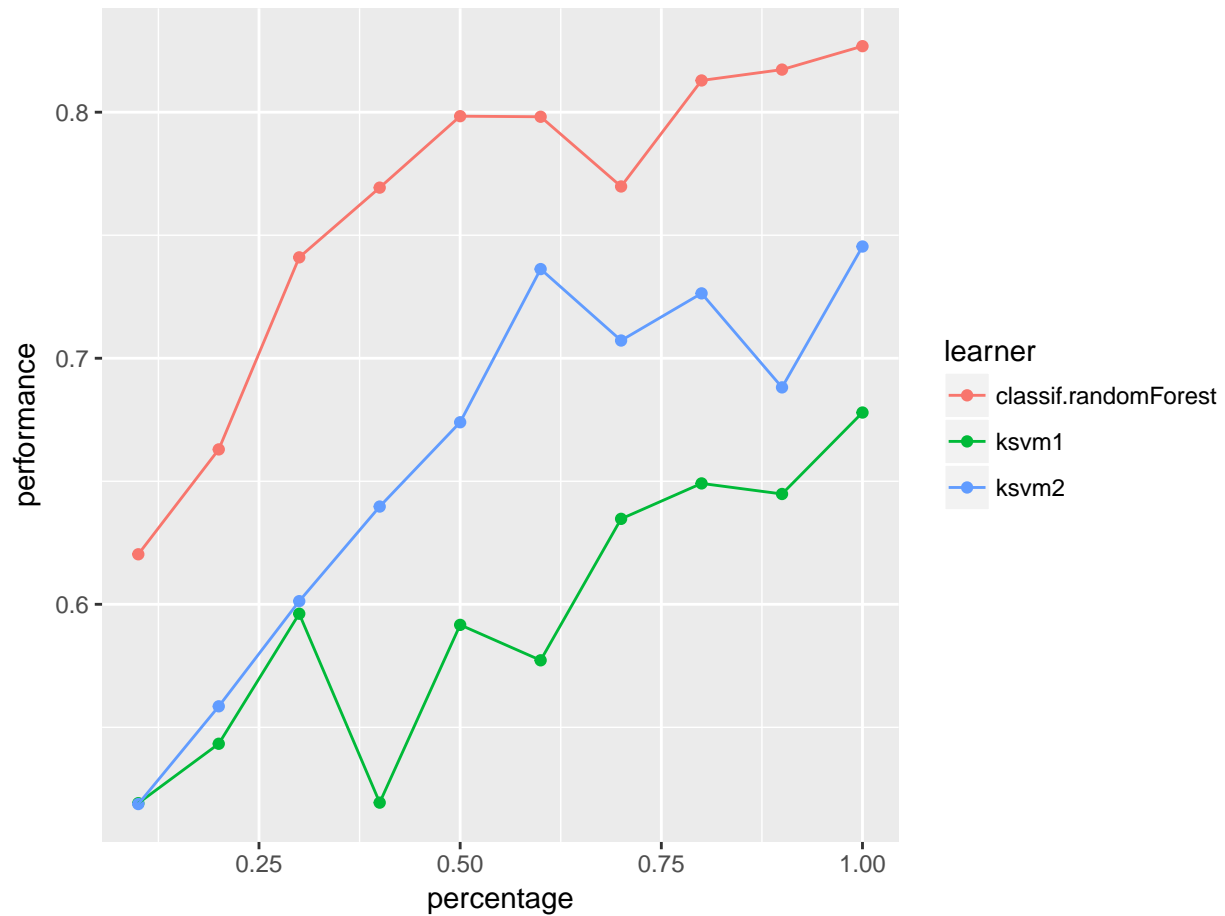
```
r = generateLearningCurveData(  
  learners = c("classif.rpart", "classif.knn"),  
  task = sonar.task,  
  percs = seq(0.1, 1, by = 0.2),  
  measures = list(tp, fp, tn, fn),  
  resampling = makeResampleDesc(method = "CV", iters = 5),  
  show.info = FALSE)  
plotLearningCurve(r)
```



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`.

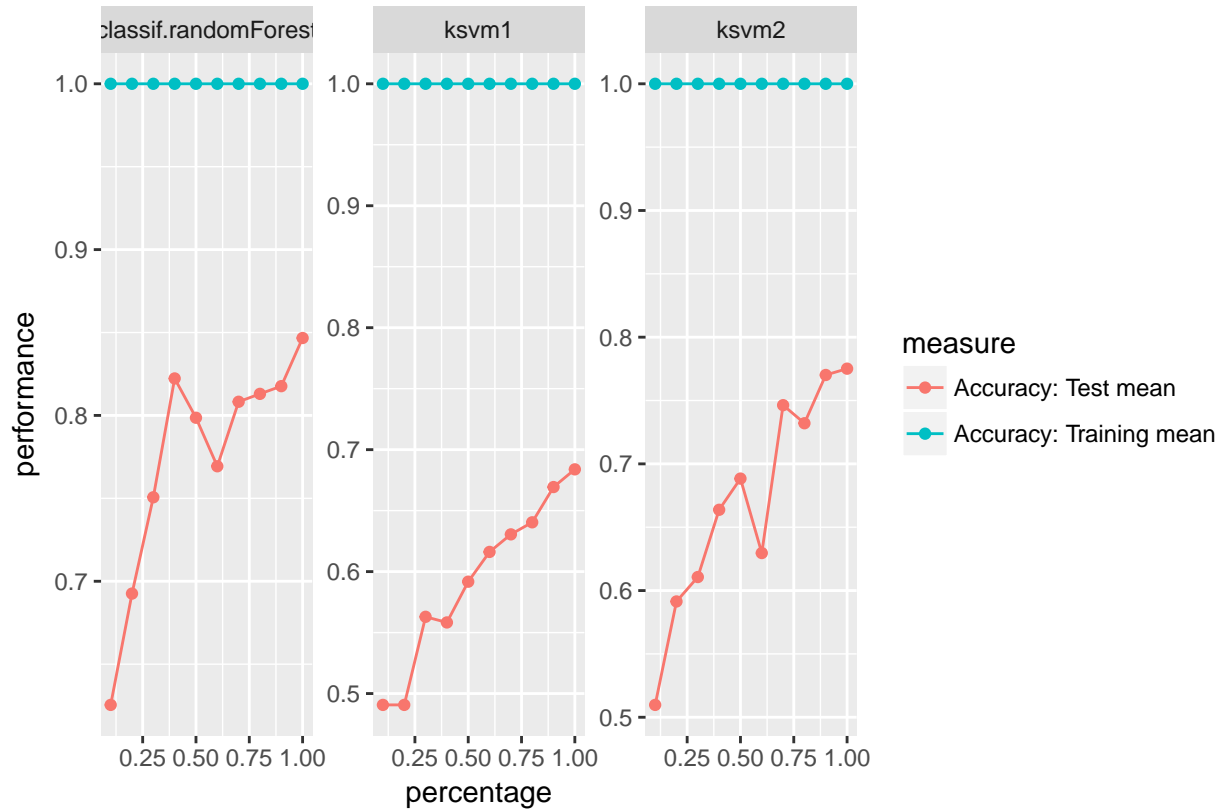
In the first example we simply passed a vector of learner names to `generateLearningCurveData()`. As usual, you can also create the learners beforehand and provide a *list* of `Learner` (`makeLearner()`) objects, or even pass a mixed *list* of `Learner` (`makeLearner()`) objects and strings. Make sure that all learners have unique `ids`.

```
lrns = list(
  makeLearner(c1 = "classif.ksvm", id = "ksvm1", sigma = 0.2, C = 2),
  makeLearner(c1 = "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 $\hat{f}_{X_s}^{(i)}$. 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, $\frac{\partial \hat{f}_{X_s}^{(i)}}{\partial X_s}$, 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 $\hat{f}_{X_s}^{(i)}$ 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 (`vignette("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    0.4846168    0.1000000
## 2 setosa    0.4380378    0.3666667
## 3 setosa    0.3764083    0.6333333
## 4 setosa    0.3156856    0.9000000
## 5 setosa    0.2405666    1.1666667
## 6 setosa    0.1659041    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$data)
##      Class Probability Petal.Width Petal.Length
## 1 setosa    0.4846168    0.1000000          NA
## 2 setosa    0.4380378    0.3666667          NA
## 3 setosa    0.3764083    0.6333333          NA
## 4 setosa    0.3156856    0.9000000          NA
## 5 setosa    0.2405666    1.1666667          NA
## 6 setosa    0.1659041    1.4333333          NA
tail(pd.lst$data)
##      Class Probability Petal.Width Petal.Length
## 55 virginica  0.2123895          NA    3.622222
## 56 virginica  0.3256245          NA    4.277778
## 57 virginica  0.4474958          NA    4.933333
## 58 virginica  0.6117391          NA    5.588889
## 59 virginica  0.7308699          NA    6.244444
## 60 virginica  0.7448237          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    0.6515998    0.1000000          1
## 2 setosa    0.6474006    0.3666667          1
## 3 setosa    0.6109337    0.6333333          1
## 4 setosa    0.5373744    0.9000000          1
## 5 setosa    0.4323750    1.1666667          1
## 6 setosa    0.3343676    1.4333333          1
## ... (#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 24.88320  1.730000
## 2 23.76059  5.756667
## 3 22.35978  9.783333
## 4 20.67762 13.810000
## 5 19.61423 17.836667
## 6 19.01239 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      lstat    lower    upper
## 1 24.88320  1.730000 21.33675 29.52434
## 2 23.76059  5.756667 20.81982 27.40836
## 3 22.35978  9.783333 19.89344 24.99834
## 4 20.67762 13.810000 18.68066 23.67203
## 5 19.61423 17.836667 16.53059 22.99491
## 6 19.01239 21.863333 14.88781 22.16996
## ... (#rows: 10, #cols: 4)
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  0.27861125      1.000000
## 2 setosa  0.22562713      1.655556
## 3 setosa  0.16369811      2.311111
## 4 setosa  0.09254299      2.966667
## 5 setosa  0.04536500      3.622222
## 6 setosa  0.02197704      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$data)
##      medv      lstat crim      lower      upper
## 1 31.74903  1.730000   NA 13.00724 50.49082
## 2 26.19066  5.756667   NA 14.35557 38.02575
## 3 23.52932  9.783333   NA 13.36752 33.69111
## 4 22.05845 13.810000   NA 14.19019 29.92671
## 5 20.38499 17.836667   NA 12.93912 27.83085
## 6 19.79760 21.863333   NA 11.87968 27.71552
tail(pd.se$data)
##      medv lstat      crim      lower      upper
## 15 21.90325   NA 39.54849 10.71407 33.09243
## 16 21.88579   NA 49.43403 10.67915 33.09242
## 17 21.87431   NA 59.31957 10.65561 33.09302
## 18 21.87462   NA 69.20512 10.65592 33.09332
## 19 21.87800   NA 79.09066 10.66475 33.09125
## 20 21.87800   NA 88.97620 10.66475 33.09125
```

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
## Predictions centered: FALSE
##      medv      lstat idx
## 1 26.98619  1.730000   1
```

```
## 2 25.91768 5.756667 1
## 3 24.68534 9.783333 1
## 4 23.47362 13.810000 1
## 5 22.40030 17.836667 1
## 6 21.51475 21.863333 1
## ... (#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 = TRUE)
pd.ind.classif
## PartialDependenceData
## Task: iris_example
## Features: Petal.Length
## Target: setosa, versicolor, virginica
## Derivative: FALSE
## Interaction: FALSE
## Individual: TRUE
## Predictions centered: FALSE
##   Class Probability Petal.Length      idx
## 1 setosa  0.9782330             1 1.setosa
## 2 setosa  0.9697583             1 2.setosa
## 3 setosa  0.9786474             1 3.setosa
## 4 setosa  0.9762750             1 4.setosa
## 5 setosa  0.9774078             1 5.setosa
## 6 setosa  0.9713166             1 6.setosa
## ... (#rows: 4500, #cols: 4)
```

Individual estimates of partial dependence can also be centered by predictions made at all n observations for a particular point in the prediction grid created by the features. This is controlled by the argument `center` which is a list of the same length as the length of the `features` argument and contains the values of the features desired.

```
iris = getTaskData(iris.task)
pd.ind.classif = generatePartialDependenceData(fit.classif, iris.task, "Petal.Length", individual = TRUE,
  center = list("Petal.Length" = min(iris$Petal.Length)))
```

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 -0.2384924  1.730000
## 2 -0.3548794  5.756667
## 3 -0.4212415  9.783333
## 4 -0.4281714 13.810000
## 5 -0.3794884 17.836667
```

```
## 6 -0.2881884 21.863333
pd.regr.der.ind = generatePartialDependenceData(fit.regr, bh.task, "lstat", derivative = TRUE,
  individual = TRUE)
head(pd.regr.der.ind$data)
##      medv      lstat idx
## 1 -0.2277286  1.730000  1
## 2 -0.2942850  5.756667  1
## 3 -0.3099532  9.783333  1
## 4 -0.2870211 13.810000  1
## 5 -0.2441946 17.836667  1
## 6 -0.1952765 21.863333  1
pd.classif.der = generatePartialDependenceData(fit.classif, iris.task, "Petal.Width", derivative = TRUE,
  individual = TRUE)
head(pd.classif.der.ind$data)
##      Class Probability Petal.Width
## 1 setosa  -0.1120082    0.1000000
## 2 setosa  -0.2236317    0.3666667
## 3 setosa  -0.2250086    0.6333333
## 4 setosa  -0.2467762    0.9000000
## 5 setosa  -0.3052195    1.1666667
## 6 setosa  -0.2326490    1.4333333
pd.classif.der.ind = generatePartialDependenceData(fit.classif, iris.task, "Petal.Width", derivative = TRUE,
  individual = TRUE)
head(pd.classif.der.ind$data)
##      Class Probability Petal.Width      idx
## 1 setosa  0.03184492      0.1 1.setosa
## 2 setosa  0.02264432      0.1 2.setosa
## 3 setosa  0.02064734      0.1 3.setosa
## 4 setosa  0.01931155      0.1 4.setosa
## 5 setosa  0.03314792      0.1 5.setosa
## 6 setosa  0.04838810      0.1 6.setosa
```

3.14.2 Functional ANOVA

Hooker (2004) proposed the decomposition of a learned function \hat{f} as a sum of lower dimensional functions

$$f(\mathbf{x}) = g_0 + \sum_{i=1}^p g_i(X_i) + \sum_{i \neq j} g_{ij}(x_{ij}) + \dots$$

where p is the number of features. `generateFunctionalANOVADData()` estimates the individual g functions using partial dependence. When functions depend only on one feature, they are equivalent to partial dependence, but a g function which depends on more than one feature is the “effect” of only those features: lower dimensional “effects” are removed.

$$\hat{g}_u(X) = \frac{1}{N} \sum_{i=1}^N \left(\hat{f}(X) - \sum_{v \subset u} g_v(X) \right)$$

Here u is a subset of $1, \dots, p$. When $|v| = 1$ g_v can be directly computed by computing the bivariate partial dependence of \hat{f} on X_u and then subtracting off the univariate partial dependences of the features contained in v .

