Flexible and Robust Machine Learning Using mlr3 in R

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Welcome to the Machine Learning in R universe. This is the electronic version of the upcoming book *Flexible and Robust Machine Learning Using mlr3 in R*. This book will teach you about the mlr3 universe of packages, from some machine learning methodology to implementations of complex algorithmic pipelines. We will cover how to use the mlr3 family of packages for data processing, fitting and training of machine learning models, tuning and hyperparameter optimization, feature selection, pipelines, data preprocessing, and model interpretability. In addition we will look at how our interface works beyond classification and regression settings to other fields including survival analysis, clustering, and more. Finally we will demonstrate how you can contribute to our universe by creating packages, learners, measures, pipelines, and other features.

We hope you enjoy reading our book and always welcome comments and feedback. If you notice any mistakes in the book we would appreciate if you could open an issue in the mlr3book issue tracker.

Preface

Welcome to the Machine Learning in R universe (mlr3verse)! Before we begin, make sure you have installed `mlr3` if you want to follow along. We recommend installing the complete `mlr3verse`, which will install all of the important packages.

```
install.packages("mlr3verse")
```

Or you can install just the base package:

```
install.packages("mlr3")
```

In our first example, we will show you some of the most basic functionality – training a model and making predictions.

```
library(mlr3)
task = tsk("penguins")
split = partition(task)
learner = lrn("classif.rpart")

learner$train(task, row_ids = split$train)
learner$model
```

```
n= 231

node), split, n, loss, yval, (yprob)
      * denotes terminal node

1) root 231 129 Adelie (0.441558442 0.199134199 0.359307359)
  2) flipper_length< 207.5 145  44 Adelie (0.696551724 0.296551724 0.006896552)
    4) bill_length< 44.65 100   2 Adelie (0.980000000 0.020000000 0.000000000) *
    5) bill_length>=44.65 45   4 Chinstrap (0.066666667 0.911111111 0.022222222) *
  3) flipper_length>=207.5 86   4 Gentoo (0.011627907 0.034883721 0.953488372) *
```

```
predictions = learner$predict(task, row_ids = split$test)
predictions
```

```
<PredictionClassif> for 113 observations:
    row_ids     truth  response
          3    Adelie    Adelie
```

```
          4    Adelie    Adelie
          5    Adelie    Adelie
---
        341 Chinstrap    Adelie
        343 Chinstrap    Gentoo
        344 Chinstrap Chinstrap
```

```
predictions$score(msr("classif.acc"))
```

```
classif.acc
  0.9380531
```

In this example, we trained a decision tree on a subset of the `penguins` dataset, made predictions on the rest of the data and then evaluated these with the accuracy measure. In Chapter 2 we will break this down in more detail.

`mlr3` makes training and predicting easy, but it also allows us to perform very complex operations in just a few lines of code:

```
library(mlr3verse)
library(mlr3pipelines)
library(mlr3benchmark)

tasks = tsks(c("breast_cancer", "sonar"))
tuned_rf = auto_tuner(
    tnr("grid_search", resolution = 5),
    lrn("classif.ranger", num.trees = to_tune(200, 500)),
    rsmp("holdout")
)
tuned_rf = pipeline_robustify(NULL, tuned_rf, TRUE) %>>%
    po("learner", tuned_rf)
stack_lrn = ppl(
    "stacking",
    base_learners = lrns(c("classif.rpart", "classif.kknn")),
    lrn("classif.log_reg"))
stack_lrn = pipeline_robustify(NULL, stack_lrn, TRUE) %>>%
    po("learner", stack_lrn)

learners = c(tuned_rf, stack_lrn)
bm = benchmark(benchmark_grid(tasks, learners, rsmp("holdout")))
```

```
bma = bm$aggregate(msr("classif.acc"))[, c("task_id", "learner_id",
  "classif.acc")]
bma$learner_id = rep(c("RF", "Stack"), 2)
bma
```

```
         task_id learner_id classif.acc
1: breast_cancer         RF   0.9605263
2: breast_cancer      Stack   0.9122807
3:         sonar         RF   0.7681159
4:         sonar      Stack   0.7101449
```

```
as.BenchmarkAggr(bm)$friedman_test()
```

```

    Friedman rank sum test

data:  ce and learner_id and task_id
Friedman chi-squared = 2, df = 1, p-value = 0.1573
```

In this (much more complex!) example we chose two tasks and two machine learning (ML) algorithms ("learners" in `mlr3` terms). We used automated tuning to optimize the number of trees in the random forest learner (Chapter 4) and a ML pipeline that imputes missing data, collapses factor levels, and creates stacked models (Chapter 6). We also showed basic features like loading learners (Chapter 2) and choosing resampling strategies for benchmarking (Chapter 3). Finally, we compared the performance of the models using the mean accuracy on the test set, and applied a statistical test to see if the learners performed significantly different (they did not!).

You will learn how to do all this and more in this book. We will walk through the functionality offered by `mlr3` and the packages in the `mlr3verse` step by step. There are a few different ways you can use this book, which we will discuss next.

How to use this book

The mlr3 ecosystem is the result of many years of methodological and applied research and improving the design and implementation of the packages over the years. This book describes the resulting features of the `mlr3verse` and discusses best practices for ML, technical implementation details, extension guidelines, and in-depth considerations for optimizing ML. It is suitable for a wide range of readers and levels of ML expertise.

Chapter 1, Chapter 2, and Chapter 3 cover the basics of mlr3. These chapters are essential to understanding the core infrastrucure of ML in mlr3. We recommend that all readers study these chapters to become familiar with basic mlr3 terminology, syntax, and style. Chapter 4, Chapter 5, and Chapter 6 contain more advanced implementation details and some ML theory. Chapter 8 delves into detail on domain-specific methods that are implemented in our extension packages. Readers may choose to selectively read sections in this chapter depending on your use cases (i.e., if you have domain-specific problems to tackle), or to use these as introductions to new domains to explore. Chapter 9 contains technical implementation details that are essential reading for advanced users who require parallelisation, custom error handling, and fine control over hyperparameters and large databases. Chapter 10 discusses packages that can be integrated with mlr3 to provide model-agnostic interpretability methods. Finally, anyone who would like to contribute to our ecosystem should read Chapter 11.

Of course, you can also read the book cover to cover from start to finish. We have marked any section that contains complex technical information with an exclamation mark (!). You may wish to skip these sections if you are only interested in basic functionality. Similarly, we have marked sections that are optional, such as parts that are more methodological focused and do not discuss the software implementation, with an asterisk (*). Readers that are interested in the more technical detail will likely want to pay attention to the tables at the end of each chapter that show the relationship between our S3 'sugar' functions and the underlying R6 classes; this is explained in more detail in Chapter 1.

This book tries to follow the Diátaxis framework[1] for documentation and so we include tutorials, how-to guides, API references, and explanations. This means that the conclusion of each chapter includes a short reference to the core functions learnt in the chapter, links to relevant posts in the mlr3gallery[2], and a few exercises that will cover content introduced in the chapter. You can find the solutions to these exercises in Appendix A.

Finally, if you want to reproduce any of the results in this book, note that the random seed is set as the chapter number and the `sessionInfo()` printed in Appendix E.

Installation guidelines

All packages in the mlr3 ecosystem can be installed from GitHub and R-universe; the majority (but not all) packages can also be installed from CRAN. We recommend adding the mlr-org R-universe[3] to your R options so that you can install all packages with `install.packages()` without having to worry which package repository it comes from. To do this, install the `usethis` package and run the following:

```
usethis::edit_r_profile()
```

In the file that opens add or change the `repos` argument in `options` so it looks something like this (you might need to add the full code block below or just edit the existing `options` function).

```
options(repos = c(
  mlrorg = "https://mlr-org.r-universe.dev",
  CRAN = "https://cloud.r-project.org/"
))
```

Save the file, restart your R session, and you are ready to go!

```
install.packages("mlr3verse")
```

If you want latest development versions of any of our packages, run

```
remotes::install_github("mlr-org/{pkg}")
```

[1] https://diataxis.fr/
[2] https://mlr-org.com/gallery.html
[3] R-universe is an alternative package repository to CRAN. The bit of code below tells R to look at both R-universe and CRAN when trying to install packages. R will always install the latest version of a package.

with `{pkg}` replaced with the name of the package you want to install. You can see an up-to-date list of all our extension packages at https://github.com/mlr-org/mlr3/wiki/Extension-Packages.

Community links

The mlr community is open to all and we welcome everybody, from those completely new to ML and R to advanced coders and professional data scientists. You can reach us on our Mattermost[4].

For case studies and how-to guides, check out the mlr3gallery[5] for extended practical blog posts. For updates on mlr you might find our blog[6] a useful point of reference.