Although this decomposition is generalizable to classification it is currently only available for regression tasks.

```

lrn.regr = makeLearner("regr.ksvm")
fit.regr = train(lrn.regr, bh.task)

fa = generateFunctionalANOVADData(fit.regr, bh.task, "lstat", depth = 1, fun = median)
fa
## FunctionalANOVADData
## Task: BostonHousing-example
## Features: lstat
## Target: medv
##
##
##   effect      medv      lstat
## 1  lstat 24.91687  1.730000
## 2  lstat 23.73687  5.756667
## 3  lstat 22.34371  9.783333
## 4  lstat 20.71830 13.810000
## 5  lstat 19.60609 17.836667
## 6  lstat 19.02202 21.863333
## ... (#rows: 10, #cols: 3)
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 24.91687  1.730000
## 2 23.73687  5.756667
## 3 22.34371  9.783333
## 4 20.71830 13.810000
## 5 19.60609 17.836667
## 6 19.02202 21.863333
## ... (#rows: 10, #cols: 2)

```

The `depth` argument is similar to the `interaction` argument in `generatePartialDependenceData()` but instead of specifying whether all of joint “effect” of all the **features** is computed, it determines whether “effects” of all subsets of the features given the specified `depth` are computed. So, for example, with p features and `depth 1`, the univariate partial dependence is returned. If, instead, `depth = 2`, then all possible bivariate functional ANOVA effects are returned. This is done by computing the univariate partial dependence for each feature and subtracting it from the bivariate partial dependence for each possible pair.

```

fa.bv = generateFunctionalANOVADData(fit.regr, bh.task, c("crim", "lstat", "age"),
  depth = 2)
fa.bv
## FunctionalANOVADData
## Task: BostonHousing-example
## Features: crim, lstat, age
## Target: medv
##
##

```

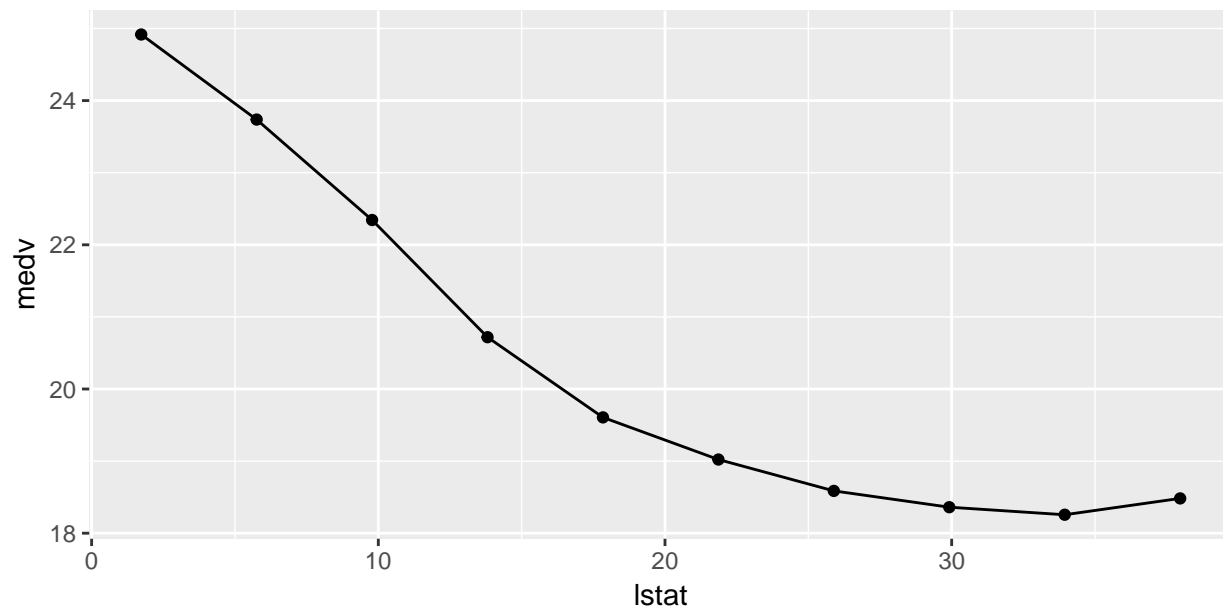
```
##      effect      medv      crim lstat age
## 1 crim:lstat -22.69321  0.006320  1.73  NA
## 2 crim:lstat -23.21905  9.891862  1.73  NA
## 3 crim:lstat -24.81861 19.777404  1.73  NA
## 4 crim:lstat -26.48423 29.662947  1.73  NA
## 5 crim:lstat -27.60245 39.548489  1.73  NA
## 6 crim:lstat -28.24694 49.434031  1.73  NA
## ... (#rows: 300, #cols: 5)
names(table(fa.bv$data$effect)) ### interaction effects estimated
## [1] "crim:age"    "crim:lstat" "lstat:age"
```

3.14.3 Plotting partial dependences

Results from `generatePartialDependenceData()` and `generateFunctionalANOVADData()` can be visualized with `plotPartialDependence()` and `plotPartialDependenceGGVIS()`.

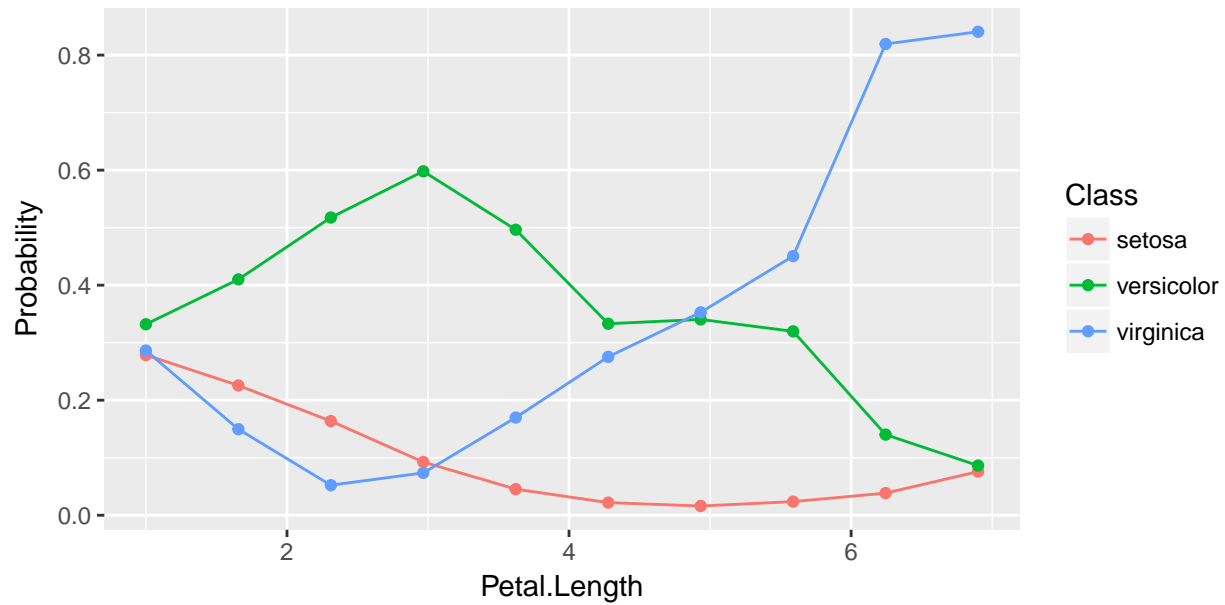
With one feature and a regression task the output is a line plot, with a point for each point in the corresponding feature's grid.

```
plotPartialDependence(pd.regr)
```



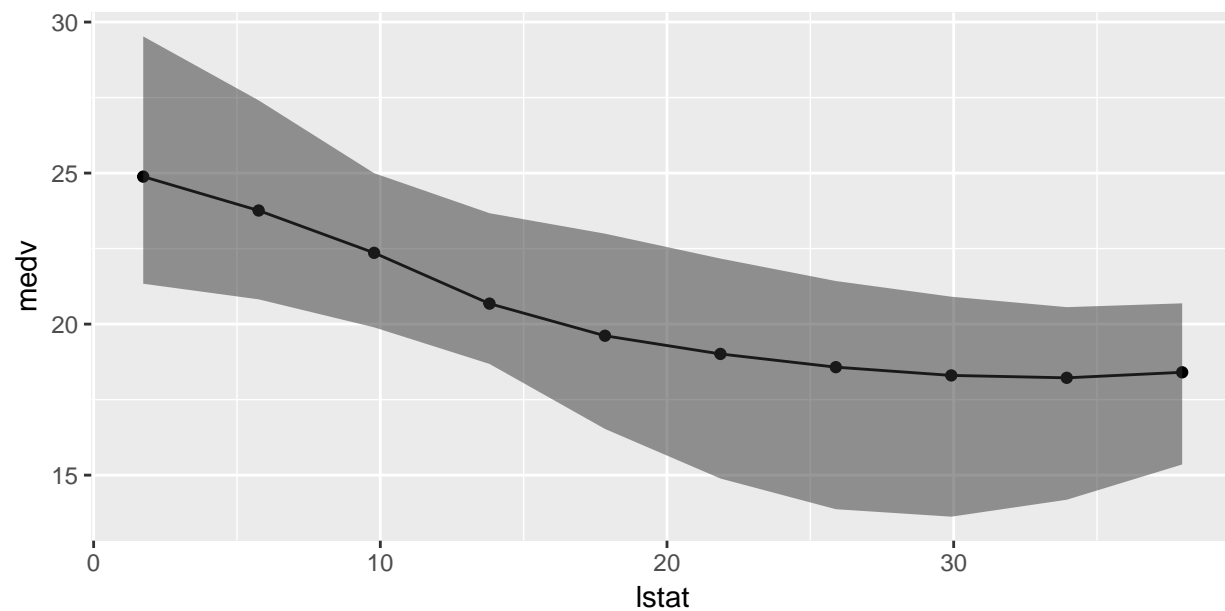
With a classification task, a line is drawn for each class, which gives the estimated partial probability of that class for a particular point in the feature grid.


```
plotPartialDependence(pd.classif)
```



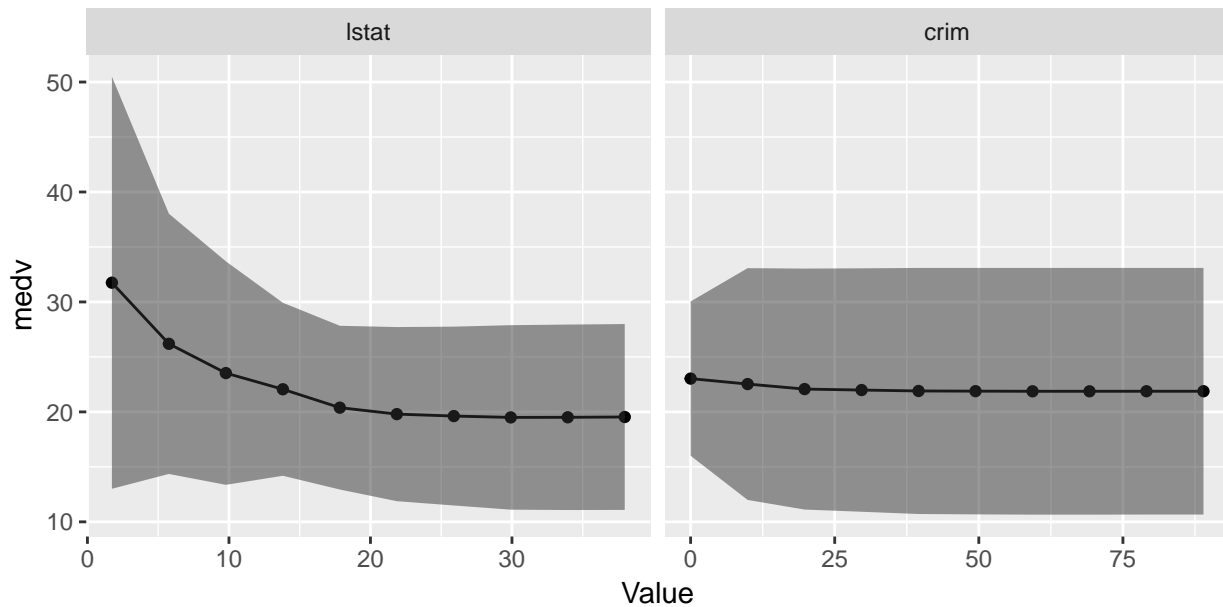
For regression tasks, when the `fun` argument of `generatePartialDependenceData()` is used, the bounds will automatically be displayed using a gray ribbon.

```
plotPartialDependence(pd.ci)
```



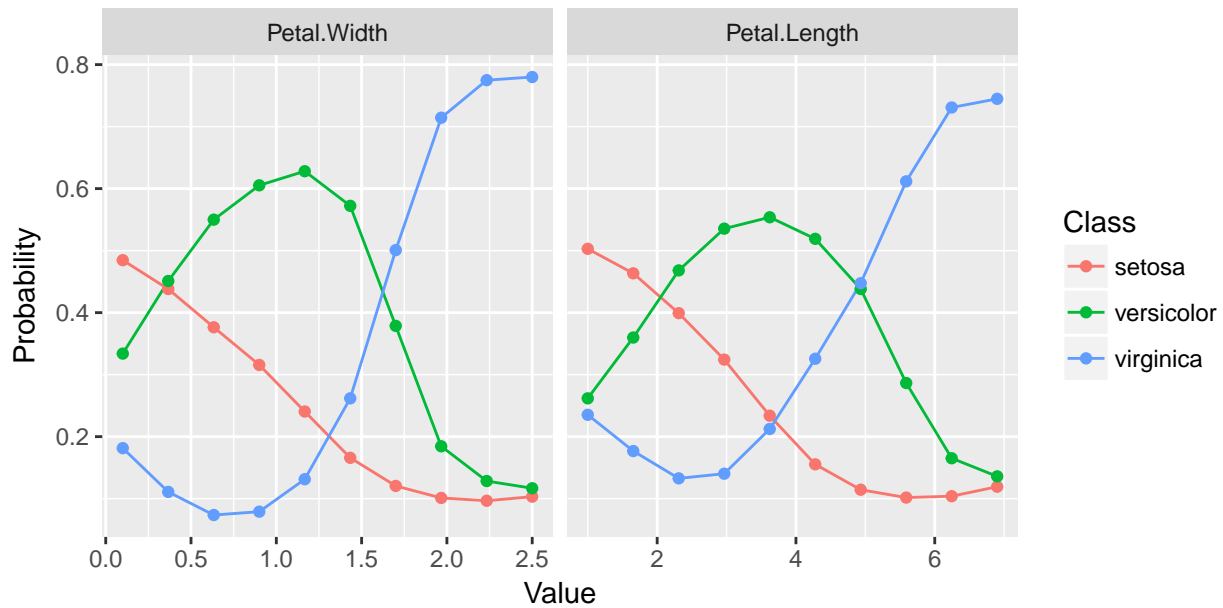
The same goes for plots of partial dependences where the learner has `predict.type = "se"`.

```
plotPartialDependence(pd.se)
```



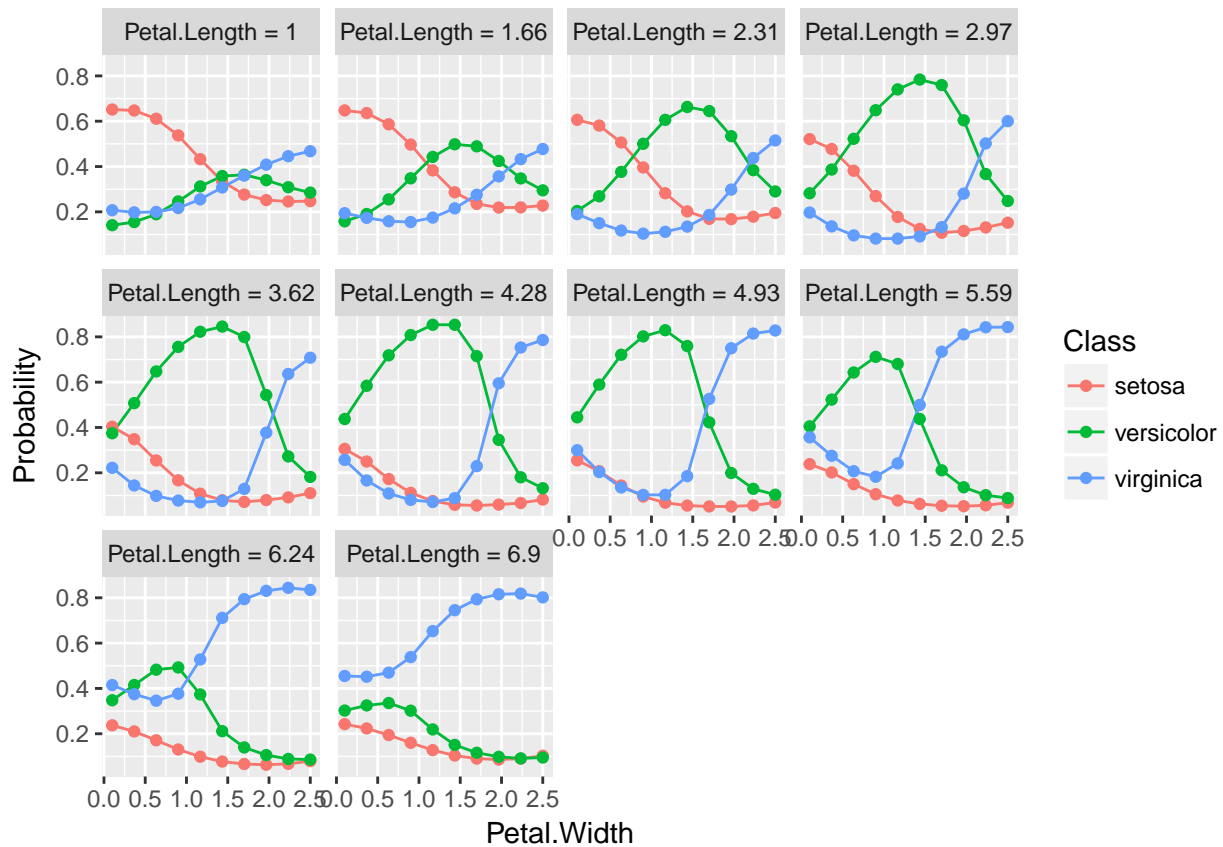
When multiple features are passed to `generatePartialDependenceData()` but `interaction = FALSE`, facetting is used to display each estimated bivariate relationship.

```
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")
```

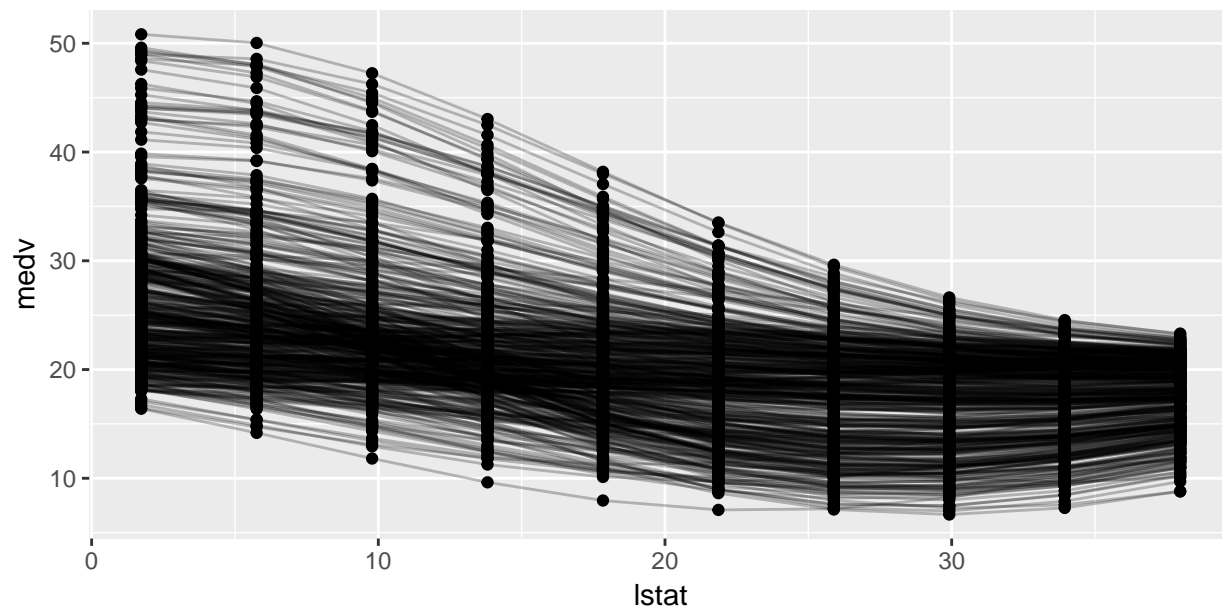


`plotPartialDependenceGGVIS()` can be used similarly, however, since `ggvis` currently lacks subplotting/facetting capabilities, the argument `interact` maps one feature to an interactive sidebar where the user can select a value of one feature.

```
plotPartialDependenceGGVIS(pd.int, interact = "Petal.Length")
```

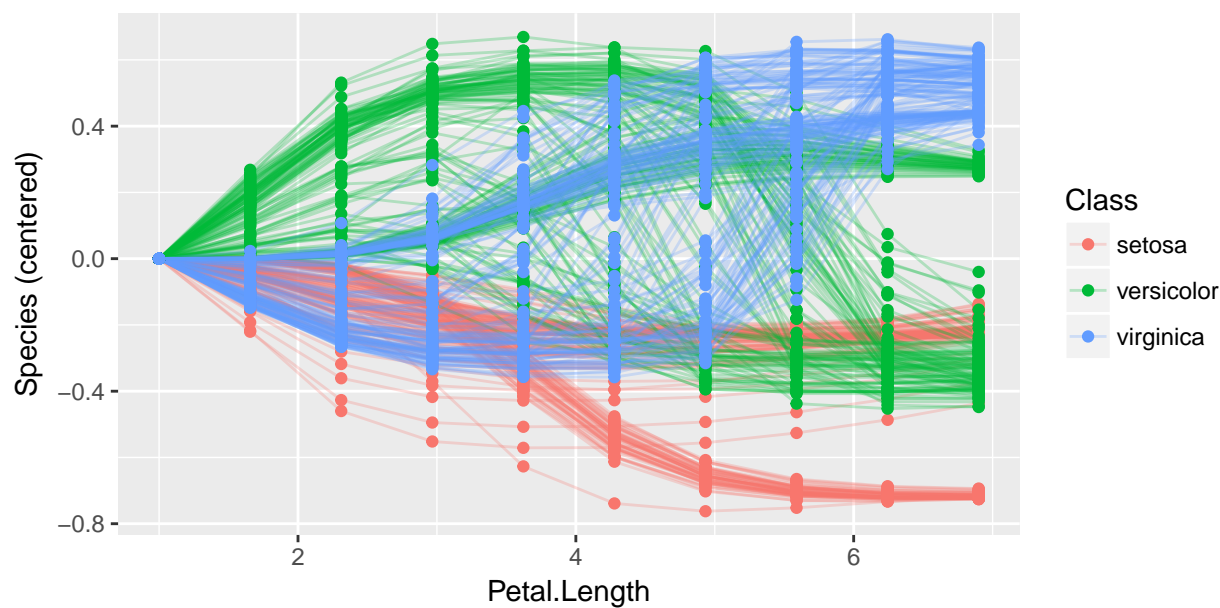
When `individual = TRUE` each individual conditional expectation curve is plotted.

```
plotPartialDependence(pd.ind.regr)
```



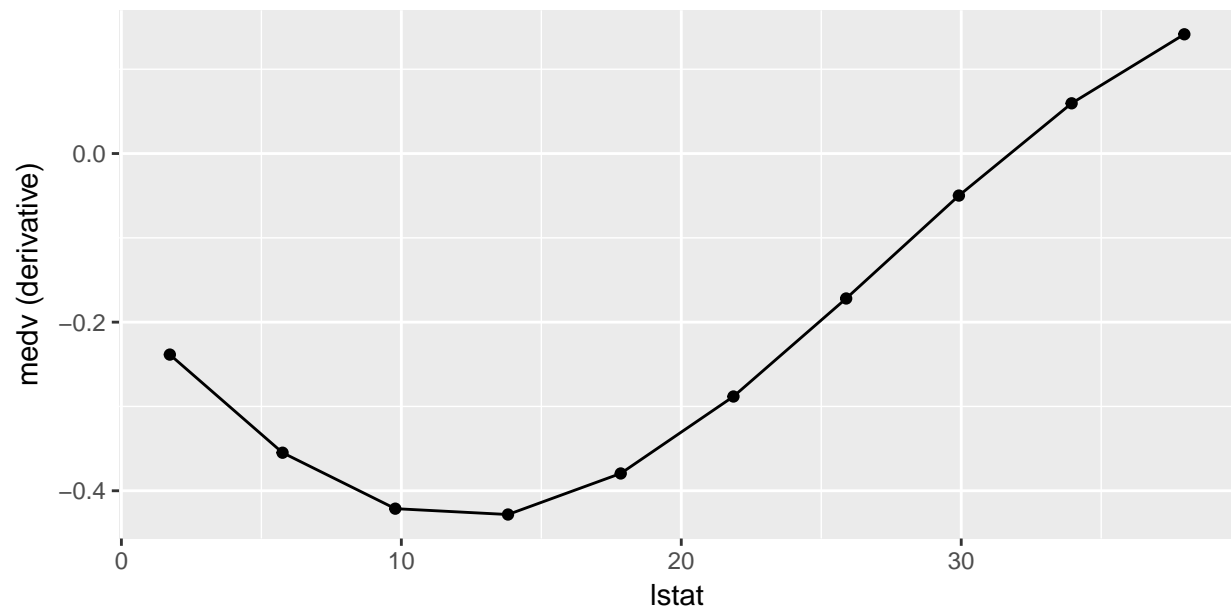
When the individual curves are centered by subtracting the individual conditional expectations estimated at a particular value of X_s this results in a fixed intercept which aids in visualizing variation in predictions made by $\hat{f}_{X_s}^{(i)}$.

```
plotPartialDependence(pd.ind.classif)
```



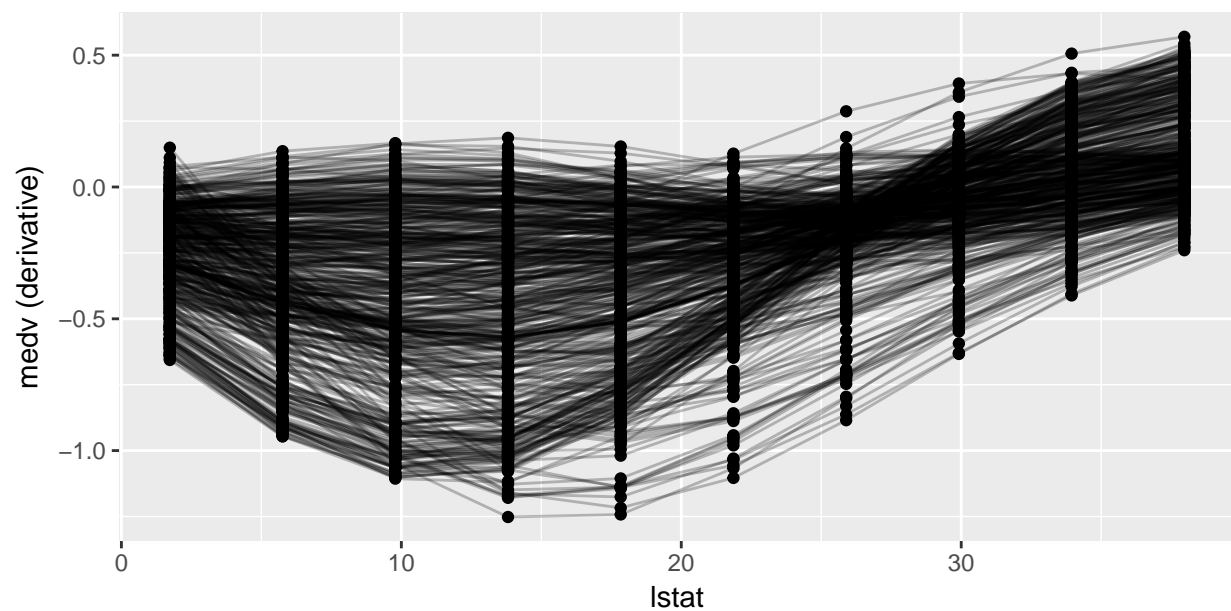
Plotting partial derivative functions works the same as partial dependence. Below are estimates of the derivative of the mean aggregated partial dependence function, and the individual partial dependence functions for a regression and a classification task respectively.

```
plotPartialDependence(pd.regr.der)
```



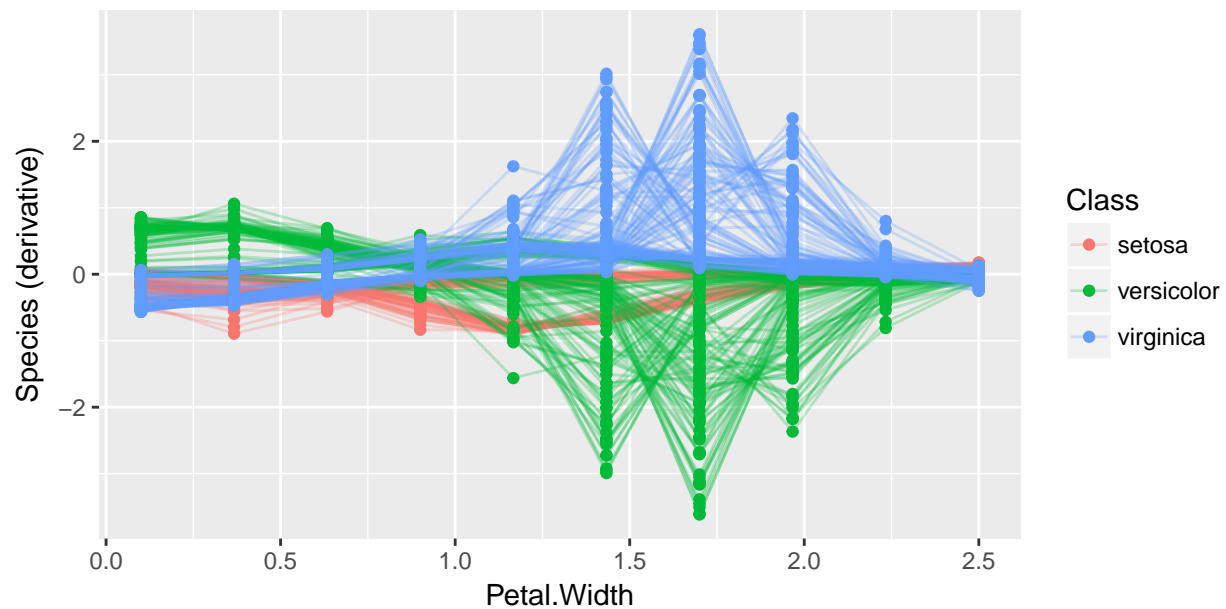
This suggests that \hat{f} is not additive in `lstat` except in the neighborhood of 25.

```
plotPartialDependence(pd.regr.der.ind)
```



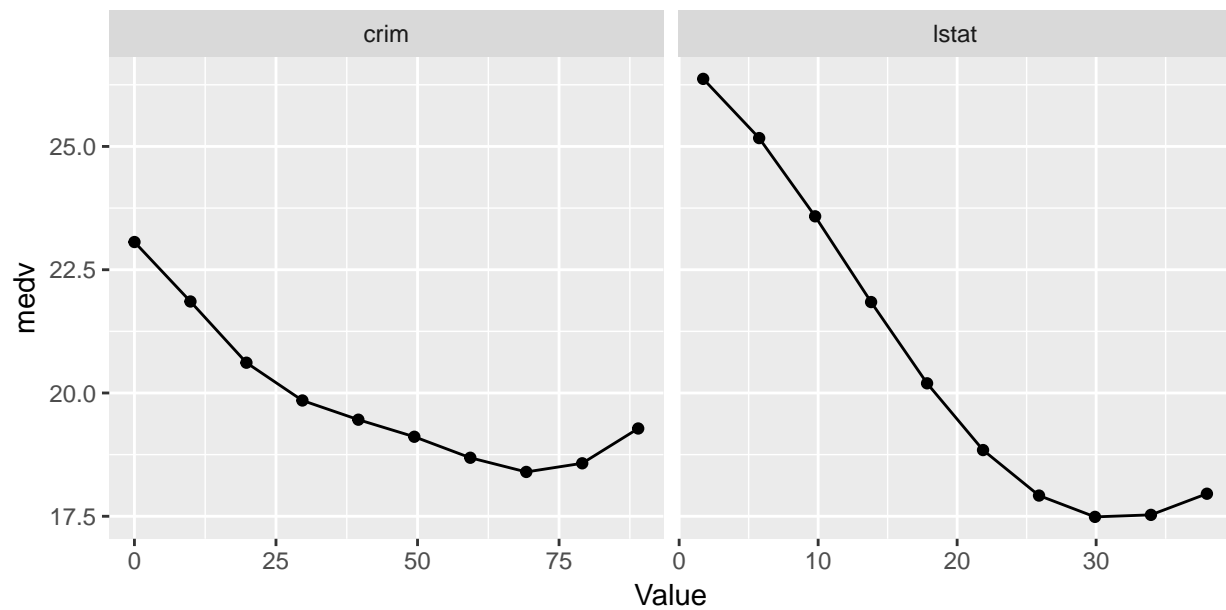
This suggests that `Petal.Width` interacts with some other feature in the neighborhood of (1.5, 2) for classes “`virginica`” and “`versicolor`”.

```
plotPartialDependence(pd.classif.der.ind)
```



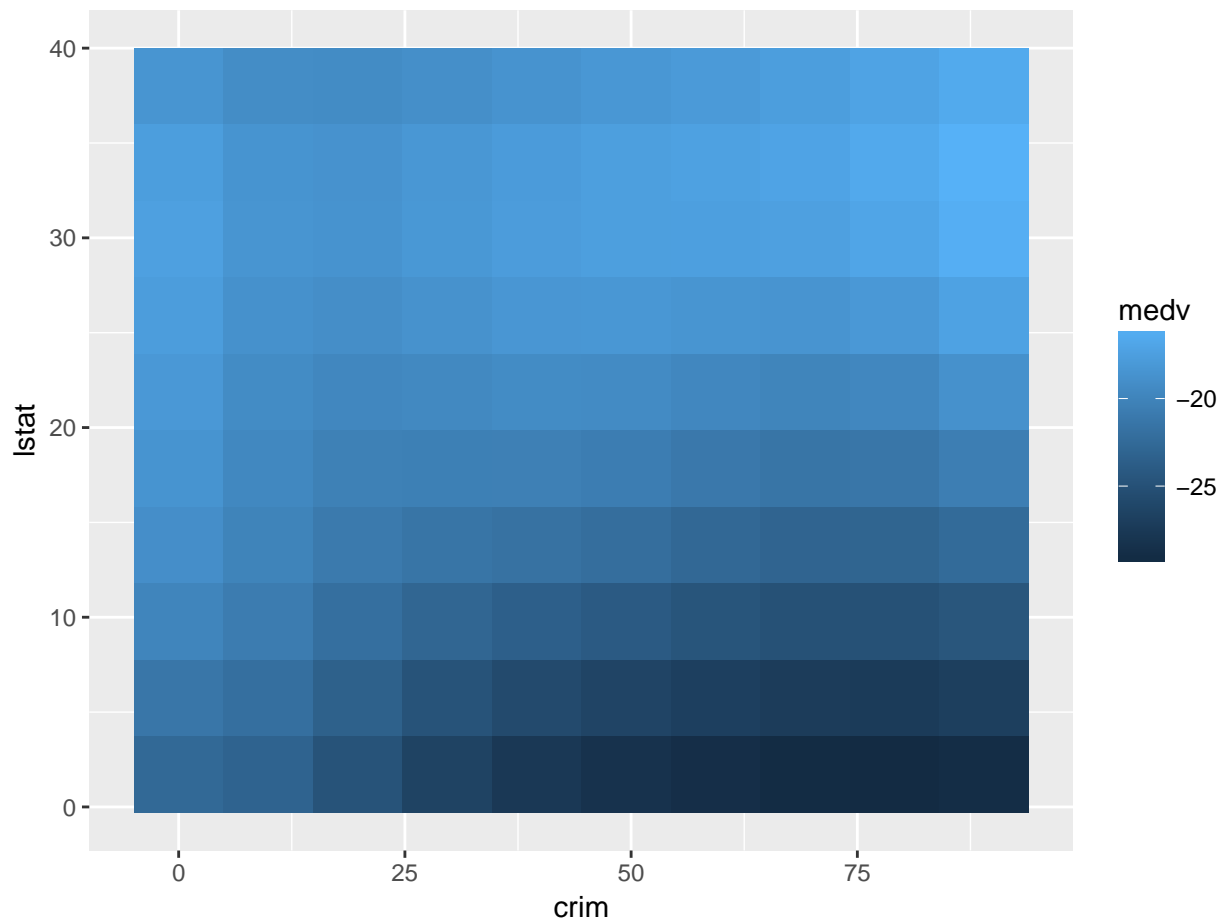
Output from `generateFunctionalANOVAData()` can also be plotted using `plotPartialDependence()`.

```
fa = generateFunctionalANOVAData(fit.regr, bh.task, c("crim", "lstat"), depth = 1)
plotPartialDependence(fa)
```