We appreciate all contributions, whether they are bug reports, feature requests, or pull requests that fix bugs or extend functionality. Each of our GitHub repositories includes issues and pull request templates to ensure we can help you as much as possible to get started. Please make sure you read our code of conduct[7] and contribution guidelines[8]. With so many packages in our universe it may be hard to keep track of where to open issues. As a general rule:

1. If you have a question about using any part of the mlr3 ecosystem, ask on StackOverflow and use the tag #mlr3 – one of our team will answer you there. Be sure to include a reproducible example (reprex) and if we think you found a bug then we will refer you to the relevant GitHub repository.
2. Bug reports or pull requests about core functionality (train, predict, etc.) should be opened in the mlr3 GitHub repository.
3. Bug reports or pull requests about learners should be opened in the mlr3extralearners GitHub repository.
4. Bug reports or pull requests about measures should be opened in the mlr3measures GitHub repository.
5. Bug reports or pull requests about domain specific functionality should be opened in the GitHub repository of the respective package (see Chapter 1).

Do not worry about opening an issue in the wrong place, we will transfer it to the right one!

Citation info

Every package in the mlr3verse has its own citation details that can be found on the respective GitHub repository.

To reference this book please use:

```
Becker M, Binder M, Bischl B, Foss N, Kotthoff L, Lang M, Pfisterer F,
Reich N G, Richter J, Schratz P, Sonabend R, Pulatov D.
2023. "Flexible and Robust Machine Learning Using mlr3 in R". https://mlr3book.mlr-org.com.
```

[4] https://lmmisld-lmu-stats-slds.srv.mwn.de/signup_email?id=6n7n67tdh7d4bnfxydqomjqspo
[5] https://mlr-org.com/gallery.html
[6] https://mlr-org.com/blog.html
[7] https://github.com/mlr-org/mlr3/blob/main/.github/CODE_OF_CONDUCT.md
[8] https://github.com/mlr-org/mlr3/blob/main/CONTRIBUTING.md

```
@misc{
    title = Flexible and Robust Machine Learning Using mlr3 in R
    author = {Marc Becker, Martin Binder, Bernd Bischl, Natalie Foss,
    Lars Kotthoff, Michel Lang, Florian Pfisterer, Nicholas G. Reich,
    Jakob Richter, Patrick Schratz, Raphael Sonabend, Damir Pulatov},
    url = {https://mlr3book.mlr-org.com},
    year = {2023}
}
```

To reference the `mlr3` package, please cite our JOSS paper:

```
Lang M, Binder M, Richter J, Schratz P, Pfisterer F, Coors S, Au Q,
Casalicchio G, Kotthoff L, Bischl B (2019). "mlr3: A modern object-oriented
machine learning framework in R." Journal of Open Source Software.
doi: 10.21105/joss.01903.
```

```
@Article{mlr3,
  title = {{mlr3}: A modern object-oriented machine learning framework in {R}},
  author = {Michel Lang and Martin Binder and Jakob Richter and Patrick Schratz and
  Florian Pfisterer and Stefan Coors and Quay Au and Giuseppe Casalicchio and
  Lars Kotthoff and Bernd Bischl},
  journal = {Journal of Open Source Software},
  year = {2019},
  month = {dec},
  doi = {10.21105/joss.01903},
  url = {https://joss.theoj.org/papers/10.21105/joss.01903},
}
```

mlr3book style guide

Throughout this book we will use our own style guide that can be found in the mlr3 wiki[9]. Below are the most important style choices relevant to the book.

1. We always use `=` instead of `<-` for assignment.
2. Class names are in `UpperCamelCase`
3. Function and method names are in `lower_snake_case`
4. When referencing functions, we will only include the package prefix (e.g., `pkg::function`) for functions outside the mlr3 universe or when there may be ambiguity about in which package the function lives. Note you can use `environment(function)` to see which namespace a function is loaded from.
5. We denote packages, fields, methods, and functions as follows:
    - `package` - With link (if online) to package CRAN, R-Universe, or GitHub page

[9] https://github.com/mlr-org/mlr3/wiki/Style-Guide

- `package::function()` (for functions *outside* the mlr-org ecosystem)
- `function()` (for functions *inside* the mlr-org ecosystem) - With link to function documentation page
- `$field` for fields (data encapsulated in a R6 class)
- `$method()` for methods (functions encapsulated in a R6 class)

1. Introduction and Overview

The (**M**achine **L**earning in **R**) `mlr3` (Lang et al. 2019) package and ecosystem provide a generic, object-oriented, and extensible framework for regression (Appendix C), classification (Section 2.4), and other machine learning tasks (Chapter 8) for the R language (R Core Team 2019). This unified interface provides functionality to extend and combine existing machine learning algorithms (learners (Section 2.2)), intelligently select and tune the most appropriate technique for a given machine learning task (Appendix C), and perform large-scale comparisons that enable meta-learning. Examples of this advanced functionality include hyperparameter tuning (Chapter 4) and feature selection (Chapter 5). Parallelization of many operations is natively supported (Section 9.1).

Classification
Regression
Tasks

Learners

`mlr3` has similar overall aims to `caret`, `tidymodels`, scikit-learn[1] for Python, and MLJ[2] for Julia. In general `mlr3` is designed to provide more flexibility than other machine learning frameworks while still offering easy ways to use advanced functionality. While in particular tidymodels makes it very easy to perform simple machine learning tasks, `mlr3` is more geared towards advanced machine learning. To get a quick overview of how to do things in the `mlr3verse`, see the mlr3 cheatsheets[3].

> **Note**
>
> `mlr3` provides a unified interface to existing learners in R. With few exceptions, we do not implement any learners ourselves, although we often augment the functionality provided by the underlying learners. This includes, in particular, the definition of hyperparameter spaces for tuning.

1.1. Target audience

We assume that users of `mlr3` have taken an introductory machine learning course or have the equivalent expertise and some basic experience with R. A background in computer science or statistics is beneficial for understanding the advanced functionality described in the later chapters of this book, but not required. (James et al. 2014) provides a comprehensive introduction for those new to machine learning.

`mlr3` provides a domain-specific language for machine learning in R that allows to do everything from simple exercises to complex projects. We target both **practitioners** who want to quickly apply machine learning algorithms and **researchers** who want to implement, benchmark, and compare their new methods in a structured environment.

[1] https://scikit-learn.org/
[2] https://alan-turing-institute.github.io/MLJ.jl/dev/
[3] https://cheatsheets.mlr-org.com/

1.2. From mlr to mlr3

The `mlr` package (Bischl et al. 2016) was first released to CRAN[4] in 2013, with the core design and architecture dating back much further. Over time, the addition of many features has led to a considerably more complex design that made it harder to build, maintain, and extend than we had hoped for. In hindsight, we saw that some design and architecture choices in `mlr` made it difficult to support new features, in particular with respect to machine learning pipelines. Furthermore, the R ecosystem and helpful packages such as `data.table` have undergone major changes after the initial design of `mlr`.

It would have been impossible to integrate all of these changes into the original design of `mlr`. Instead, we decided to start working on a reimplementation in 2018, which resulted in the first release of `mlr3` on CRAN in July 2019.

The new design and the integration of further and newly-developed R packages (especially `R6`, `future`, and `data.table`) makes `mlr3` much easier to use, maintain, and in many regards more efficient than its predecessor `mlr`. The packages in the ecosystem are less tightly coupled, making them easier to maintain and easier to develop, especially very specialized packages.

1.3. Design principles

> **Some readers may want to skip this section of the book.**

We follow these general design principles in the `mlr3` package and `mlr3verse` ecosystem.

- **Separation of computation and presentation**. Most packages of the `mlr3` ecosystem focus on processing and transforming data, applying machine learning algorithms, and computing results. Our core packages do not provide graphical user interfaces (GUIs) because their dependencies would make installation unnecessarily complex, especially on headless servers. For the same reason, visualizations of data and results are provided in the extra package `mlr3viz`, which avoids dependencies on `ggplot2`. `mlr3shiny` provides an interface for some basic machine learning tasks using the `shiny` package.
- **Object-oriented programming (OOP)**. Embrace `R6` for a clean, object-oriented design, object state-changes, and reference semantics.
- **Tabular data**. Embrace `data.table` for its top-notch computation performance as well as tabular data as a data structure which can be easily processed further.
- **Unify input and output data formats.** This considerably simplifies the API and allows easy selection and "split-apply-combine" (aggregation) operations. We combine `data.table` and `R6` to place references to non-atomic and compound objects in tables and make heavy use of list columns.
- **Defensive programming and type safety**. All user input is checked with `checkmate` (Lang 2017). We document return types, and avoid mechanisms popular in base R which "simplify" the result unpredictably (e.g., `sapply()` or the `drop` argument for indexing data.frames). And we have extensive unit tests!