Interactions can often be more easily visualized by using functional ANOVA.

```
fa.bv = generateFunctionalANOVAData(fit.regr, bh.task, c("crim", "lstat"), depth = 2)
plotPartialDependence(fa.bv, "tile")
```



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 probabilities (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
```

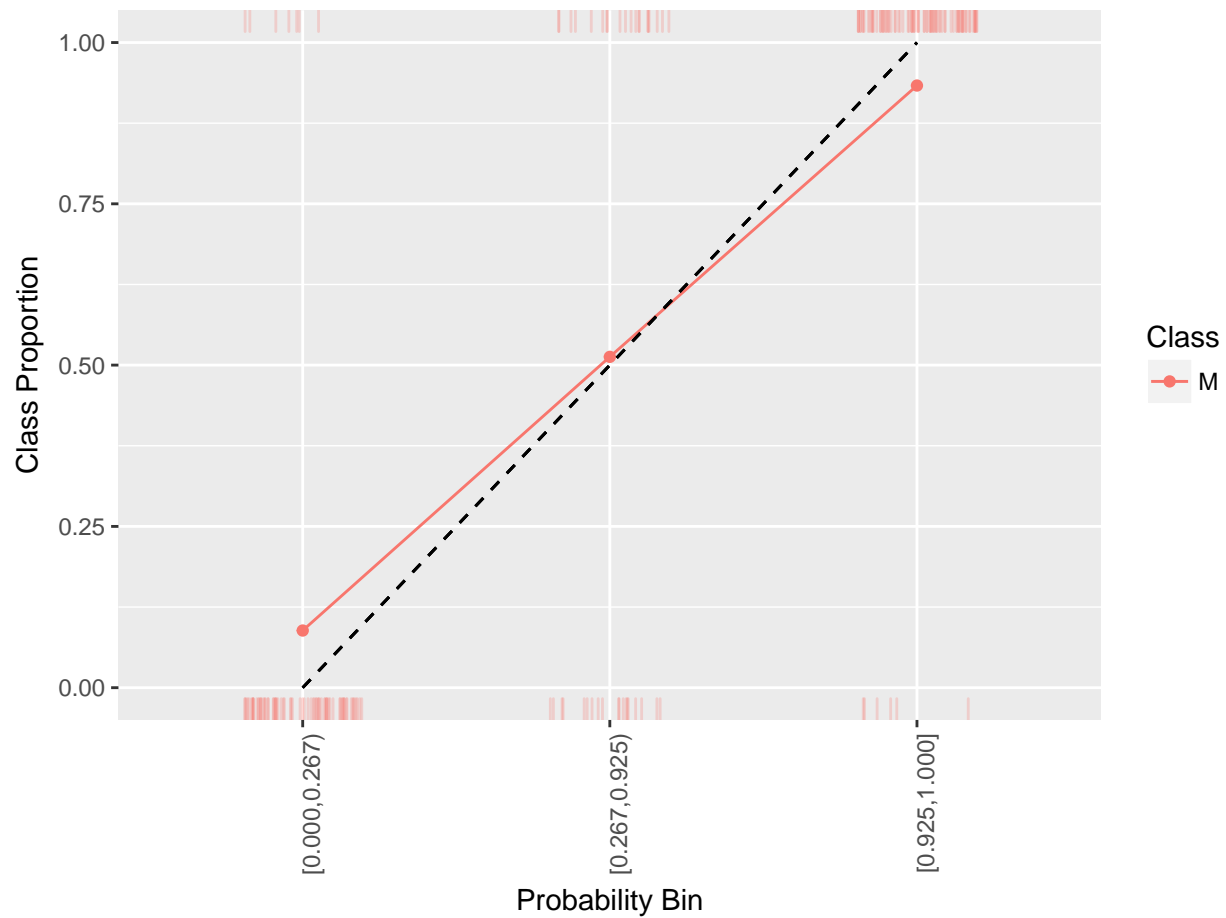
```
## 5 prediction (0.2,0.3]      M 0.2727273
## 6 prediction (0.4,0.5]      M 0.4615385
## 7 prediction (0.8,0.9]      M 0.0000000
## 8 prediction (0.5,0.6]      M 0.0000000
```

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
```

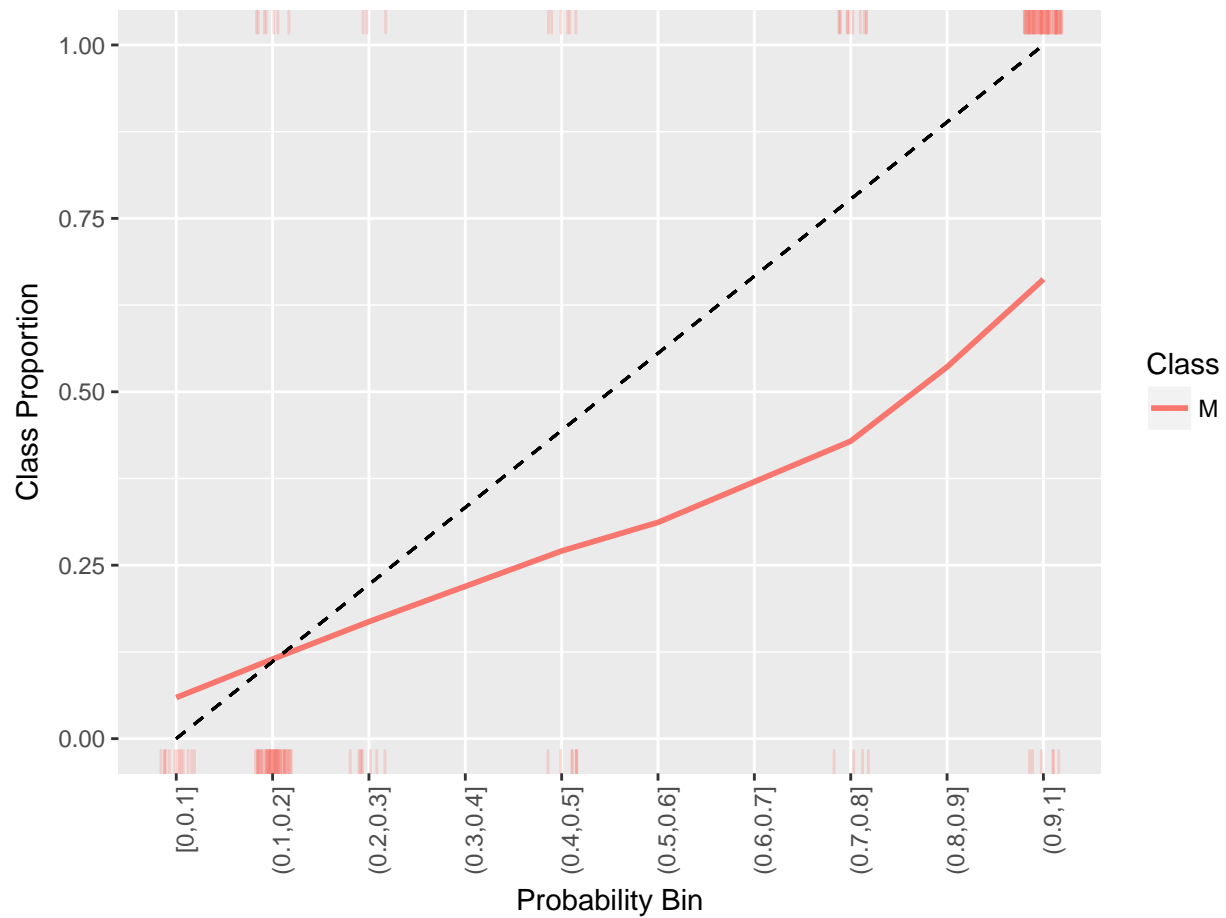
`generateCalibrationData()` objects can be plotted using `plotCalibration()`. `plotCalibration()` by default plots a reference line which shows perfect calibration and a “rag” plot, which is a rug plot on the top and bottom of the graph, where the top pertains to “positive” cases, where the predicted 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)
```

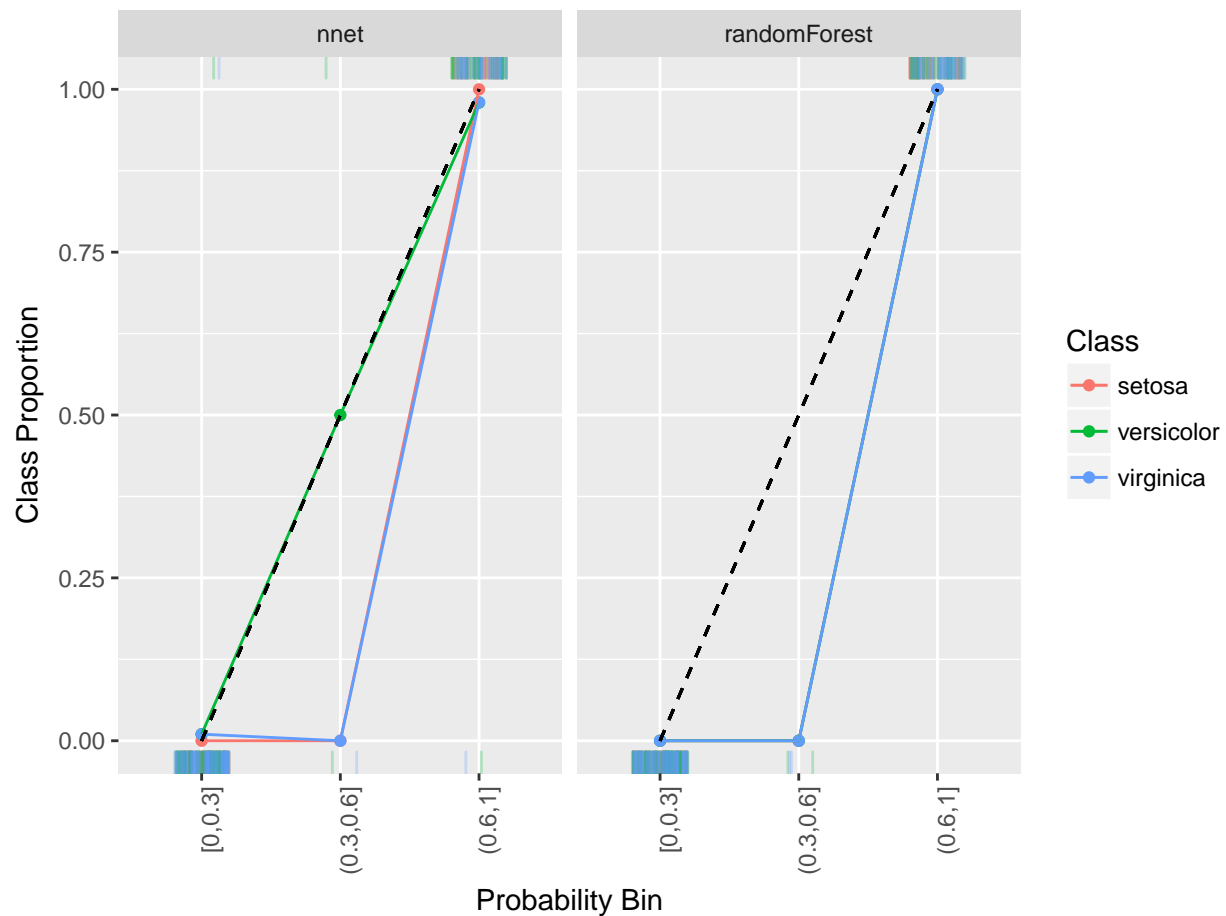
Because of the discretization of the probabilities, sometimes it is advantageous to smooth the calibration plot. Though `smooth = FALSE` by default, setting this option to `TRUE` replaces the estimated proportions with a loess smoother.

```
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 (`vignette("tune")`) 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 27.59337940    0.7122396    0.2877604         1     0.090
## 2  0.03409938    0.6510417    0.3489583         2     0.084
## 3 11.39021547    0.7291667    0.2708333         3     0.084
## 4  0.64800028    0.7721354    0.2278646         4     0.079
## 5  0.18618607    0.7434896    0.2565104         5     0.083
## 6  0.03195475    0.6510417    0.3489583         6     0.076
```

As a reminder from the resampling (`vignette("resample")`) 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 30.3216272      0.7109375      0.9440104      0.2890625      0.05598958
## 2  0.2974239      0.7617188      0.8085938      0.2382812      0.19140625
## 3  0.1717653      0.7473958      0.7799479      0.2526042      0.22005208
## 4 26.5614772      0.7161458      0.9388021      0.2838542      0.06119792
## 5  0.3338512      0.7539062      0.8033854      0.2460938      0.19661458
## 6  3.0735887      0.7578125      0.8645833      0.2421875      0.13541667
## iteration exec.time
## 1          1      0.114
## 2          2      0.100
## 3          3      0.100
## 4          4      0.108
## 5          5      0.115
## 6          6      0.106

```

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      0.6197917      0.3802083          1      0.051
## 2 -3.8888889      0.6197917      0.3802083          2      0.065
## 3 -2.7777778      0.6927083      0.3072917          3      0.057
## 4 -1.6666667      0.7500000      0.2500000          4      0.052
## 5 -0.5555556      0.7421875      0.2578125          5      0.050
## 6  0.5555556      0.7109375      0.2890625          6      0.050
## 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.

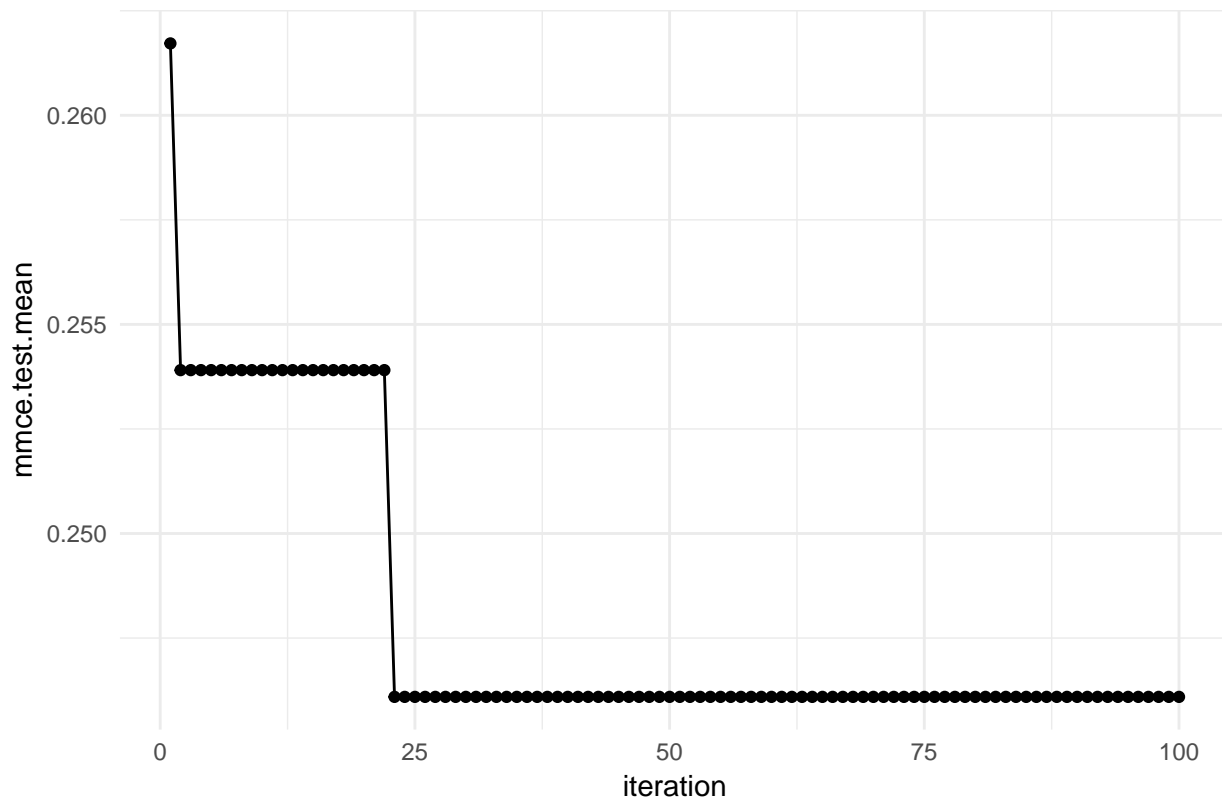
In the example below, we tune the number of clusters against the silhouette score on the Pima dataset. We specify the x-axis with the `x` argument and the y-axis with the `y` argument. If the `plot.type` argument is not specified, `mlr` will attempt to plot a scatterplot by default. Since `plotHyperParsEffect()` 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.