[4] https://cran.r-project.org

- **Light on dependencies**. One of the main maintenance burdens for `mlr` was to keep up with changing learner interfaces and behavior of the many packages it depended on. We require far fewer packages in `mlr3` to make installation and maintenance easier. We still provide the same functionality, but it is split into more packages that have fewer dependencies individually. As mentioned above, this is particularly the case for all visualization functionality, which is contained in a separate package to avoid unnecessary dependencies in all other packages.

1.4. Package ecosystem

`mlr3` depends on the following popular and well-established packages that are not developed by core members of the `mlr3` team:

- `R6`: The class system predominantly used in mlr3.
- `data.table`: High-performance extension of R's `data.frame`.
- `digest`: Cryptographic hash functions.
- `uuid`: Generation of universally unique identifiers.
- `lgr`: Highly configurable logging library.
- `mlbench` and `palmerpenguins`: More machine learning data sets.
- `evaluate`: For capturing output, warnings, and exceptions (Section 9.2).
- `future` / `future.apply`: For parallelization (Section 9.1).

The `mlr3` package itself provides the base functionality that the rest of ecosystem (`mlr3verse`) relies on and the fundamental building blocks for machine learning. **?@fig-mlr3verse** shows the packages in the `mlr3verse` that extend `mlr3` with capabilities for preprocessing, pipelining, visualizations, additional learners, additional task types, and more.

> Tip
>
> A complete list with links to the repositories for the respective packages can be found on our package overview page[a].
>
> [a] https://mlr-org.com/ecosystem.html

We build on `R6` for object orientation and `data.table` to store and operate on tabular data. Both are core to `mlr3`; we briefly introduce both packages for beginners. While in-depth expertise with these packages is not necessary, a basic understanding is required to work effectively with `mlr3`.

1.5. Quick R6 introduction for beginners

`R6` is one of R's more recent paradigm for object-oriented programming (OOP). It addresses shortcomings of earlier OO implementations in R, such as S3, which we used in `mlr`. If you have done any object-oriented programming before, R6 should feel familiar. We focus on the parts of R6 that you need to know to use `mlr3`.

Objects are created by calling the constructor of an `R6::R6Class()` object, specifically the initialization method `$new()`. For example, `foo = Foo$new(bar = 1)` creates a new object of class `Foo`, setting the `bar` argument of the constructor to the value `1`.

Objects have mutable state that is encapsulated in their fields, which can be accessed through the dollar operator. We can access the `bar` value in the `foo` variable from above through `foo$bar` and set its value by assigning the field, e.g. `foo$bar = 2`.

In addition to fields, objects expose methods that allow to inspect the object's state, retrieve information, or perform an action that changes the internal state of the object. For example, the `$train()` method of a learner changes the internal state of the learner by building and storing a model, which can then be used to make predictions.

Objects can have public and private fields and methods. The public fields and methods define the API to interact with the object. Private methods are only relevant for you if you want to extend `mlr3`, e.g. with new learners.

Technically, R6 objects are environments, and as such have reference semantics. For example, `foo2 = foo` does not create a copy of `foo` in `foo2`, but another reference to the same actual object. Setting `foo$bar = 3` will also change `foo2$bar` to `3` and vice versa.

To copy an object, use the `$clone()` method and the `deep = TRUE` argument for nested objects, for example, `foo2 = foo$clone(deep = TRUE)`.

> **Tip**
>
> For more details on R6, have a look at the excellent R6 vignettes[a], especially the introduction[b]. For comprehensive R6 information, we refer to the R6 chapter from Advanced R[c].
>
> [a] https://r6.r-lib.org/
> [b] https://r6.r-lib.org/articles/Introduction.html
> [c] https://adv-r.hadley.nz/r6.html

1.6. Quick `data.table` introduction for beginners

The package `data.table` implements a popular alternative to R's `data.frame()`, i.e. an object to store tabular data. We decided to use `data.table` because it is blazingly fast and scales well to bigger data.

> **Note**
>
> Many `mlr3` functions return `data.table`s which can conveniently be subsetted or combined with other outputs. If you do not like the syntax or are feeling more comfortable with other tools, base `data.frame`s or `tibble`/`dplyr`s are just a single `as.data.frame()` or `as_tibble()` away.

Data tables are constructed with the `data.table()` function (whose interface is similar to `data.frame()`) or by converting an object with `as.data.table()`.

```
library("data.table")
dt = data.table(x = 1:6, y = rep(letters[1:3], each = 2))
dt
```

```
   x y
1: 1 a
2: 2 a
3: 3 b
4: 4 b
5: 5 c
6: 6 c
```

data.tables can be used much like data.frames, but they do provide additional functionality that makes complex operations easier. For example, data can be summarized by groups with the [operator:

```
dt[, mean(x), by = "y"]
```

```
   y  V1
1: a 1.5
2: b 3.5
3: c 5.5
```

There is also extensive support for many kinds of database join operations (see e.g. this RPubs post by Ronald Stalder[5]) that make it easy to combine multiple data.tables in different ways.

> **Tip**
>
> For an in-depth introduction, we refer the reader to the excellent data.table introduction vignette[a].
>
> [a] https://cran.r-project.org/web/packages/data.table/vignettes/datatable-intro.html

1.7. Essential mlr3 utilities

Sugar functions

Most objects in mlr3 can be created through convenience functions called *sugar functions*. They provide shortcuts for common code idioms, reducing the amount of code a user has to write. We heavily use sugar functions throughout this book and give the equivalent "full form" for full detail. In most cases, the sugar functions will achieve what you want to do, and you only have to consider using the full R6 code if you program custom objects or extensions. For example lrn("regr.rpart") is the sugar version of LearnerRegrRpart$new().

[5] https://rstudio-pubs-static.s3.amazonaws.com/52230_5ae0d25125b544caab32f75f0360e775.html

Dictionaries

mlr3 uses dictionaries to store objects like learners or tasks. These are key-value stores that allow to associate a key with a value that can be an R6 object, much like paper dictionaries associate words with their definitions. Often, values in dictionaries are accessed through sugar functions that automatically use the applicable dictionary without the user having to specify it; only the key to be retrieved needs to be specified. Dictionaries are used to group relevant objects so that they can be listed and retrieved easily. For example, a learner can be retrieved directly from the `mlr_learners` dictionary using the key `"classif.featureless"` (`mlr_learners$get("classif.featureless")`) and you can get an overview over all stored learners with `as.data.table(mlr_learners)`.

mlr3viz

mlr3viz is the package for all plotting functionality in the mlr3 ecosystem. The package uses a common theme (`ggplot2::theme_minimal()`) so that all generated plots have a similar aesthetic. Under the hood, mlr3viz uses `ggplot2`. mlr3viz extends `fortify` and `autoplot`for use with common mlr3 outputs including Prediction, Learner, and Benchmark objects (these objects will be introduced and covered in the next chapter). The most common use of mlr3viz is the `autoplot()` function, where the type of the object passed determines the type of the plot. Plot types are documented in the respective manual page that can be accessed through `?autoplot.X`. For example, the documentation of plots for regression tasks can be found by running `?autoplot.TaskRegr`.

2. Fundamentals

We describe and explain the basic building blocks of mlr3 and how to train and evaluate simple machine learning models. The chapter introduces the different types of tasks that mlr3 supports and how to work with them, learners and how to train models, how to make predictions using those trained models, and how to evaluate the quality of the predictions in a principled fashion. Only the basic concepts are introduced, but we give pointers on where to learn more in the rest of the book, and overviews of other concepts. After reading this chapter, you will be able to use mlr3 for most machine learning workflows.

In this chapter, we will introduce the `mlr3` objects and corresponding `R6` classes that implement the essential building blocks of machine learning. These building blocks include the data (and the methods of creating training and test sets), the machine learning algorithm (and its training and prediction process), and evaluation measures to assess the quality of predictions.

In essence, machine learning means learning relationships from data. In supervised learning, datasets consist of observations (rows in tabular data) that are labeled, which means that each data point includes features (columns in tabular data) and a quantity that we are trying to predict, also called 'target'. For example, we might want to predict the miles per gallon a car gets based on features such as its horsepower and the number of gears. Data and information on what they represent, along with what quantities to predict are called "tasks" in `mlr3` (Appendix C) – they can be thought of as machine learning tasks we are trying to solve. There can be more than one task per dataset, for example ones that include different sets of features, observations, or predict different target quantities.