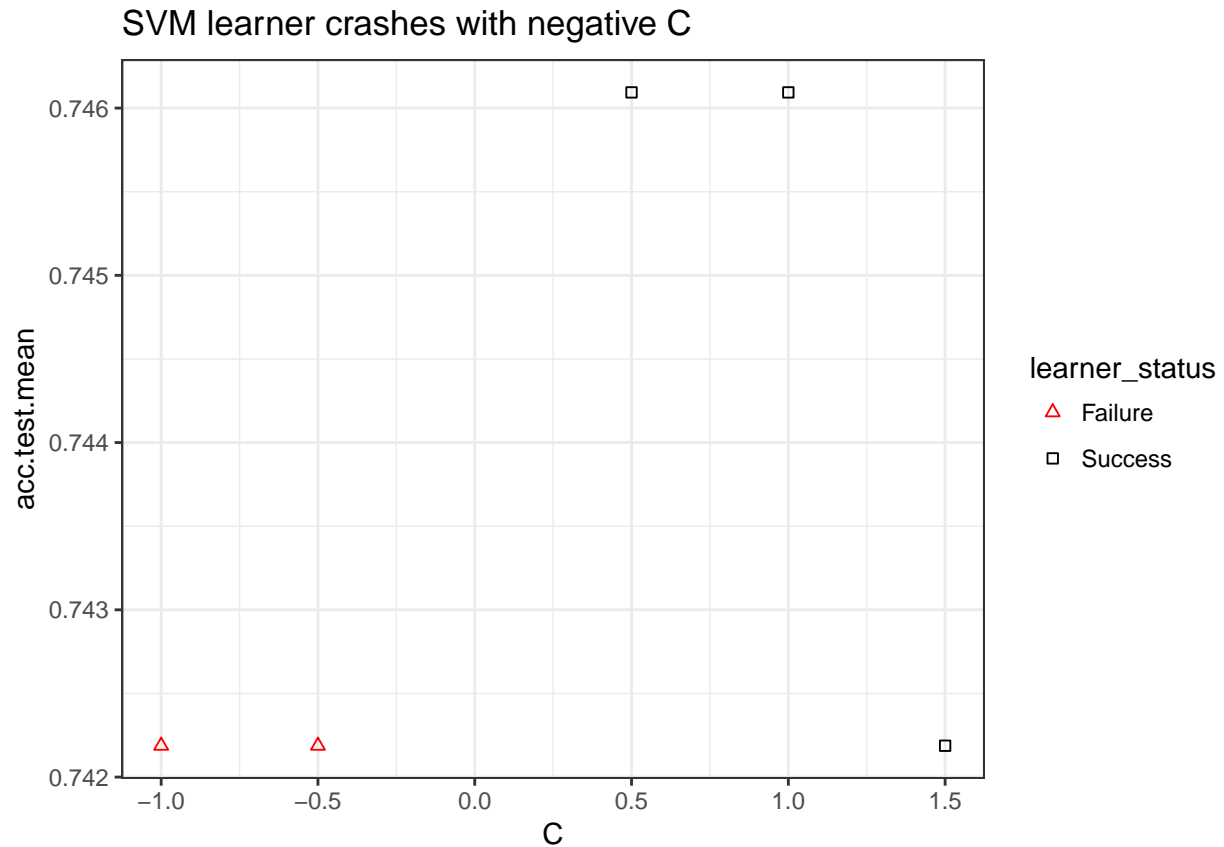
```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x)
)
ctrl = makeTuneControlGenSA(budget = 100L)
rdesc = makeResampleDesc("Holdout")
res = tuneParams("classif.ksvm", task = pid.task, control = ctrl,
  resampling = rdesc, par.set = ps, show.info = FALSE)
data = generateHyperParsEffectData(res)
plt = plotHyperParsEffect(data, x = "iteration", y = "mmce.test.mean",
  plot.type = "line")
plt + ggtitle("Analyzing convergence of simulated annealing") +
  theme_minimal()
```

Analyzing convergence of simulated annealing



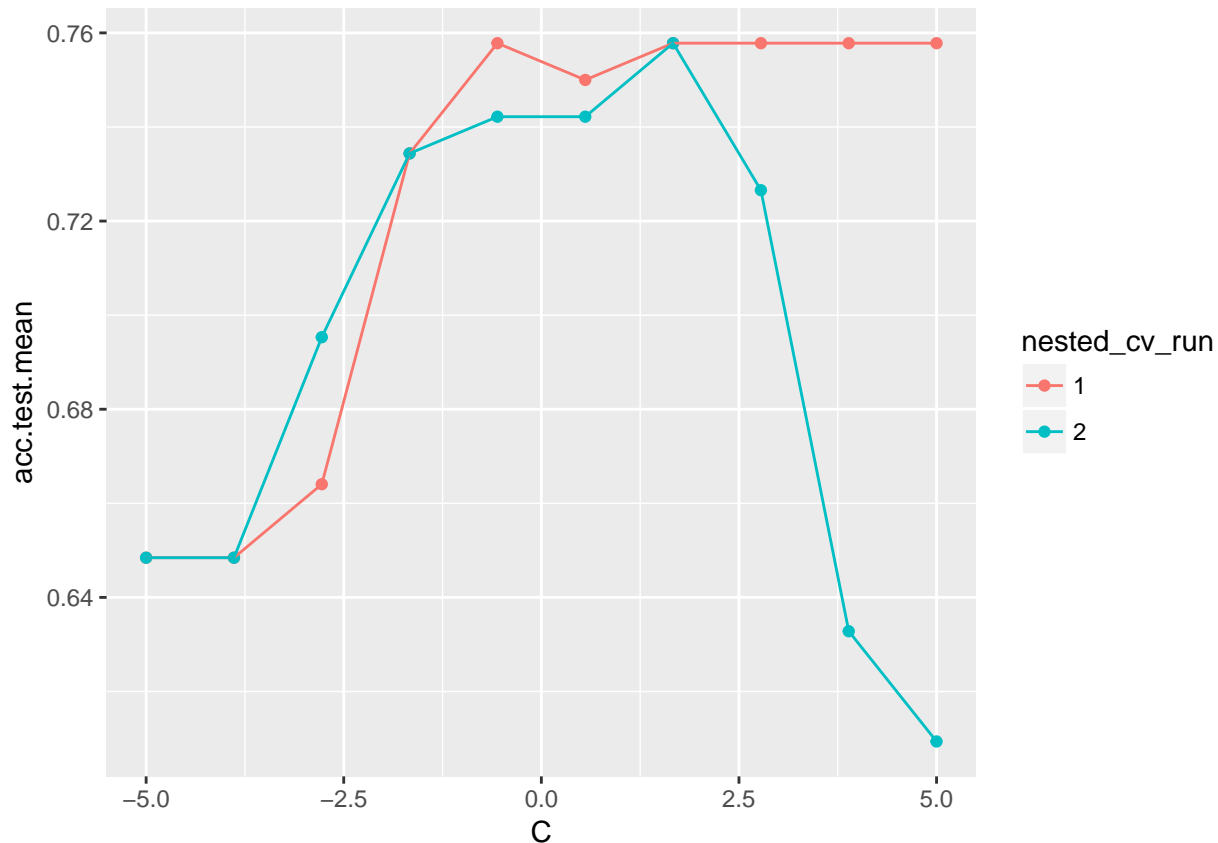
In the case of a learner crash, `mlr` will impute the crash with the worst value graphically and indicate the point. In the example below, we give the `C` parameter negative values, which will result in a learner crash for SVM.

```
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 (`vignette("nested_resampling")`) 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")
```

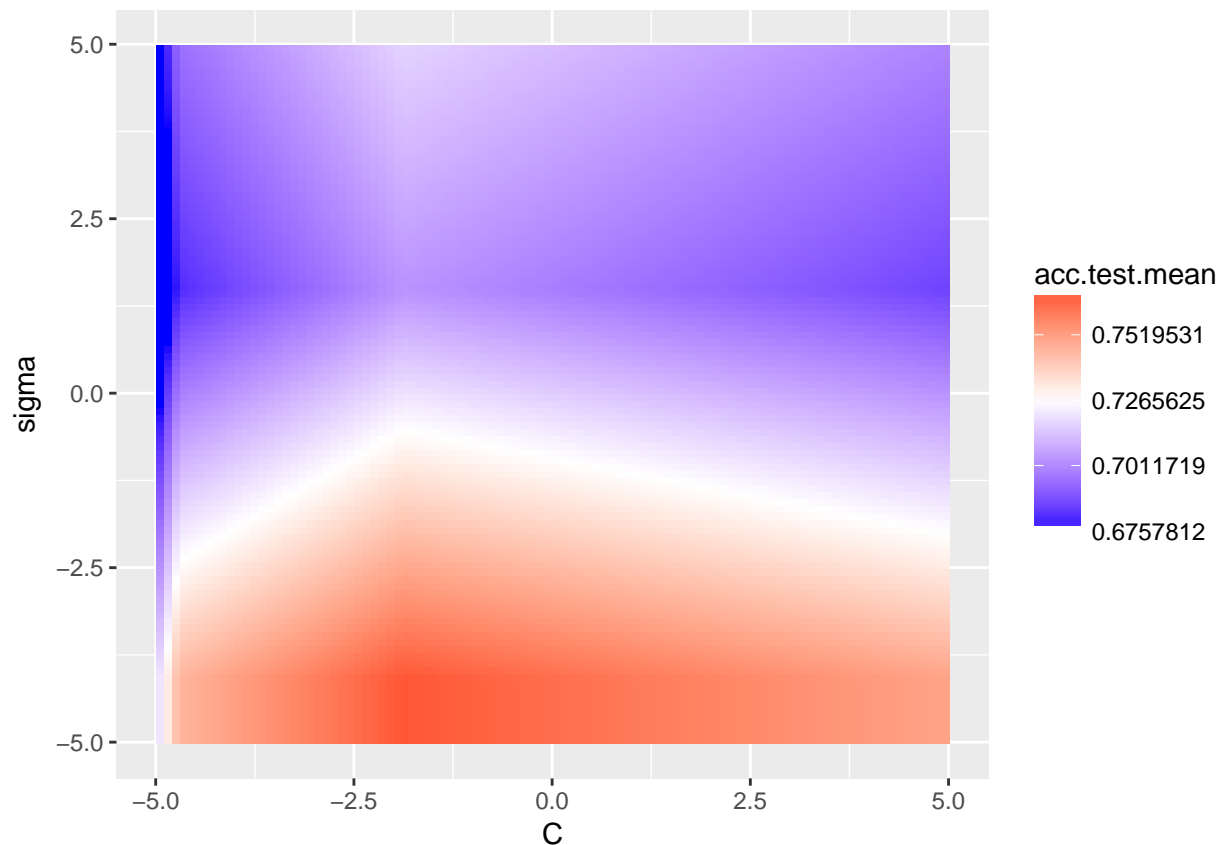



3.16.3 Visualizing the effect of 2 hyperparameters

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.

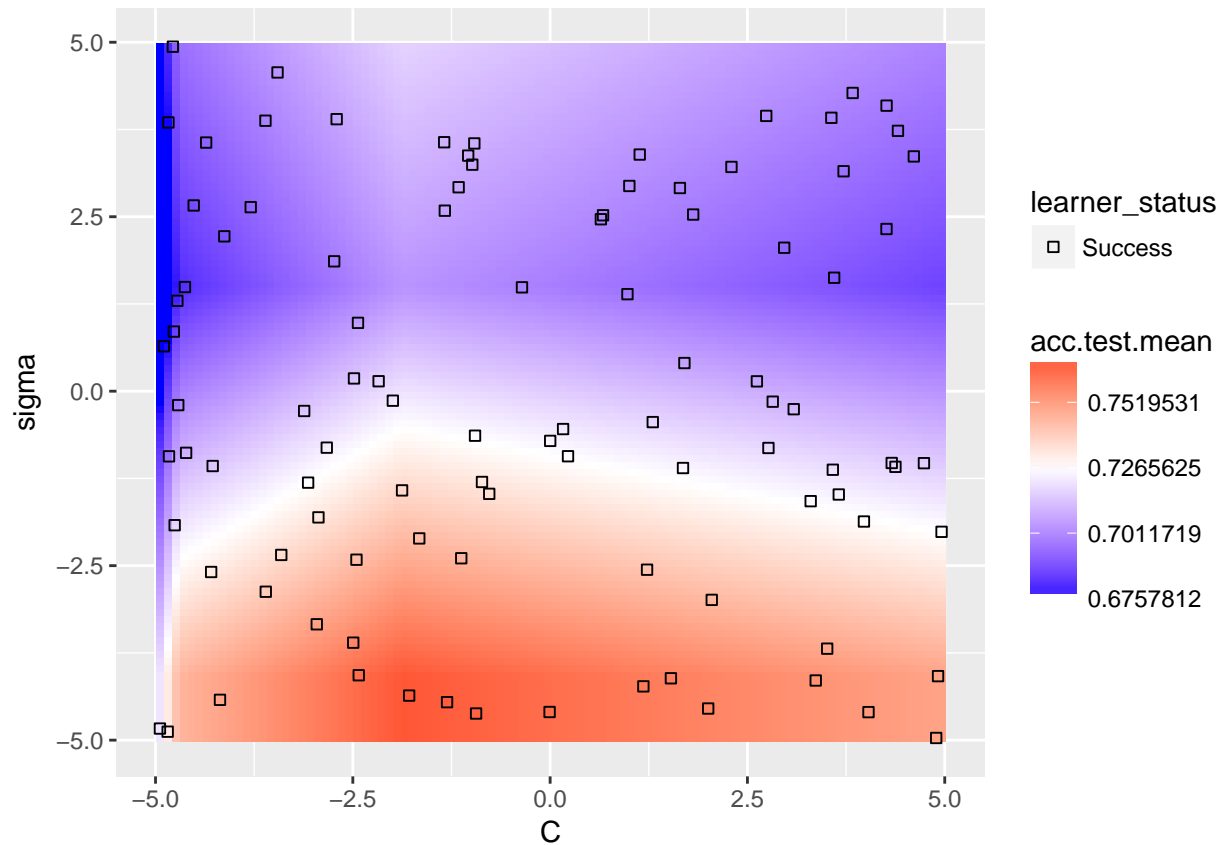
In the example below, we tune the `C` and `sigma` parameters for SVM on the Pima dataset. We use interpolation to produce a regular grid for plotting the heatmap. The `interpolation` argument accepts any regression learner from `mlr` to perform the interpolation. The `z` argument will be used to fill 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)
```



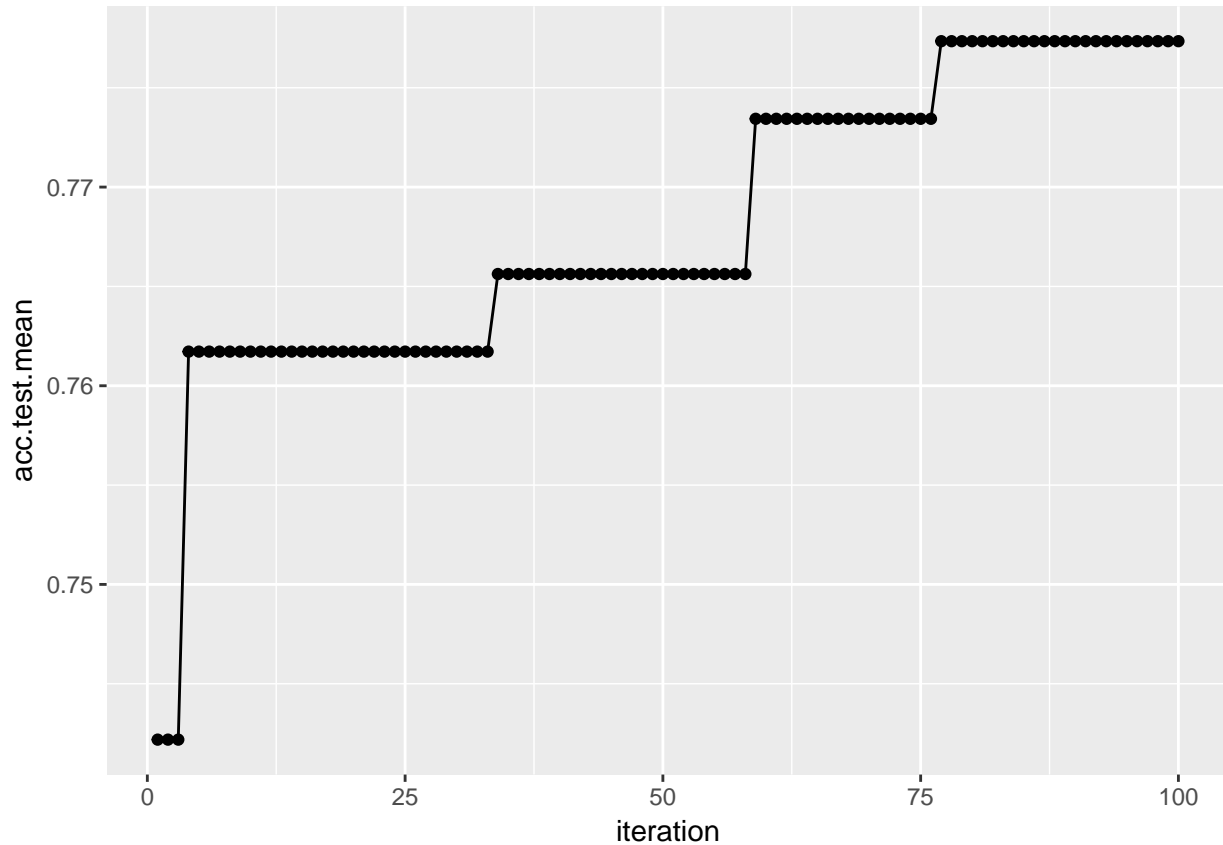
We can use the `show.experiments` argument in order to visualize which points were specifically passed to the learner in the original experiment and which points were interpolated by `mlr`:

```
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)
```



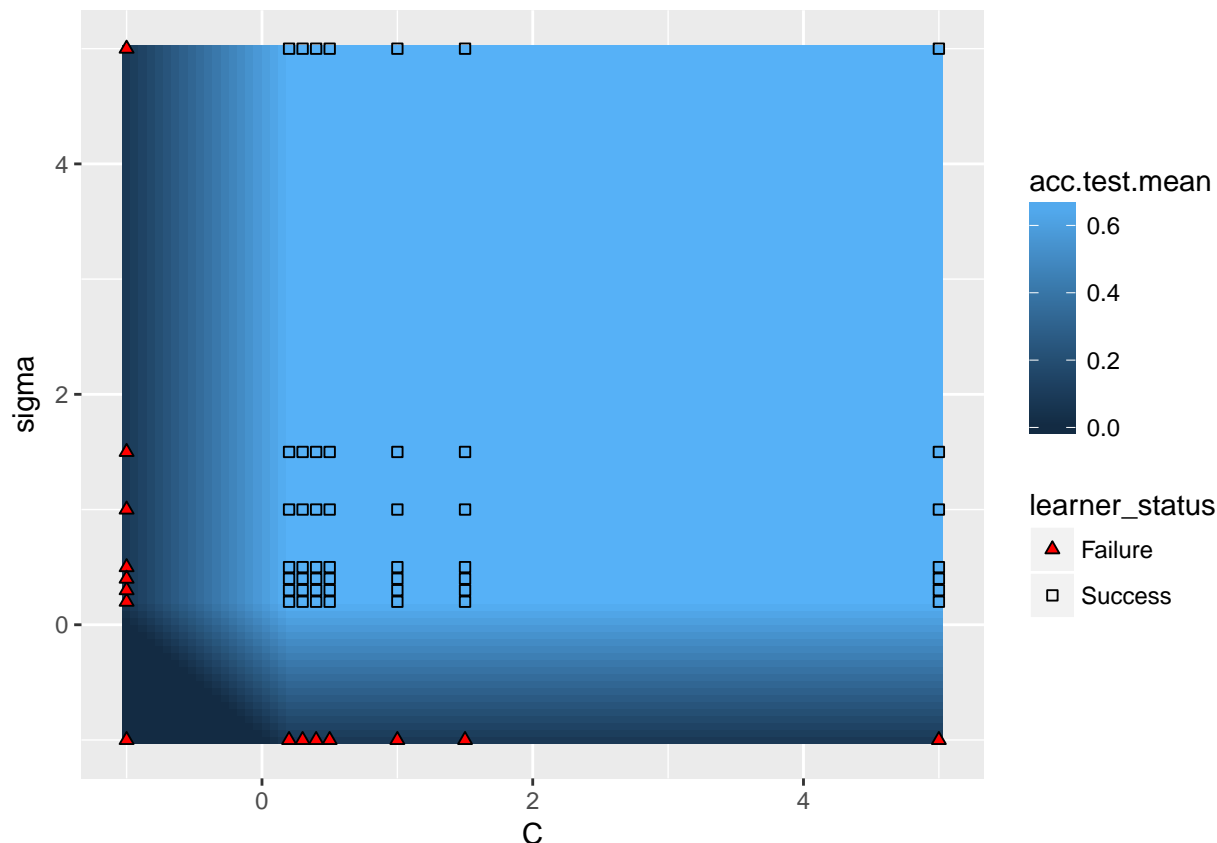
We can also visualize how long the optimizer takes to reach an optima for the same example:

```
plotHyperParsEffect(data, x = "iteration", y = "acc.test.mean",
  plot.type = "line")
```



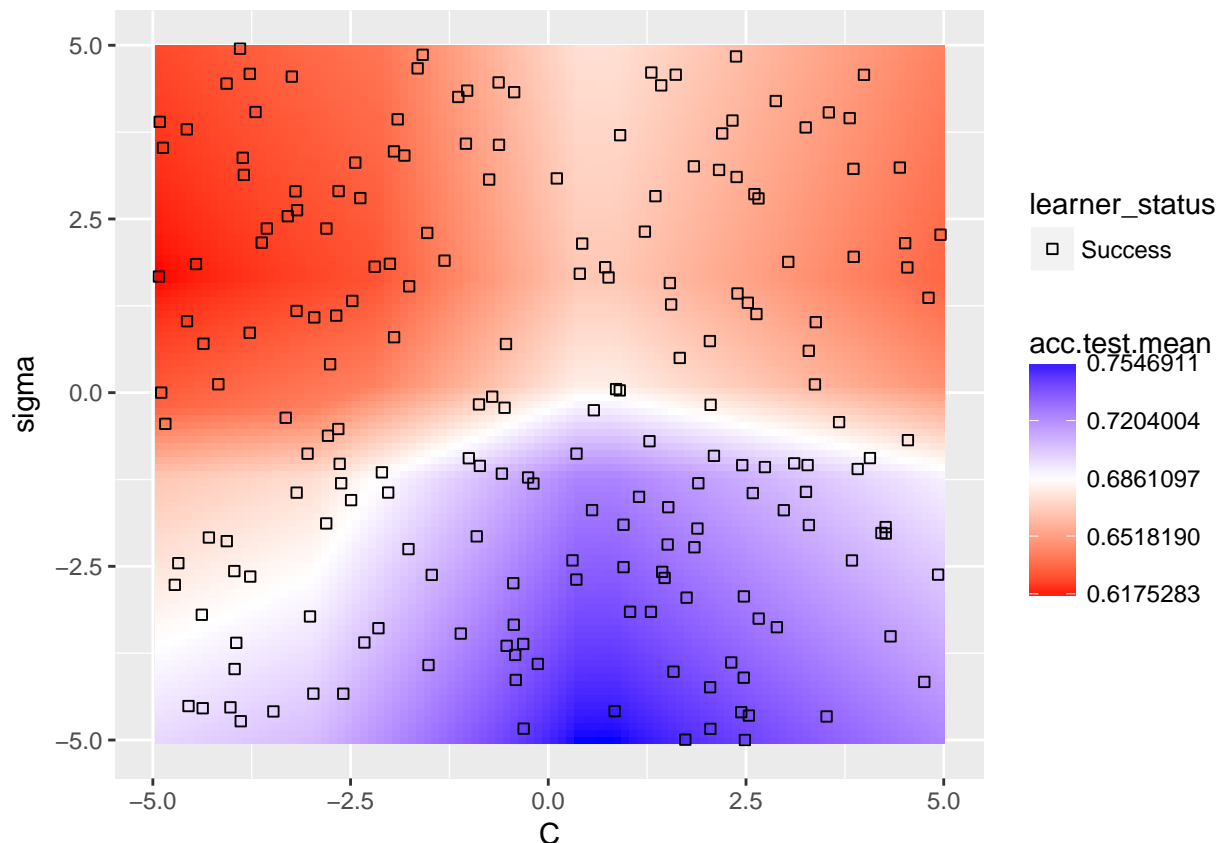
In the case where we are tuning 2 hyperparameters and we have a learner crash, `mlr` will indicate the respective points and impute them with the worst value. In the example below, we tune `C` and `sigma`, forcing `C` to be negative for some instances which will crash SVM. We perform interpolation to 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)
```



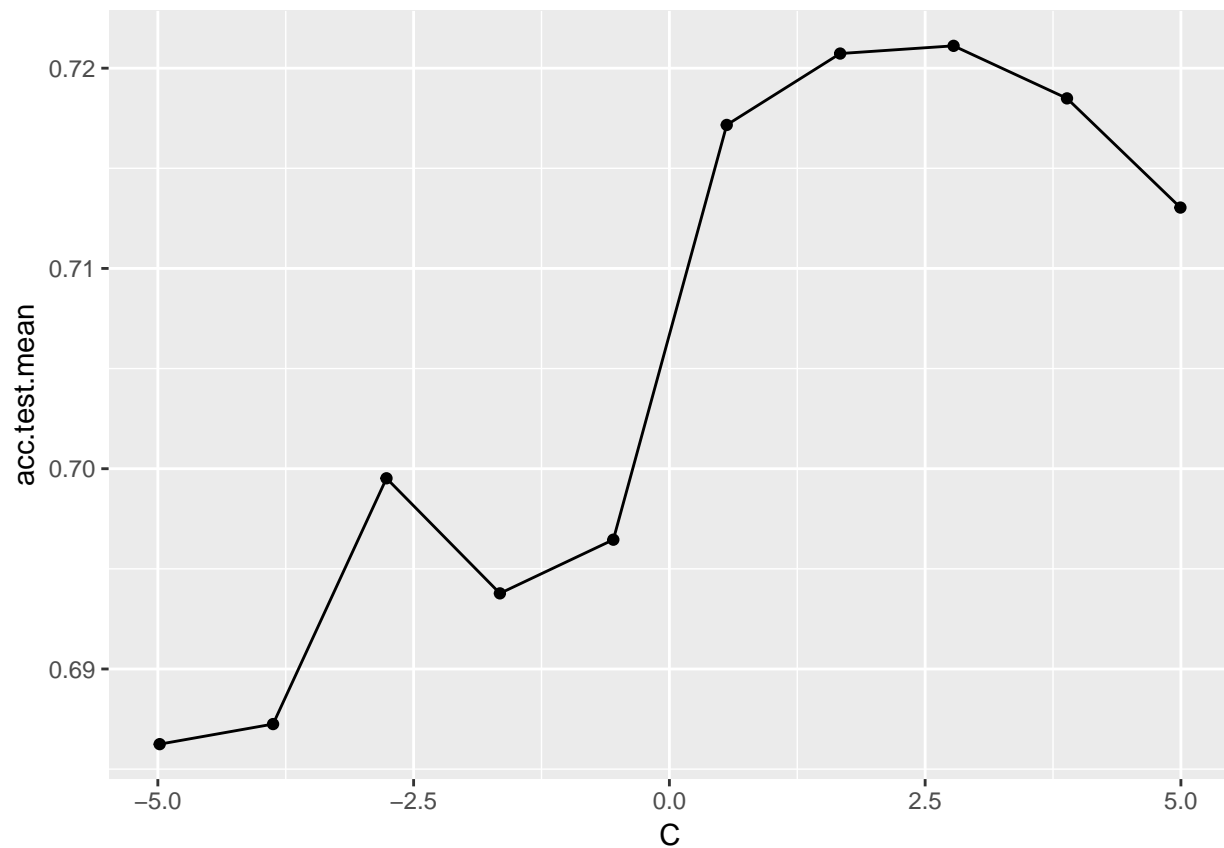
3.16.4 Visualizing the effects of more than 2 hyperparameters

In order to visualize the result when tuning 3 or more hyperparameters simultaneously we can take advantage of partial dependence plots (`vignette("partial_dependence")`) 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)
```

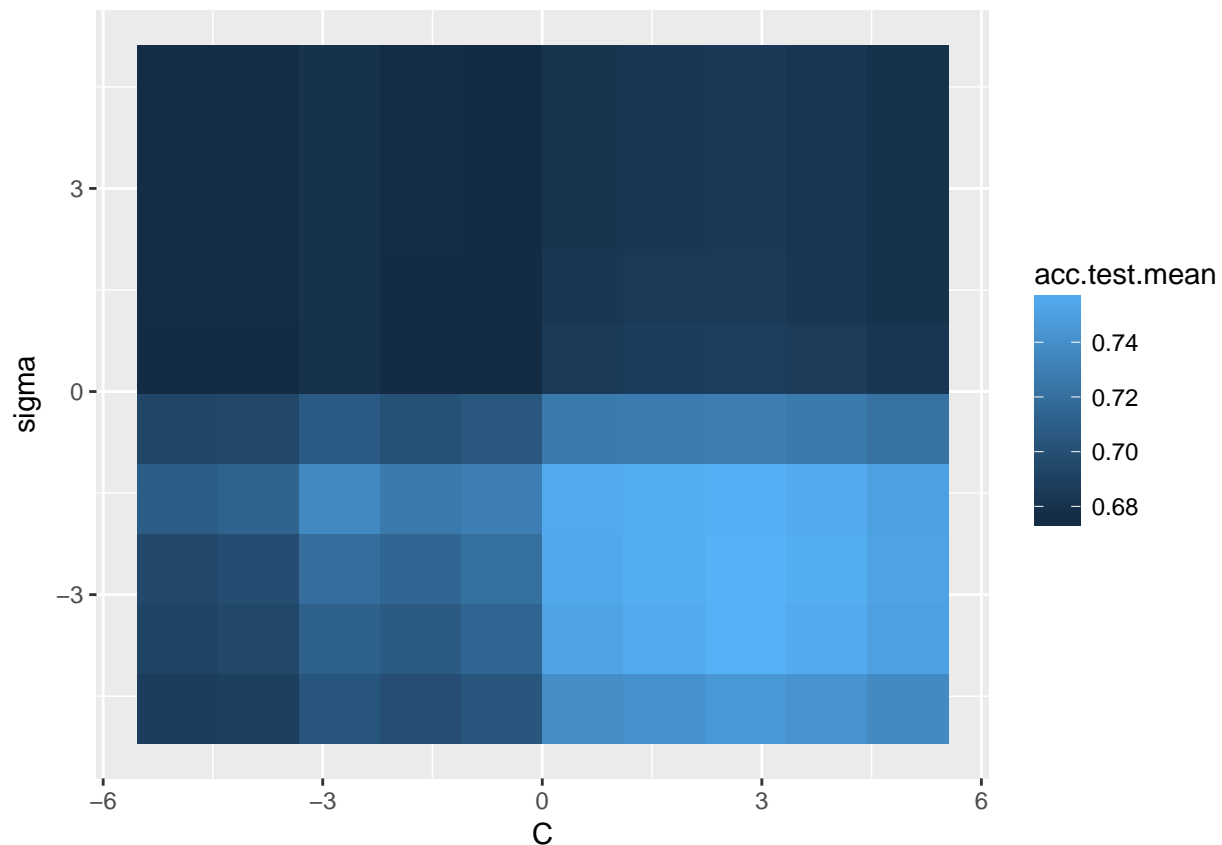
You can generate a plot for a single hyperparameter like `C` as shown below. The `partial.dep.learn` can be any regression Learner (`makeLearner()`) in `mlr` and is used to regress the attained performance values on the values of the 3 hyperparameters visited during tuning. The fitted model serves as 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")]
##           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 0.5390803 0.4609197        R
## 2  2     R 0.5475413 0.4524587        R
## 3  3     R 0.6423390 0.3576610        M
## 4  4     R 0.4588889 0.5411111        R
## 5  5     R 0.4858746 0.5141254        R
## 6  6     R 0.4833310 0.5166690        R
## ... (#rows: 208, #cols: 5)
performance(oob, measures = list(auc, mmce))
##           auc           mmce
## 0.9385158 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.

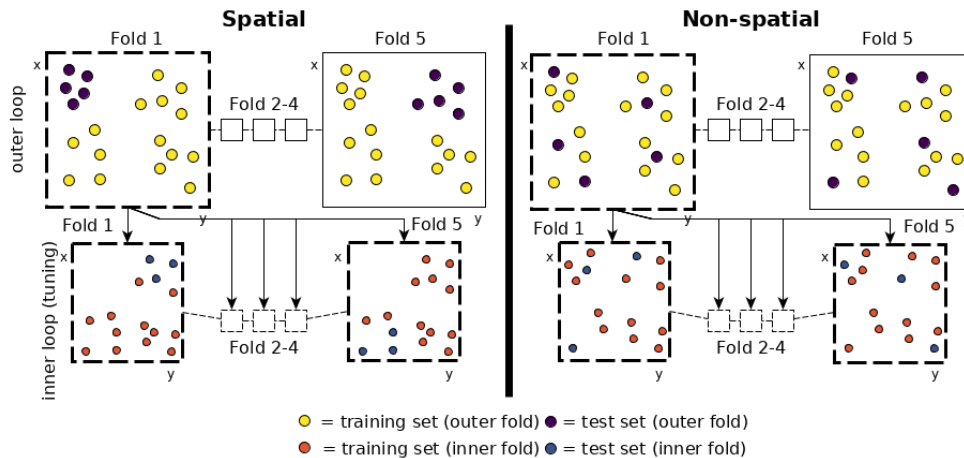


Figure 3: Nested Spatial and Non-Spatial Cross-Validation

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 (`vignette("task")`), you need to explicitly state that the task is `spatial` one by setting `spatial = TRUE`. Next, there need to be two variables named `x` and `y` in your data set that store the coordinate information. If this applies, the coordinates will be used for spatial partitioning if `SpCV` or `SpRepCV` are selected as resampling strategies.

Also, these variables **will be removed** for any `train()` or `predict()` call. This means they will not be used as predictors within the specified learner but only to set up the sampling for the cross-validation task.

Coordinates must be named `x` and `y` to be used for spatial partitioning. If named differently and `spatial = TRUE` was set during task creation, an error will occur.

3.18.3 Examples

The `bc.task.spatial` data set serves as an example data set for spatial modeling tasks in `mlr`. The task (`vignette("task")`) attribute `spatial` is set to `TRUE` to indicate that the data set also stores coordinate information.

In this example, the “Random Forest” algorithm (package `ranger::ranger()`) is used to model a binomial response variable.

For performance assessment, a repeated spatial cross-validation with 5 folds and 10 repetitions is chosen.

3.18.3.1 Spatial Cross-Validation