Supervised learning can be further divided into regression (predicting numeric target values) and classification (predicting categorical target values/labels). In either case, the goal is to build a model that captures the relationship between features and target. We can build such models using machine learning algorithms, for example decision trees, support vector machines, neural networks, and many more. A machine learning algorithm, given training data, induces such a model. Machine learning algorithms are called "learners" in `mlr3` (Section 2.2) – given data, they learn models. Each learner has a parameterized space that potential models are drawn from and during the training process, these parameters are fitted to best match the data. For example, the parameters could be the weights given to individual features when predicting a quantity in linear regression. For other learners, the parameters are not as explicit, for example for decision tree learners where a fitted model corresponds to a particular decision tree. All learners optimize a so-called loss function during training, i.e. training a learner means finding the model that optimizes the loss. In general, a loss function quantifies the mismatch between ground truth target values in the training data and the predictions of the model.

Given a model, we can make predictions (Section 2.2.2) on new data. A model is only useful though if it generalizes beyond the training data. Otherwise, we could build a perfect model by simply memorizing the training data. Therefore, separate test data is used to evaluate models in an unbiased way and to assess to what extent they have learned the true relationships that underlie the data (Chapter 3). We can evaluate models in `mlr3` in many ways (Section 2.3). In general, we use the same kind of loss function that the learner used to build the model, but now with data that was not used during training. The performance of a model, quantified by the value of the loss function when evaluated on new data, is called the estimated of the generalization error – how well do we expect this model to do in general? `mlr3` calls loss functions "measures". We can use different measures for training and testing, although it makes most sense for the measures to be the same.

Much more information on (supervised) machine learning can be found in Hastie, Friedman, and Tibshirani (2001), James et al. (2014), or Bishop (2006).

The basic idea is illustrated in the following figure:

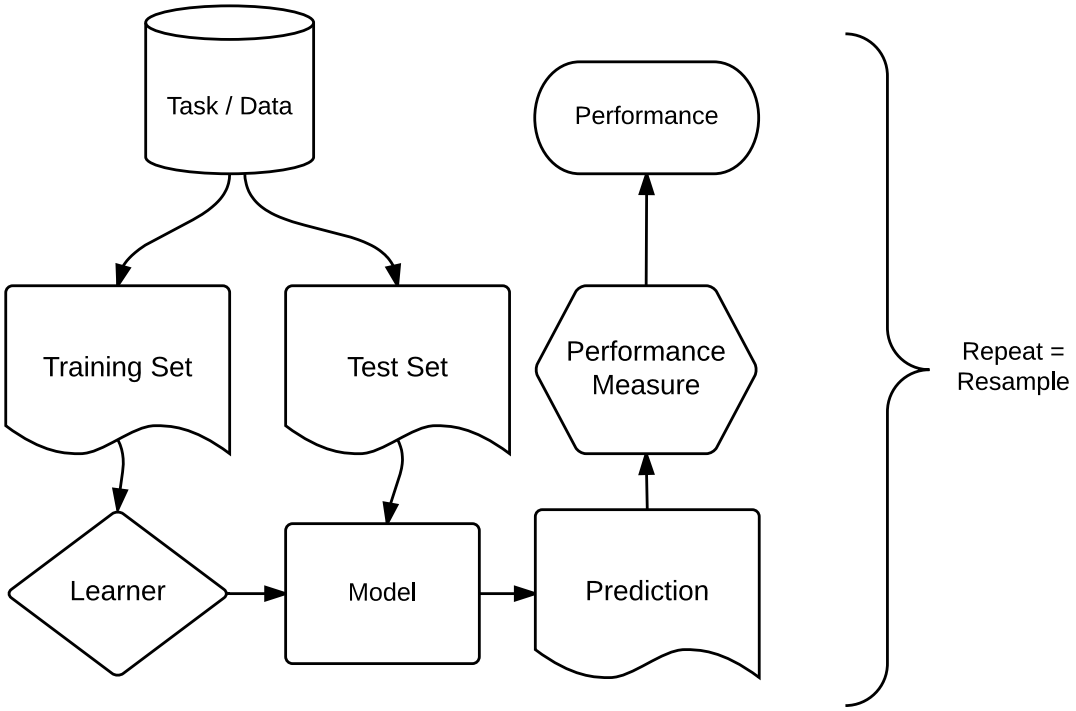


Figure 2.1.: General overview of the machine learning process.

2.1. Tasks

Tasks are objects that contain the (usually tabular) data and additional meta-data that define a machine learning problem. The meta-data contain, for example, the name of the target feature for supervised machine learning problems. This information is used automatically by operations that

can be performed on a task so that for example the user does not have to specify the prediction target every time a model is trained.

2.1.1. Built-in Tasks

mlr3 includes a few predefined machine learning tasks in an R6 `Dictionary` named `mlr_tasks`.

```
mlr_tasks
```

```
<DictionaryTask> with 19 stored values
Keys: bike_sharing, boston_housing, breast_cancer, german_credit, ilpd,
  iris, kc_housing, moneyball, mtcars, optdigits, penguins,
  penguins_simple, pima, sonar, spam, titanic, usarrests, wine, zoo
```

To get a task from the dictionary, use the `tsk()` function and assign the return value to a new variable. Here, we retrieve the `mtcars regression task`, which is provided by the package datasets:

```
task_mtcars = tsk("mtcars")
task_mtcars
```

```
<TaskRegr:mtcars> (32 x 11): Motor Trends
* Target: mpg
* Properties: -
* Features (10):
  - dbl (10): am, carb, cyl, disp, drat, gear, hp, qsec, vs, wt
```

To get more information about a particular task, it is easiest to use the `help()` method that all mlr3-objects come with:

```
task_mtcars$help()
```

> **Tip**
>
> If you are familiar with R's help system (i.e. the `help()` and `?` functions), this may seem confusing. `task_mtcars` is the variable that holds the mtcars task, not a function, and hence we cannot use `help()` or `?`.

Alternatively, the corresponding man page can be found under `mlr_tasks_<id>`, e.g.

```
help("mlr_tasks_mtcars")
```

We can also load the data separately and convert it to a task, without using the `tsk()` function that mlr3 provides. If the data we want to use does not come with mlr3, it has to be done this way.

For example, the data for `mtcars` is also available separately, as a `data.frame()` and not a task. `mtcars` contains characteristics for different types of cars, along with their fuel consumption. We want to predict the numeric target feature stored in column `"mpg"` (miles per gallon).

```
data("mtcars", package = "datasets")
str(mtcars)
```

```
'data.frame':   32 obs. of  11 variables:
 $ mpg : num  21 21 22.8 21.4 18.7 18.1 14.3 24.4 22.8 19.2 ...
 $ cyl : num  6 6 4 6 8 6 8 4 4 6 ...
 $ disp: num  160 160 108 258 360 ...
 $ hp  : num  110 110 93 110 175 105 245 62 95 123 ...
 $ drat: num  3.9 3.9 3.85 3.08 3.15 2.76 3.21 3.69 3.92 3.92 ...
 $ wt  : num  2.62 2.88 2.32 3.21 3.44 ...
 $ qsec: num  16.5 17 18.6 19.4 17 ...
 $ vs  : num  0 0 1 1 0 1 0 1 1 1 ...
 $ am  : num  1 1 1 0 0 0 0 0 0 0 ...
 $ gear: num  4 4 4 3 3 3 3 4 4 4 ...
 $ carb: num  4 4 1 1 2 1 4 2 2 4 ...
```

We create the regression task, i.e. we construct a new instance of the R6 class `TaskRegr`. An easy way to do this is to use the function `as_task_regr()` to convert our `data.frame()` to a regression task, specifying the target feature in an additional argument. Before we give the data to `as_task_regr()`, we can process it using the usual R functions, for example to select a subset of data.

```
library("mlr3")
mtcars_subset = subset(mtcars, select = c("mpg", "cyl", "disp"))

task_mtcars = as_task_regr(mtcars_subset, target = "mpg", id = "cars")
task_mtcars
```

```
<TaskRegr:cars> (32 x 3)
* Target: mpg
* Properties: -
* Features (2):
  - dbl (2): cyl, disp
```

> **Tip**
>
> The task constructors `as_task_regr()` and `as_task_classif()` will check for non-ASCII characters in the column names of your data. As many ML models do not work properly with arbitrary UTF8 names, `mlr3` defaults to throw an error if any of the column names contains either a non-ASCII character or does not comply with R's variable naming scheme. We generally recommend converting names with `make.names()` first, but you can also set the

option `mlr3.allow_utf8_names` to true to relax the check (but do not be surprised if a model fails).

The data can be any rectangular data format, e.g. a `data.frame()`, `data.table()`, or `tibble()`. Internally, the data is converted and stored in a DataBackend. The `target` argument specifies the prediction target column. The `id` argument is optional and specifies an identifier for the task that is used in plots and summaries. If no `id` is given provided, the deparsed name of the data will be used (an R way of turning data into strings).