```
data("bc.task.spatial")
bc.task.spatial
## Supervised task: basque
```

```

## Type: classif
## Target: diplo01
## Observations: 944
## Features:
##   numerics      factors    ordered functionals
##         9          2          0          0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Is spatial: TRUE
## Classes: 2
##   0   1
## 720 224
## Positive class: 1
learner.glm = makeLearner("classif.ranger", predict.type = "prob")

resampling = makeResampleDesc("SpRepCV", fold = 5, reps = 10)

set.seed(123)
out = resample(learner = learner.glm, task = bc.task.spatial,
  resampling = resampling, measures = list(auc))
## Resampling: repeated spatial cross-validation
## Measures:          auc
## [Resample] iter 1:   0.8564829
## [Resample] iter 2:   0.8903922
## [Resample] iter 3:   0.8018739
## [Resample] iter 4:   0.8170660
## [Resample] iter 5:   0.8626639
## [Resample] iter 6:   0.8888889
## [Resample] iter 7:   0.9200000
## [Resample] iter 8:   0.8844538
## [Resample] iter 9:   0.7644215
## [Resample] iter 10:  0.7704265
## [Resample] iter 11:  0.8883220
## [Resample] iter 12:  0.8430926
## [Resample] iter 13:  0.7603609
## [Resample] iter 14:  0.7996886
## [Resample] iter 15:  0.9112150
## [Resample] iter 16:  0.8575808
## [Resample] iter 17:  0.8758170
## [Resample] iter 18:  0.9722531
## [Resample] iter 19:  0.7683578
## [Resample] iter 20:  0.7707363
## [Resample] iter 21:  0.8282783
## [Resample] iter 22:  0.8040078
## [Resample] iter 23:  0.8559476
## [Resample] iter 24:  0.8466709
## [Resample] iter 25:  0.8556985
## [Resample] iter 26:  0.9694784
## [Resample] iter 27:  0.8534002
## [Resample] iter 28:  0.8696655
## [Resample] iter 29:  0.7530708
## [Resample] iter 30:  0.7707363

```

```
## [Resample] iter 31: 0.7859410
## [Resample] iter 32: 0.8797678
## [Resample] iter 33: 0.7657106
## [Resample] iter 34: 0.8925759
## [Resample] iter 35: 0.9153037
## [Resample] iter 36: 0.8602616
## [Resample] iter 37: 0.8804180
## [Resample] iter 38: 0.7662884
## [Resample] iter 39: 0.7716682
## [Resample] iter 40: 0.9719888
## [Resample] iter 41: 0.7636481
## [Resample] iter 42: 0.7815193
## [Resample] iter 43: 0.9147196
## [Resample] iter 44: 0.8892013
## [Resample] iter 45: 0.8720978
## [Resample] iter 46: 0.8436748
## [Resample] iter 47: 0.7144397
## [Resample] iter 48: 0.7679477
## [Resample] iter 49: 0.8233804
## [Resample] iter 50: 0.7238220
##
## Aggregated Result: auc.test.mean=0.8379085
##
mean(out$measures.test$auc)
## [1] 0.8379085
```

We can check for the introduced spatial autocorrelation bias here by performing the same modeling task using a non-spatial partitioning setting. To force non-spatial cross-validation here, variables `x` and `y` need to be removed from the data set because they are not used for partitioning when using `RepCV` and also should not be used as predictors.

Additionally, the `spatial` task attribute needs to be set to `FALSE`. Finally, `RepCV` is chosen instead of `SpRepCV`.

3.18.3.2 Non-Spatial Cross-Validation

```
data("bc.task.spatial")
bc.task.spatial
## Supervised task: basque
## Type: classif
## Target: diplo01
## Observations: 944
## Features:
##      numerics      factors      ordered functionals
##           9           2           0           0
## Missings: FALSE
## Has weights: FALSE
## Has blocking: FALSE
## Is spatial: TRUE
## Classes: 2
##    0    1
## 720 224
## Positive class: 1
bc.task.spatial$task.desc$spatial = FALSE
```

```

bc.task.spatial$env$data$x = NULL
bc.task.spatial$env$data$y = NULL

learner.glm = makeLearner("classif.ranger", predict.type = "prob")

resampling = makeResampleDesc("RepCV", fold = 5, reps = 10)

set.seed(123)
out = resample(learner = learner.glm, task = bc.task.spatial,
  resampling = resampling, measures = list(auc))
## Resampling: repeated cross-validation
## Measures:          auc
## [Resample] iter 1:  0.8967930
## [Resample] iter 2:  0.9045999
## [Resample] iter 3:  0.9294306
## [Resample] iter 4:  0.8802067
## [Resample] iter 5:  0.9297806
## [Resample] iter 6:  0.9167055
## [Resample] iter 7:  0.9145773
## [Resample] iter 8:  0.9190111
## [Resample] iter 9:  0.9230211
## [Resample] iter 10: 0.8920038
## [Resample] iter 11: 0.9174018
## [Resample] iter 12: 0.9216362
## [Resample] iter 13: 0.8649985
## [Resample] iter 14: 0.9400488
## [Resample] iter 15: 0.9335277
## [Resample] iter 16: 0.8901363
## [Resample] iter 17: 0.8874161
## [Resample] iter 18: 0.9116547
## [Resample] iter 19: 0.9056988
## [Resample] iter 20: 0.9353667
## [Resample] iter 21: 0.9007716
## [Resample] iter 22: 0.9178832
## [Resample] iter 23: 0.9260784
## [Resample] iter 24: 0.8679113
## [Resample] iter 25: 0.9532938
## [Resample] iter 26: 0.8807246
## [Resample] iter 27: 0.9007646
## [Resample] iter 28: 0.9112245
## [Resample] iter 29: 0.9021704
## [Resample] iter 30: 0.9442953
## [Resample] iter 31: 0.9243403
## [Resample] iter 32: 0.9407455
## [Resample] iter 33: 0.8723823
## [Resample] iter 34: 0.9146044
## [Resample] iter 35: 0.8980796
## [Resample] iter 36: 0.9012854
## [Resample] iter 37: 0.9103448
## [Resample] iter 38: 0.9683020
## [Resample] iter 39: 0.9169096
## [Resample] iter 40: 0.8891844
## [Resample] iter 41: 0.8992375

```

```
## [Resample] iter 42: 0.8888889
## [Resample] iter 43: 0.9168440
## [Resample] iter 44: 0.9027697
## [Resample] iter 45: 0.9038690
## [Resample] iter 46: 0.9262346
## [Resample] iter 47: 0.8470183
## [Resample] iter 48: 0.8931188
## [Resample] iter 49: 0.9615858
## [Resample] iter 50: 0.9296015
##
## Aggregated Result: auc.test.mean=0.9104896
##
mean(out$measures.test$auc)
## [1] 0.9104896
```

The introduced bias (caused by spatial autocorrelation) in performance in this example is around 0.07 AUROC.

3.18.4 Notes

- Usually, coordinates are not used as predictors in spatial modeling. If you insist on using them and also want to perform spatial cross-validation, add them to the data set with a different name than `x` or `y`, e.g. `x1` and `y1`. That way they will be treated as normal predictors.
- 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()`), `makeRLearnerRegr` (`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`) (`vignette("cost_sensitive_classif")`) with example-specific costs. This type of learning task is currently exclusively handled through wrappers (`vignette("wrapper")`) 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 (`vignette("tune")`)).

Next, we add information on the properties of the learner (see also the section on learners (`vignette("learner")`)). 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 from the `[%earth]` package.

```

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 (`vignette("measures")`) (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 (`vignette("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_c
```

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 (`vignette("measure")`) 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` (`vignette("measure")`) (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: 0x12588c48>
## <environment: namespace:mlr>
measureMSE
## function (truth, response)
## {
##     mean((response - truth)^2)
## }
## <bytecode: 0x127c8648>
## <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 (`vignette("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 (`vignette("tune")`) or feature selection (`vignette("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: 0xb3133f0>
## <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 (`vignette("resample")`) 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` (`vignette("measure")`). 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 (`vignette("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)

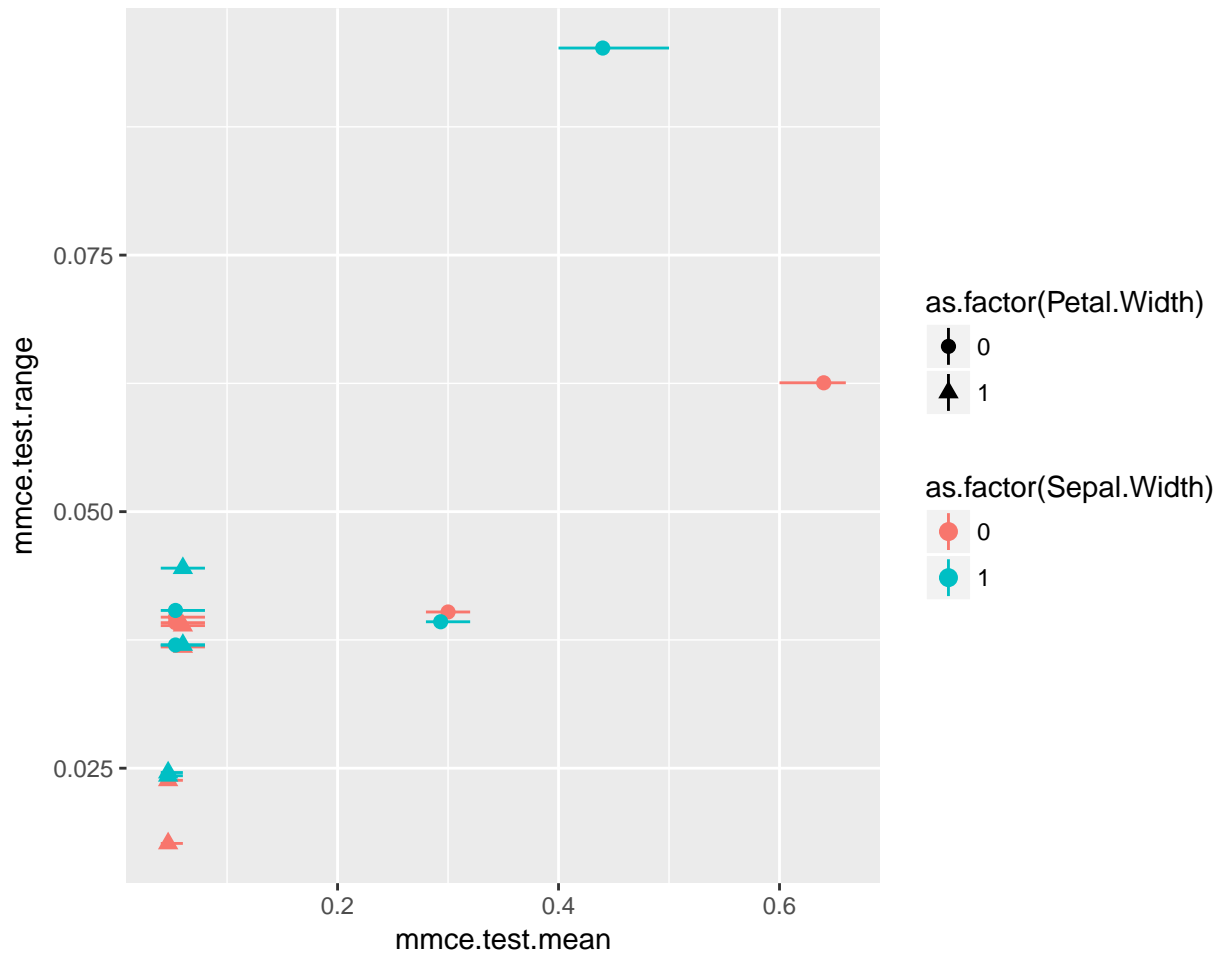
```

```

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      0.64000000
## 2           1           0           0           0      0.30000000
## 3           0           1           0           0      0.44000000
## 4           0           0           1           0      0.05333333
## 5           0           0           0           1      0.04666667
## 6           1           1           0           0      0.29333333
##   mmce.test.range mmce.test.min mmce.test.max
## 1           0.06           0.60           0.66
## 2           0.04           0.28           0.32
## 3           0.10           0.40           0.50
## 4           0.04           0.04           0.08
## 5           0.02           0.04           0.06
## 6           0.04           0.28           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 (`vignette("filter_methods")`) 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: 0x185297d0>
## <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 resources 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 `NA`s 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

```

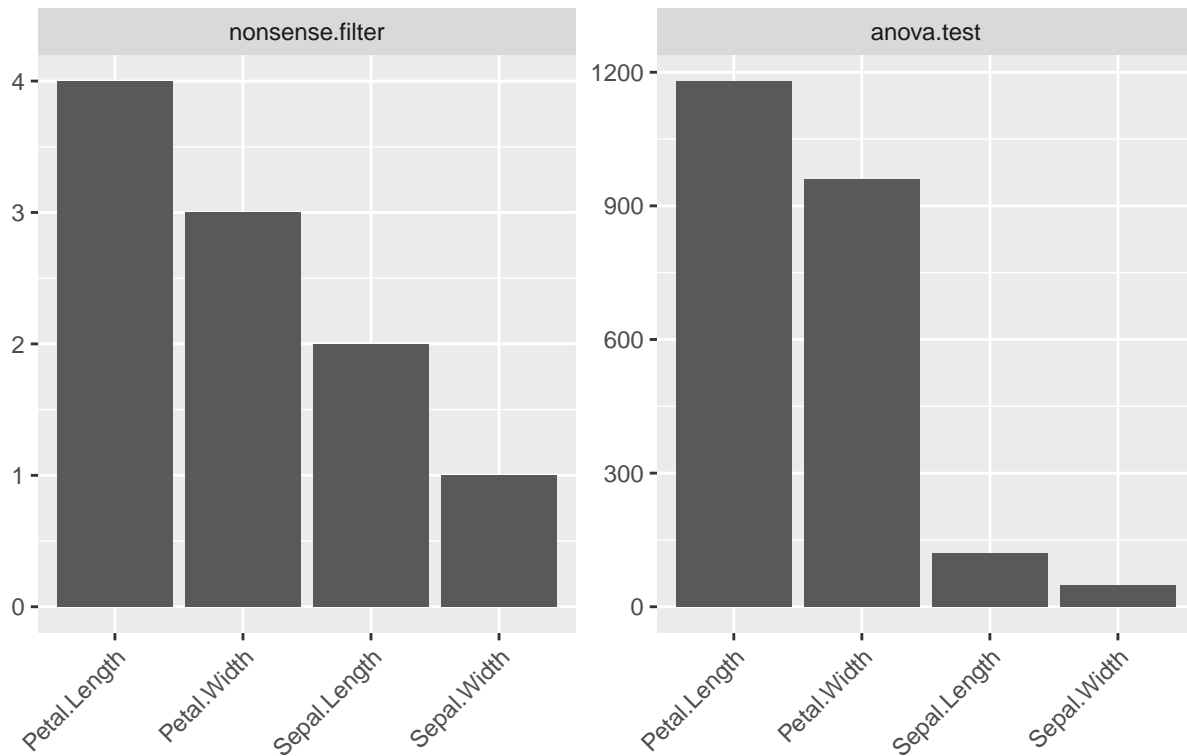
You can use it like any other filter method already integrated in `mlr` (i.e., via the `method` argument of `generateFilterValuesData()` or the `fw.method` argument of `makeFilterWrapper()`; see also the page on feature selection (`vignette("feature_selection")`).

```

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_example (4 features)



```
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
## Is spatial: 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
classif	bc.task
	bc.task.spatial
	gunpoint.task
	iris.task
	phoneme.task
	pid.task
	sonar.task
cluster	agri.task
	mtcars.task
costsens	costiris.task
multilabel	yeast.task
regr	bh.task
	fuelsubset.task
surv	lung.task
	wpbc.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 (84)

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

classif.ada *ada* ada Boosting

classif.adaboostm1 *adaboostm1* ada Boosting M1

classif.bartMachine *bartmachine* Bayesian Additive Regression Trees

classif.binomial *binomial* Binomial Regression

classif.blackboost *blackboost* Gradient Boosting With Regression Trees

classif.boosting *adabag* Adabag Boosting

Class / Short Name / Name

classif.bst *bst* Gradient Boosting
classif.C50 *C50* C50
classif.cforest *cforest* Random forest based on conditional inference trees
classif.clusterSVM *clusterSVM* Clustered Support Vector Machines
classif.ctree *ctree* Conditional Inference Trees
classif.cvglmnet *cvglmnet* GLM with Lasso or Elasticnet Regularization (Cross Validated Lambda)
classif.dbnDNN *dbn.dnn* Deep neural network with weights initialized by DBN
classif.dcSVM *dcSVM* Divided-Conquer Support Vector Machines
classif.earth *fda* Flexible Discriminant Analysis
classif.evtree *evtrees* Evolutionary learning of globally optimal trees
classif.extraTrees *extraTrees* Extremely Randomized Trees
classif.fdausc.glm *fdausc.glm* Generalized Linear Models classification on FDA

classif.featureless *featureless* Featureless classifier
classif.fnn *fnn* Fast k-Nearest Neighbour
classif.gamboost *gamboost* Gradient boosting with smooth components
classif.gaterSVM *gaterSVM* Mixture of SVMs with Neural Network Gater Function
classif.gausspr *gausspr* Gaussian Processes
classif.gbm *gbm* Gradient Boosting Machine
classif.geoDA *geoda* Geometric Predictive Discriminant Analysis
classif.glmboost *glmboost* Boosting for GLMs
classif.glmnet *glmnet* GLM with Lasso or Elasticnet Regularization
classif.h2o.deeplearning *h2o.dl* h2o.deeplearning
classif.h2o.gbm *h2o.gbm* h2o.gbm
classif.h2o.glm *h2o.glm* h2o.glm
classif.h2o.randomForest *h2o.rf* h2o.randomForest
classif.IBk *ibk* k-Nearest Neighbours
classif.J48 *j48* J48 Decision Trees
classif.JRip *jrip* Propositional Rule Learner
classif.kknn *kknn* k-Nearest Neighbor
classif.knn *knn* k-Nearest Neighbor
classif.ksvm *ksvm* Support Vector Machines
classif.lda *lda* Linear Discriminant Analysis
classif.LiblineaRL1L2SVC *liblinl1l2svc* L1-Regularized L2-Loss Support Vector Classification
classif.LiblineaRL1LogReg *liblinl1logreg* L1-Regularized Logistic Regression
classif.LiblineaRL2L1SVC *liblinl2l1svc* L2-Regularized L1-Loss Support Vector Classification
classif.LiblineaRL2LogReg *liblinl2logreg* L2-Regularized Logistic Regression
classif.LiblineaRL2SVC *liblinl2svc* L2-Regularized L2-Loss Support Vector Classification
classif.LiblineaRMultiClassSVC *liblinmulticlasssvc* Support Vector Classification by Crammer and Singer
classif.linDA *linda* Linear Discriminant Analysis
classif.logreg *logreg* Logistic Regression
classif.lqa *lqa* Fitting penalized Generalized Linear Models with the LQA algorithm
classif.lssvm *lssvm* Least Squares Support Vector Machine
classif.lvq1 *lvq1* Learning Vector Quantization
classif.mda *mda* Mixture Discriminant Analysis
classif.mlp *mlp* Multi-Layer Perceptron
classif.multinom *multinom* Multinomial Regression
classif.naiveBayes *nbayes* Naive Bayes
classif.neuralnet *neuralnet* Neural Network from neuralnet
classif.nnet *nnet* Neural Network
classif.nnTrain *nn.train* Training Neural Network by Backpropagation
classif.nodeHarvest *nodeHarvest* Node Harvest

Class / Short Name / Name

classif.OneR *oner* 1-R Classifier
classif.pamr *pamr* Nearest shrunken centroid
classif.PART *part* PART Decision Lists
classif.penalized *penalized* Penalized Logistic Regression
classif.plr *plr* Logistic Regression with a L2 Penalty
classif.plsdaCaret *plsdacaret* Partial Least Squares (PLS) Discriminant Analysis
classif.probit *probit* Probit Regression
classif.qda *qda* Quadratic Discriminant Analysis
classif.quaDA *quada* Quadratic Discriminant Analysis
classif.randomForest *rf* Random Forest
classif.randomForestSRC *rfsrc* Random Forest
classif.ranger *ranger* Random Forests
classif.rda *rda* Regularized Discriminant Analysis
classif.rFerns *rFerns* Random ferns
classif.rknn *rknn* Random k-Nearest-Neighbors
classif.rotationForest *rotationForest* Rotation Forest
classif.rpart *rpart* Decision Tree
classif.RRF *RRF* Regularized Random Forests
classif.rrllda *rrlda* Robust Regularized Linear Discriminant Analysis
classif.saeDNN *sae.dnn* Deep neural network with weights initialized by Stacked AutoEncoder
classif.sda *sda* Shrinkage Discriminant Analysis
classif.sparseLDA *sparseLDA* Sparse Discriminant Analysis
classif.svm *svm* Support Vector Machines (libsvm)
classif.xgboost *xgboost* eXtreme Gradient Boosting

5.2.0.2 Regression (61)

Additional learner properties:

- *se*: Standard errors can be predicted.

Class / Short Name / Name

regr.bartMachine *bartmachine* Bayesian Additive Regression Trees
regr.bcart *bcart* Bayesian CART
regr.bgp *bgp* Bayesian Gaussian Process
regr.bgppllm *bgppllm* Bayesian Gaussian Process with jumps to the Limiting Linear Model
regr.blackboost *blackboost* Gradient Boosting with Regression Trees
regr.blm *blm* Bayesian Linear Model
regr.brnn *brnn* Bayesian regularization for feed-forward neural networks
regr.bst *bst* Gradient Boosting
regr.btgp *btgp* Bayesian Treed Gaussian Process
regr.btgppllm *btgppllm* Bayesian Treed Gaussian Process with jumps to the Limiting Linear Model
regr.btlm *btlm* Bayesian Treed Linear Model
regr.cforest *cforest* Random Forest Based on Conditional Inference Trees
regr.crs *crs* Regression Splines
regr.ctree *ctree* Conditional Inference Trees
regr.cubist *cubist* Cubist
regr.cvglmnet *cvglmnet* GLM with Lasso or Elasticnet Regularization (Cross Validated Lambda)
regr.earth *earth* Multivariate Adaptive Regression Splines
regr.elmNN *elmNN* Extreme Learning Machine for Single Hidden Layer Feedforward Neural Networks

Class / Short Name / Name

regr.evtree *evtree* Evolutionary learning of globally optimal trees
regr.extraTrees *extraTrees* Extremely Randomized Trees
regr.FDboost *FDboost* Functional linear array regression boosting
regr.featureless *featureless* Featureless regression
regr.fnn *fnn* Fast k-Nearest Neighbor
regr.frbs *frbs* Fuzzy Rule-based Systems
regr.gamboost *gamboost* Gradient Boosting with Smooth Components
regr.gausspr *gausspr* Gaussian Processes
regr.gbm *gbm* Gradient Boosting Machine
regr.glm *glm* Generalized Linear Regression
regr.glmboost *glmboost* Boosting for GLMs
regr.glmnet *glmnet* GLM with Lasso or Elasticnet Regularization
regr.GPfit *GPfit* Gaussian Process
regr.h2o.deeplearning *h2o.dl* h2o.deeplearning
regr.h2o.gbm *h2o.gbm* h2o.gbm
regr.h2o.glm *h2o.glm* h2o.glm
regr.h2o.randomForest *h2o.rf* h2o.randomForest
regr.IBk *ibk* K-Nearest Neighbours
regr.kknn *kknn* K-Nearest-Neighbor regression
regr.km *km* Kriging
regr.ksvm *ksvm* Support Vector Machines
regr.laGP *laGP* Local Approximate Gaussian Process
regr.LiblineaRL2L1SVR *liblinl2l1svr* L2-Regularized L1-Loss Support Vector Regression
regr.LiblineaRL2L2SVR *liblinl2l2svr* L2-Regularized L2-Loss Support Vector Regression
regr.lm *lm* Simple Linear Regression
regr.mars *mars* Multivariate Adaptive Regression Splines
regr.mob *mob* Model-based Recursive Partitioning Yielding a Tree with Fitted Models Associated with each Terminal Node
regr.nnet *nnet* Neural Network
regr.nodeHarvest *nodeHarvest* Node Harvest
regr.pcr *pcr* Principal Component Regression
regr.penalized *penalized* Penalized Regression
regr.plsr *plsr* Partial Least Squares Regression
regr.randomForest *rf* Random Forest
regr.randomForestSRC *rfsrc* Random Forest
regr.ranger *ranger* Random Forests
regr.rknn *rknn* Random k-Nearest-Neighbors
regr.rpart *rpart* Decision Tree
regr.RRF *RRF* Regularized Random Forests
regr.rsm *rsm* Response Surface Regression
regr.rvm *rvm* Relevance Vector Machine
regr.slim *slim* Sparse Linear Regression using Nonsmooth Loss Functions and L1 Regularization
regr.svm *svm* Support Vector Machines (libsvm)
regr.xgboost *xgboost* eXtreme Gradient Boosting

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

surv.cforest *crf* Random Forest based on Conditional Inference Trees
surv.CoxBoost *coxboost* Cox Proportional Hazards Model with Componentwise Likelihood based Boosting
surv.coxph *coxph* Cox Proportional Hazard Model
surv.cv.CoxBoost *cv.CoxBoost* Cox Proportional Hazards Model with Componentwise Likelihood based Boosting, tuned
surv.cvglmnet *cvglmnet* GLM with Regularization (Cross Validated Lambda)
surv.gamboost *gamboost* Gradient boosting with smooth components
surv.gbm *gbm* Gradient Boosting Machine
surv.glmboost *glmboost* Gradient Boosting with Componentwise Linear Models
surv.glmnet *glmnet* GLM with Regularization
surv.randomForestSRC *rfsrc* Random Forest
surv.ranger *ranger* Random Forests
surv.rpart *rpart* Survival Tree

5.2.0.4 Cluster analysis (9)

Additional learner properties:

- *prob*: Probabilities can be predicted.

Class / Short Name / Name

cluster.cmeans <i>cmeans</i> Fuzzy C-Means Clustering	Package: e1071cluster
cluster.Cobweb <i>cobweb</i> Cobweb Clustering Algorithm	Package: RWeka
cluster.dbscan <i>dbscan</i> DBScan Clustering	Package: fpc
cluster.EM <i>em</i> Expectation-Maximization Clustering	Package: RWeka
cluster.FarthestFirst <i>farthestfirst</i> FarthestFirst Clustering Algorithm	Package: RWeka
cluster.kkmeans <i>kkmeans</i> Kernel K-Means	Package: kernlab
cluster.kmeans <i>kmeans</i> K-Means	Package: statscluster
cluster.SimpleKMeans <i>simplekmeans</i> K-Means Clustering	Package: RWeka
cluster.XMeans <i>xmeans</i> XMeans (k-means with automatic determination of k)	Package: RWeka

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 (`vignette("cost_sensitive_classif")`) and the documentation of `makeCostSensClassifWrapper()`, `makeCostSensRegrWrapper()` and `makeCostSensWeightedPairsWrapper()` for details.

5.2.0.6 Multilabel classification (3)

Class / Short Name / Name

multilabel.cforest <i>cforest</i> Random forest based on conditional inference trees	Package: par
multilabel.randomForestSRC <i>rfsrc</i> Random Forest	Package: randomForestSRC
multilabel.rFerns <i>rFerns</i> Random ferns	Package: rFerns

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 (`vignette("multilabel")`) 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 (`vignette("create_measure")`).

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

acc Accuracy
auc Area under the curve
bac Balanced accuracy
ber Balanced error rate
brier Brier score
brier.scaled Brier scaled
f1 F1 measure
fdr False discovery rate
fn False negatives
fnr False negative rate
fp False positives
fpr False positive rate
gmean G-mean
gpr Geometric mean of precision and recall.
kappa Cohen's kappa
logloss Logarithmic loss
lsr Logarithmic Scoring Rule
mcc Matthews correlation coefficient
mmce Mean misclassification error
multiclass.au1p Weighted average 1 vs. 1 multiclass AUC
multiclass.au1u Average 1 vs. 1 multiclass AUC
multiclass.aunp Weighted average 1 vs. rest multiclass AUC
multiclass.aunu Average 1 vs. rest multiclass AUC

ID / Name

multiclass.brier Multiclass Brier score
npv Negative predictive value
ppv Positive predictive value
qsr Quadratic Scoring Rule
ssr Spherical Scoring Rule
tn True negatives
tnr True negative rate
tp True positives
tpr True positive rate
wkappa Mean quadratic weighted kappa

5.3.0.2 Regression

ID / Name

arsq Adjusted coefficient of determination
expvar Explained variance
kendalltau Kendall's tau
mae Mean of absolute errors
mape Mean absolute percentage error
medae Median of absolute errors
medse Median of squared errors
mse Mean of squared errors
msle Mean squared logarithmic error
rae Relative absolute error
rmse Root mean squared error
rmsle Root mean squared logarithmic error
rrse Root relative squared error
rsq Coefficient of determination
sae Sum of absolute errors
spearmanrho Spearman's rho
sse Sum of squared errors

5.3.0.3 Survival analysis

ID / Name

cindex Harrell's Concordance index
cindex.uno Uno's Concordance index
iauc.uno Uno's estimator of cumulative AUC for right censored time-to-event data
ibrier Integrated brier score using Kaplan-Meier estimator for weighting

5.3.0.4 Cluster analysis

ID / Name

db Davies-Bouldin cluster separation measure
dunn Dunn index
G1 Calinski-Harabasz pseudo F statistic
G2 Baker and Hubert adaptation of Goodman-Kruskal's gamma statistic

ID / Name
silhouette Rousseeuw's silhouette internal cluster quality index

5.3.0.5 Cost-sensitive classification

ID / Name
mcp Misclassification penalty
meancosts Mean costs of the predicted choices

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 (`vignette("cost_sensitive_classif")`) and also the page on custom performance measures (`vignette("create_measure")`).

5.3.0.6 Multilabel classification

ID / Name
multilabel.acc Accuracy (multilabel)
multilabel.f1 F1 measure (multilabel)
multilabel.hamloss Hamming loss
multilabel.ppv Positive predictive value (multilabel)
multilabel.subset01 Subset-0-1 loss
multilabel.tpr TPR (multilabel)

5.3.0.7 General performance measures

ID / Name
featperc Percentage of original features used for model
timeboth timetrain + timepredict
timepredict Time of predicting test set
timetrain Time of fitting the model

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
anova.test	Rfast
auc	
carscore	care

Method	Package
cforest.importance	party
chi.squared	FSelector
gain.ratio	FSelector
information.gain	FSelector
kruskal.test	
linear.correlation	Rfast
mrmr	mRMRe
oneR	FSelector
permutation.importance	
randomForest.importance	randomForest
randomForestSRC.rfsrc	randomForestSRC
randomForestSRC.var.select	randomForestSRC
rank.correlation	Rfast
relief	FSelector
symmetrical.uncertainty	FSelector
univariate.model.score	
variance	

5.4.2 Deprecated methods

Method	Package	Description
rf.importance	randomForestSRC	Importance of
rf.min.depth	randomForestSRC	Minimal depth
univariate		Resamples an