Printing a task gives a short summary: it has 32 observations and 3 columns, of which `mpg` is the target and 2 are features stored in double-precision floating point format.

We can plot the task using the `mlr3viz` package, which gives a graphical summary of the distribution of the target and feature values:

```
library("mlr3viz")
autoplot(task_mtcars, type = "pairs")
```

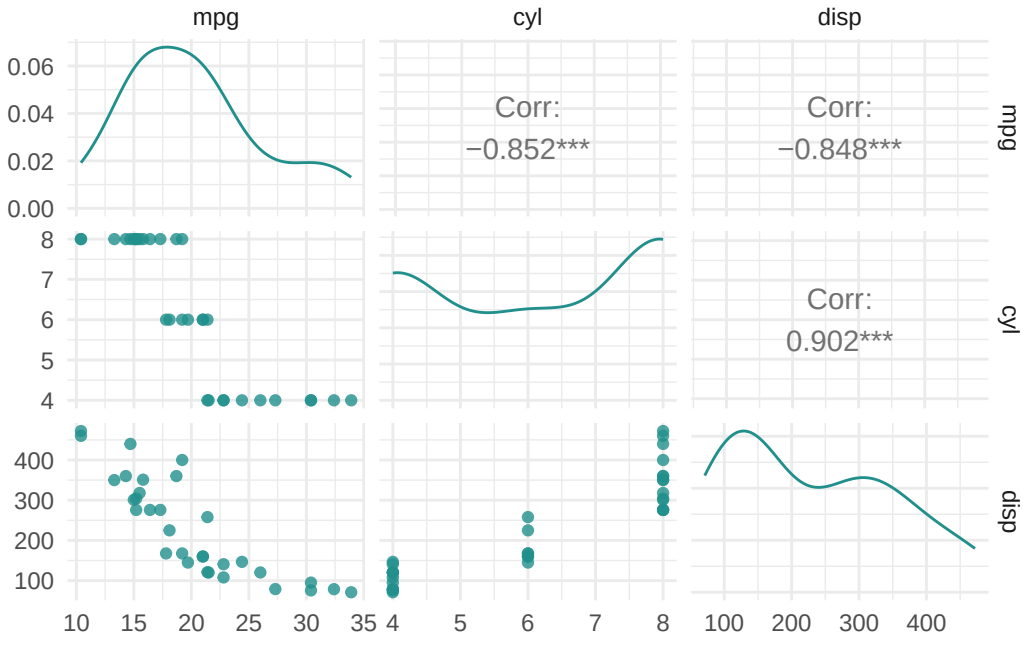


Figure 2.2.: Overview of the mtcars dataset.

Tip

Instead of loading multiple extension packages individually, it is often more convenient to load the `mlr3verse` package instead. It makes the functions from most `mlr3` packages that are used for common machine learning and data science tasks available.

2.1.2. Retrieving Data

The Task object primarily represents a tabular dataset, combined with meta-data about which columns of that data should be used to predict which other columns in what way, and some more information about column data types.

Various fields can be used to retrieve meta-data about a task. The dimensions, for example, can be retrieved using `$nrow` and `$ncol`:

```
task_mtcars$nrow
```

```
[1] 32
```

```
task_mtcars$ncol
```

```
[1] 3
```

The names of the feature and target columns are stored in the `$feature_names` and `$target_names` slots, respectively. Here, "target" refers to the feature we want to predict and "feature" to the predictors for the task.

```
task_mtcars$feature_names
```

```
[1] "cyl"  "disp"
```

```
task_mtcars$target_names
```

```
[1] "mpg"
```

While the columns of a task have unique `character`-valued names, their rows are identified by unique natural numbers, called row IDs. They can be accessed through the `$row_ids` slot:

```
head(task_mtcars$row_ids)
```

```
[1] 1 2 3 4 5 6
```

Row IDs are not used as features when predicting; they are meta-data that allows to access individual observations.

> **Warning**
>
> Although the row IDs are typically just the sequence from `1` to `nrow(data)`, they are only guaranteed to be unique natural numbers. It is possible that they do not start at `1`, that they are not increasing by 1 each, or that they are not even in increasing order. This allows to transparently operate on real database management systems, where uniqueness is the only requirement for primary keys.

The data contained in a task can be accessed through `$data()`, which returns a `data.table` object. It has optional `rows` and `cols` arguments to specify subsets of the data to retrieve. When a database backend is used, this avoids loading unnecessary data into memory, making it more efficient than retrieving the entire data first and then subsetting it using `[<rows>, <cols>]`.

```
task_mtcars$data()
```

```
     mpg cyl  disp
 1: 21.0   6 160.0
 2: 21.0   6 160.0
 3: 22.8   4 108.0
 4: 21.4   6 258.0
 5: 18.7   8 360.0
---
28: 30.4   4  95.1
29: 15.8   8 351.0
30: 19.7   6 145.0
31: 15.0   8 301.0
32: 21.4   4 121.0
```

```
# retrieve data for rows with IDs 1, 5, and 10 and column "mpg"
task_mtcars$data(rows = c(1, 5, 10), cols = "mpg")
```

```
    mpg
1: 21.0
2: 18.7
3: 19.2
```

A shortcut to extract all data from a task is to simply convert it to a `data.table`:

```
# show summary of all data
summary(as.data.table(task_mtcars))
```

```
      mpg             cyl             disp
 Min.   :10.40   Min.   :4.000   Min.   : 71.1
 1st Qu.:15.43   1st Qu.:4.000   1st Qu.:120.8
```

```
 Median :19.20   Median :6.000   Median :196.3
 Mean   :20.09   Mean   :6.188   Mean   :230.7
 3rd Qu.:22.80   3rd Qu.:8.000   3rd Qu.:326.0
 Max.   :33.90   Max.   :8.000   Max.   :472.0
```

2.1.3. Task Mutators

It is often necessary to create tasks that encompass subsets of other tasks' data, for example to manually create train-test-splits, or to fit models on a subset of given features. Restricting tasks to a given set of features can be done by calling `$select()` with the desired feature names. Restriction to rows (observations) is done with `$filter()` with the row IDs.

```
task_mtcars_small = tsk("mtcars") # initialize with the full task
task_mtcars_small$select(c("am", "carb")) # keep only these features
task_mtcars_small$filter(2:4) # keep only these rows
task_mtcars_small$data()
```

```
    mpg am carb
1: 21.0  1    4
2: 22.8  1    1
3: 21.4  0    1
```

These methods are so-called *mutators*; they modify the given `Task` in place. If you want to have an unmodified version of the task, you need to use the `$clone()` method to create a copy first.

```
task_mtcars_smaller = task_mtcars_small$clone()
task_mtcars_smaller$filter(2)
task_mtcars_smaller$data()
```

```
   mpg am carb
1:  21  1    4
```

```
task_mtcars_small$data()  # the original task is unmodified
```

```
    mpg am carb
1: 21.0  1    4
2: 22.8  1    1
3: 21.4  0    1
```

Note also how the last call to `$filter(2)` did not select the second row of `task_mtcars_small`, but the row with ID 2, which is the *first* row of `task_mtcars_small`.

> **Tip**
>
> If you need to work with row numbers instead of row IDs, you can work on the vector of row IDs:

```
# keep the 2nd row:
keep = task_mtcars_small$row_ids[2] # extracts ID of 2nd row
task_mtcars_smaller$filter(keep)
```

The methods above allow to subset the data; the methods `$rbind()` and `$cbind()` allow to add extra rows and columns to a task.

```
task_mtcars_smaller$rbind( # add another row
  data.frame(mpg = 23, am = 0, carb = 3)
)
task_mtcars_smaller$data()
```

```
   mpg am carb
1:  21  1    4
2:  23  0    3
```

2.1.4. Roles (Rows and Columns)

> **Some readers may want to skip this section of the book.**

We have seen that certain columns are designated as "targets" and "features" during task creation; mlr3 calls this "roles". Target refers to the column(s) we want to predict and features are the predictors (also called co-variates or descriptors) for the target. Besides these two, there are other possible roles for columns. The roles affect the behavior of the task for different operations.

The `task_mtcars_small` task, for example, has the following column roles:

```
task_mtcars_small$col_roles
```

```
$feature
[1] "am"   "carb"

$target
[1] "mpg"

$name
[1] "model"

$order
```

```
character(0)

$stratum
character(0)

$group
character(0)

$weight
character(0)
```

As you can see, there are additional column roles; the interested reader is referred to the documentation of `Task` for more detail. We can list all supported column roles by printing the names of the field `$col_roles`:

```
# supported column roles, see ?Task
names(task_mtcars_small$col_roles)
```

```
[1] "feature" "target"  "name"    "order"   "stratum" "group"   "weight"
```

Columns can have multiple roles. It is also possible for a column to have no role at all, in which case they are ignored. This is, in fact, how `$select()` and `$filter()` operate: They unassign the `"feature"` (for columns) or `"use"` (for rows) role without modifying the data which is stored in an immutable backend:

```
task_mtcars_small$backend
```

```
<DataBackendDataTable> (32x13)
             model  mpg cyl disp  hp drat    wt  qsec vs am gear carb ..row_id
         Mazda RX4 21.0   6  160 110 3.90 2.620 16.46  0  1    4    4        1
     Mazda RX4 Wag 21.0   6  160 110 3.90 2.875 17.02  0  1    4    4        2
        Datsun 710 22.8   4  108  93 3.85 2.320 18.61  1  1    4    1        3
    Hornet 4 Drive 21.4   6  258 110 3.08 3.215 19.44  1  0    3    1        4
 Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2        5
           Valiant 18.1   6  225 105 2.76 3.460 20.22  1  0    3    1        6
[...] (26 rows omitted)
```

There are two main ways to manipulate the column roles of a `Task`:

1. Use the `Task` method `$set_col_roles()` (recommended).
2. Directly modify the field `$col_roles`, which is a named list of vectors of column names. Each vector in this list corresponds to a column role, and the column names contained in that vector have the corresponding role.

Just as `$select()`/`$filter()`, these are in-place operations, i.e. the task object itself is modified. To retain an unmodified version of a task, use `$clone()`.

Changing the column or row roles, whether through `$select()`/`$filter()` or directly, does not change the underlying data, it just updates the view on it. Because the underlying data are still there (and accessible through `$backend`), we can add the `"cyl"` column back into the task by setting its column role to `"feature"`.

```
task_mtcars_small$set_col_roles("cyl", roles = "feature")
task_mtcars_small$feature_names  # cyl is now a feature again
```

```
[1] "am"   "carb" "cyl"
```

```
task_mtcars_small$data()
```

```
    mpg am carb cyl
1: 21.0  1    4   6
2: 22.8  1    1   4
3: 21.4  0    1   6
```

Just like columns, it is also possible to assign different roles to rows. Rows can have two different roles:

1. Role `use`: Rows that are generally available for training (although they may also be used for the test set). This role is the default role. The `$filter()` call changes this role, in the same way that `$select()` changes the `"feature"` column role.
2. Role `validation`: Rows that are not used for training. Rows that have missing values in the target column during task creation are automatically set to the validation role.

There are several reasons to hold some observations back or treat them differently:

1. It is often good practice to validate the final model on an external validation set to identify overfitting.
2. Some observations may be unlabeled in the original data, e.g. in competitions like Kaggle[1].

These observations cannot be used for training a model, but can be used for getting predictions from a trained model.

[1] https://www.kaggle.com/

2.2. Learners

Objects of class `Learner` provide a unified interface to many popular machine learning algorithms in R. They are available through the `mlr_learners` dictionary. The list of learners supported in the base package `mlr3` is deliberately small to avoid dependencies; support for additional learners is provided by the `mlr3learners` and `mlr3extralearners` packages.

Learners encapsulate methods to train a model and make predictions using it given a `Task` and provide meta-data about the learners. The base class of each learner is `Learner`.

To retrieve a `Learner` from the `mlr_learners` dictionary, use the function `lrn()`:

```
learner_rpart = lrn("regr.rpart")
```

Each learner provides the following meta-data:

- `$feature_types`: the type of features the learner can deal with.
- `$packages`: the packages required to train a model with this learner and make predictions.
- `$properties`: additional properties and capabilities. For example, a learner has the property "missings" if it is able to handle missing feature values, and "importance" if it computes and allows to extract data on the relative importance of the features.
- `$predict_types`: possible prediction types. For example, a regression learner can predict numerical values ("response") and may be able to predict the standard error of a prediction ("se").

This information can be queried through these slots, or seen at a glance when printing the learner:

```
learner_rpart
```

```
<LearnerRegrRpart:regr.rpart>: Regression Tree
* Model: -
* Parameters: xval=0
* Packages: mlr3, rpart
* Predict Types:  [response]
* Feature Types: logical, integer, numeric, factor, ordered
* Properties: importance, missings, selected_features, weights
```

All learners work in two stages:

- **Training**: A training task (features and target data) is passed to the learner's `$train()` function which trains and stores a model, i.e. the learned relationship of the features to the target.
- **Prediction**: New data, usually a different partition of the original dataset, is passed to the `$predict()` method of the trained learner. The model trained in the first step is used to predict the target values, e.g. the numerical value for regression problems.

> **Warning**
>
> A learner that has not been trained cannot make predictions and will throw an error if `$predict()` is called on it.

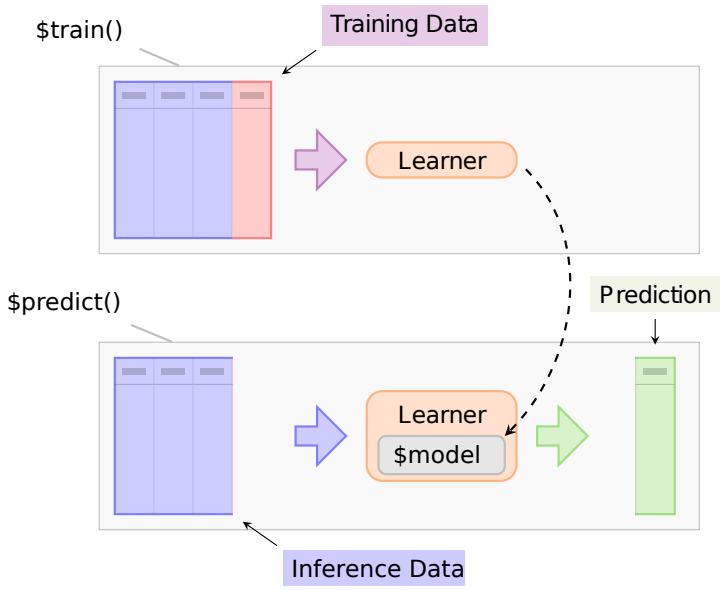


Figure 2.3.: Overview of the different stages of a learner.

2.2.1. Training the learner

We train the model by giving a task to the learner. It is a good idea to hold back some data from the training process use to assess the quality of the predictions made by the trained model. The `partition()` function randomly splits the task into two disjoint sets: a training set (67% of the total data, the default) and a test set (33% of the total data, the data not part of the training set).

```
splits = partition(task_mtcars)
splits
```

```
$train
 [1]  1  2  3  4  5  8 25 30 32  6 11 13 17 22 23 24 29 31 19 20 28

$test
 [1]  9 10 21 27  7 12 14 15 16 18 26
```

We learn a regression tree by calling the `$train()` method of the learner, specifying the task and the part of it to use for training (`splits$train`). This operation adds the learned model to the existing `Learner` object. We can now access the stored model via the field `$model`.

```
learner_rpart$train(task_mtcars, splits$train)
learner_rpart$model
```

```
n= 21

node), split, n, deviance, yval
      * denotes terminal node

1) root 21 617.38670 20.33333
  2) disp>=153.35 14  88.36857 17.42857 *
  3) disp< 153.35 7 174.63710 26.14286 *
```

We see that the learner has identified features in the task that are predictive of the class (`mpg`) and uses them to partition observations in the tree. The textual representation of the model depends on the type of learner. For more information on this particular type of model and how it is printed, see `rpart::print.rpart()`.

The model seems rather simplistic, using only a single feature and a single set of branches. Each learner has hyperparameters that control its behavior and allow to influence the way a model is learned. Setting hyperparameters to values appropriate for a given machine learning task is crucial for good predictive performance. The field `param_set` stores a description of the hyperparameters the learner has, their ranges, defaults, and current values:

```
learner_rpart$param_set
```

```
<ParamSet>
                id    class lower upper nlevels        default value
 1:             cp ParamDbl     0     1     Inf           0.01
 2:     keep_model ParamLgl    NA    NA       2          FALSE
 3:     maxcompete ParamInt     0   Inf     Inf              4
 4:       maxdepth ParamInt     1    30      30             30
 5:   maxsurrogate ParamInt     0   Inf     Inf              5
 6:      minbucket ParamInt     1   Inf     Inf <NoDefault[3]>
 7:       minsplit ParamInt     1   Inf     Inf             20
 8: surrogatestyle ParamInt     0     1       2              0
 9:   usesurrogate ParamInt     0     2       3              2
10:           xval ParamInt     0   Inf     Inf             10     0
```

The set of current hyperparameter values is stored in the `values` field of the `param_set` field. You can access and change the current hyperparameter values by accessing this field, which stores a named list:

```
learner_rpart$param_set$values
```

```
$xval
[1] 0
```

```
learner_rpart$param_set$values$minsplit = 10
learner_rpart$param_set$values
```

```
$xval
[1] 0

$minsplit
[1] 10
```

> **Tip**
>
> It is possible to assign all hyperparameters in one go by assigning a named list to `$values`: `learner$param_set$values = list(minsplit = 10, ...)`. This operation removes all previously-set hyperparameters.

The `lrn()` function also accepts additional arguments to update hyperparameters or set fields of the learner when constructing it:

```
learner_rpart = lrn("regr.rpart", minsplit = 10)
learner_rpart$param_set$values
```

```
$xval
[1] 0

$minsplit
[1] 10
```

```
learner_rpart$train(task_mtcars, splits$train)
learner_rpart$model
```

```
n= 21

node), split, n, deviance, yval
      * denotes terminal node

1) root 21 617.386700 20.33333
  2) disp>=101.55 18 167.562800 18.46111
    4) cyl>=7 9  30.075560 16.07778 *
    5) cyl< 7 9  35.242220 20.84444 *
  3) disp< 101.55 3   8.166667 31.56667 *
```

With the changed hyperparameters, we have a more complex (and more reasonable) model.

> **Note**
>
> Details on the hyperparameters of our `rpart` learner can be found at `rpart::rpart.control()`. Hyperparameters in general are discussed in more detail in the section on Hyperparameter Tuning.

2.2.2. Predicting

After the model has been created, we can now use it to make predictions. We can give the test partition to the `$predict()` function:

```
predictions = learner_rpart$predict(task_mtcars, splits$test)
predictions
```

```
<PredictionRegr> for 11 observations:
    row_ids truth response
          9  22.8 20.84444
         10  19.2 20.84444
         21  21.5 20.84444
---
         16  10.4 16.07778
         18  32.4 31.56667
         26  27.3 31.56667
```

The `$predict()` method returns a `Prediction` object, in this case a `PredictionRegr` for predicting a numeric quantity. The "truth" column contains the ground truth data, which was not given to the model to get a prediction. The "response" column contains the value predicted by the model, allowing for easy comparison with the ground truth data.

We can also use separate data to make predictions, which can be part of a separate task or simply a separate `data.frame`:

```
mtcars_new = data.frame(cyl = c(5, 6),
                        disp = c(100, 120),
                        hp = c(100, 150),
                        drat = c(4, 3.9),
                        wt = c(3.8, 4.1),
                        qsec = c(18, 19.5),
                        vs = c(1, 0),
                        am = c(1, 1),
                        gear = c(6, 4),
                        carb = c(3, 5))
mtcars_new
```

```
  cyl disp  hp drat  wt qsec vs am gear carb
```

```
1   5  100 100  4.0 3.8 18.0  1  1    6    3
2   6  120 150  3.9 4.1 19.5  0  1    4    5
```

The learner does not need to know more meta-data about this data to make predictions, as this was given when training the model. We can use the `$predict_newdata()` method to make predictions for our separate dataset:

```
predictions = learner_rpart$predict_newdata(mtcars_new)
predictions
```

```
<PredictionRegr> for 2 observations:
 row_ids truth response
       1    NA 31.56667
       2    NA 20.84444
```

Note that the "truth" column is now `NA`, as we did not give the ground truth data.

We can also access the predictions directly:

```
predictions$response
```

```
[1] 31.56667 20.84444
```

Similar to plotting tasks, `mlr3viz` provides an `autoplot()` method for `Prediction` objects.

```
library("mlr3viz")
predictions = learner_rpart$predict(task_mtcars, splits$test)
autoplot(predictions)
```

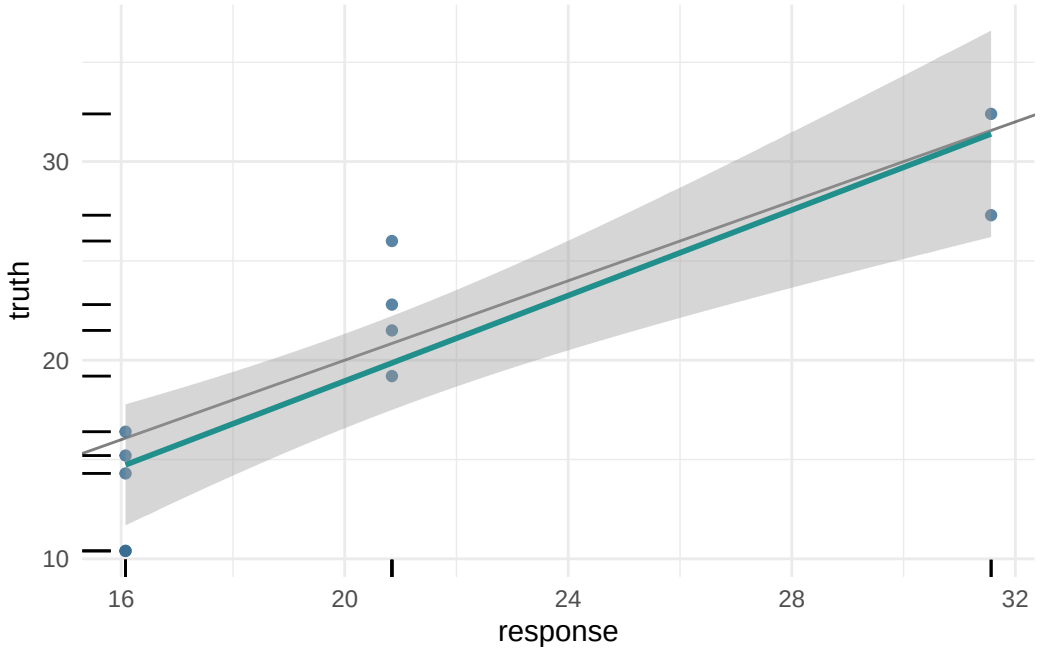


Figure 2.4.: Comparing predicted and ground truth values for the mtcars dataset.

2.2.3. Changing the Prediction Type

Regression learners default to predicting a numeric quantity. However, many regression models can also give you bounds on the prediction by providing the standard error. To predict these standard errors, the `predict_type` field of a `LearnerRegr` must be changed from "response" (the default) to "se" before training. The `rpart` learner we used above does not support predicting standard errors, so we use the `lm` linear model instead, from the `mlr3learners` package:

```
library(mlr3learners)

learner_lm = lrn("regr.lm")
learner_lm$predict_type = "se"
learner_lm$train(task_mtcars, splits$train)
predictions = learner_lm$predict(task_mtcars, splits$test)
predictions
```

```
<PredictionRegr> for 11 observations:
    row_ids truth response        se
          9  22.8 26.35691 1.4217357
         10  19.2 21.30664 0.9926847
         21  21.5 26.44570 1.2694455
---
         16  10.4 15.11714 2.1783078
         18  32.4 26.62327 1.1895495
         26  27.3 26.62199 1.1888914
```

> **Tip**
>
> Section 2.6.1 shows how to list learners that support the standard error prediction type.

The prediction object now contains the standard error for the predictions.

```
predictions
```

```
<PredictionRegr> for 11 observations:
    row_ids truth response        se
          9  22.8 26.35691 1.4217357
         10  19.2 21.30664 0.9926847
         21  21.5 26.44570 1.2694455
---
         16  10.4 15.11714 2.1783078
         18  32.4 26.62327 1.1895495
         26  27.3 26.62199 1.1888914
```

2.3. Evaluation

An important step of modeling is evaluating the performance of the trained model. We have seen how to inspect the model and plot its predictions above, but a more rigorous way that allows to compare different types of models more easily is to compute a performance measure. `mlr3` offers many performance measures, which can be created with the `msr()` function. Measures are stored in the dictionary `mlr_measures`, and a measure has to be supported by `mlr3` to be used, just like learners. For example, we can list all measures that are available for regression tasks:

```
mlr_measures$keys("regr")
```

```
 [1] "regr.bias"  "regr.ktau"  "regr.mae"   "regr.mape"  "regr.maxae"
 [6] "regr.medae" "regr.medse" "regr.mse"   "regr.msle"  "regr.pbias"
[11] "regr.rae"   "regr.rmse"  "regr.rmsle" "regr.rrse"  "regr.rse"
[16] "regr.rsq"   "regr.sae"   "regr.smape" "regr.srho"  "regr.sse"
```

Measure objects can be created with a single performance measure (`msr()`) or multiple (`msrs()`):

```
measure = msr("regr.rmse")
measures = msrs(c("regr.rmse", "regr.sse"))
```

At the core of all performance measures is a quantification of the difference between the predicted value and the ground truth value (except for unsupervised tasks, which we will discuss later). This means that in order to assess performance, we usually need the ground truth data – observations for which we do not know the true value cannot be used to assess the quality of the predictions of

a model. This is why we make predictions on the data the model did not use during training (the test set).

As we have seen above, mlr3's Prediction objects contain both predictions and ground truth. The Measure objects define how prediction and ground truth are compared, and how differences between them are quantified. We choose root mean squared error (regr.rmse) as our performance measure for this example. Once the measure is created, we can pass it to the $score() method of the Prediction object to quantify the predictive performance of our model.

```
measure = msr("regr.rmse")
measure
```

```
<MeasureRegrSimple:regr.rmse>: Root Mean Squared Error
* Packages: mlr3, mlr3measures
* Range: [0, Inf]
* Minimize: TRUE
* Average: macro
* Parameters: list()
* Properties: -
* Predict type: response
```

```
predictions$score(measure)
```

```
regr.rmse
 3.328844
```

> **Note**
>
> $score() can be called without a measure; in this case the default measure for the type of task is used. Regression defaults to mean squared error (regr.mse).

It is possible to calculate multiple measures at the same time by passing multiple measures to $score(). For example, to compute both root mean squared error regr.rmse and mean squared error regr.mse:

```
measures = msrs(c("regr.rmse", "regr.mse"))
predictions$score(measures)
```

```
regr.rmse  regr.mse
 3.328844 11.081203
```

mlr3 also provides measures that do not quantify the quality of the predictions of a model, but other information we may be interested in, for example the time it took to train the model and make predictions:

```
measures = msrs(c("time_train", "time_predict"))
predictions$score(measures, learner = learner_lm)
```

```
time_train time_predict
     0.004        0.003
```

Note that these measures require a trained learner in addition to the predictions.

Some measures have hyperparameters themselves, for example `selected_features`. This measure gives information on the features the model used and is only supported by learners that have the "selected_features" property. It requires a task and a learner in addition to the predictions. The `lm` model does not support showing selected features; we use the `rpart` learner again and the full `mtcars` task.

```
task_mtcars = tsk("mtcars")
splits = partition(task_mtcars)
learner_rpart = lrn("regr.rpart", minsplit = 10)

learner_rpart$train(task_mtcars, splits$train)
predictions = learner_rpart$predict(task_mtcars, splits$test)
measure = msr("selected_features")
predictions$score(measure, task = task_mtcars, learner = learner_rpart)
```

```
selected_features
                2
```

The hyperparameter of the measure specifies whether the number of selected features should be normalized by the total number of features. The default is `FALSE`, giving the absolute number of features that, in this case, the trained decision tree uses. We can change the hyperparameter in the same way as for learners, for example:

```
measure = msr("selected_features", normalize = TRUE)
predictions$score(measure, task = task_mtcars, learner = learner_rpart)
```

```
selected_features
              0.2
```

We have now seen the basic building blocks of `mlr3` – creating and partitioning a task, instantiating a learner and setting its hyperparameters, training a model and inspecting it, making predictions, and assessing the quality of the model with a performance measure. So far, we have focused on regression, where we want to predict a numeric quantity. The rest of this chapter looks at other task types. The general procedure it the same, but some details are different.

2.4. Classification

Classification predicts a discrete, categorical target instead of the continuous numeric quantity for regression. The models that learn to classify data are different from regression models, and regression learners are not applicable for classification problems (although for some learners, there are both regression and classification versions). mlr3 distinguishes between the different tasks and learner types through different R6 classes and different prefixes – regression learners and measures start with `regr.`, whereas classification learners and measures start with `classif.`.

2.4.1. Classification Tasks

The mlr_tasks dictionary that comes with mlr3 contains several classification tasks (TaskClassif). We can show only the classification tasks by converting the dictionary to a `data.table` and filtering on the `task_type`:

```
as.data.table(mlr_tasks)[task_type == "classif"]
```

```
               key                                    label task_type nrow
 1:   breast_cancer                  Wisconsin Breast Cancer   classif  683
 2:   german_credit                           German Credit   classif 1000
 3:           ilpd                Indian Liver Patient Data   classif  583
 4:           iris                             Iris Flowers   classif  150
 5:      optdigits Optical Recognition of Handwritten Digits   classif 5620
 6:       penguins                           Palmer Penguins   classif  344
 7: penguins_simple               Simplified Palmer Penguins   classif  333
 8:           pima                    Pima Indian Diabetes   classif  768
 9:          sonar                  Sonar: Mines vs. Rocks   classif  208
10:           spam                       HP Spam Detection   classif 4601
11:        titanic                                 Titanic   classif 1309
12:           wine                           Wine Regions   classif  178
13:            zoo                            Zoo Animals   classif  101
9 variables not shown: [ncol, properties, lgl, int, dbl, chr, fct, ord, pxc]
```

We will use the penguins dataset as a running example:

```
task_penguins = tsk("penguins")
task_penguins
```

```
<TaskClassif:penguins> (344 x 8): Palmer Penguins
* Target: species
* Properties: multiclass
* Features (7):
  - int (3): body_mass, flipper_length, year
  - dbl (2): bill_depth, bill_length
  - fct (2): island, sex
```

Just like for regression tasks, printing it gives an overview of the task, including the number of observations and features, and their types.

The target variable, species, is of type factor and has the following three classes or levels:

```
unique(task_penguins$data(cols = "species"))
```

```
     species
1:    Adelie
2:    Gentoo
3: Chinstrap
```

Classification tasks (`TaskClassif`) can also be plotted using `autoplot()`. Apart from the "pairs" plot type that we show here, "target" and "duo" are available. We refer the interested reader to the documentation of `mlr3viz::autoplot.TaskClassif` for an explanation of the other options. To keep the plot readable, we select only the first two features of the dataset.

```
library("mlr3viz")

task_penguins_small = task_penguins$clone()
task_penguins_small$select(head(task_penguins_small$feature_names, 2))
autoplot(task_penguins_small, type = "pairs")
```

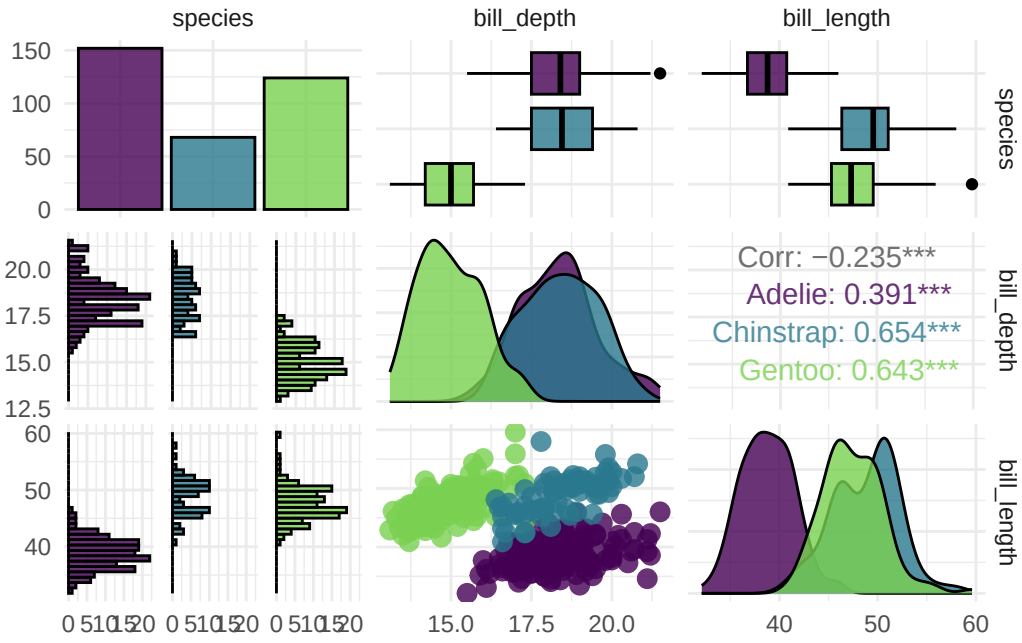


Figure 2.5.: Overview of the penguins dataset.

2.4.2. Classification Learners

Classification learners (`LearnerClassif`) are a different R6 class than regression learners (`LearnerRegr`), but also inherit from the base class `Learner`. We can instantiate a classification learner in the same way as a regression learner, by retrieving it from the `mlr_learners` dictionary using `lrn()`. Note the `classif.` prefix to denote that we want a learner that classifies observations:

```
learner_rpart = lrn("classif.rpart")
learner_rpart
```

```
<LearnerClassifRpart:classif.rpart>: Classification Tree
* Model: -
* Parameters: xval=0
* Packages: mlr3, rpart
* Predict Types:  [response], prob
* Feature Types: logical, integer, numeric, factor, ordered
* Properties: importance, missings, multiclass, selected_features,
  twoclass, weights
```

Just like regression learners, classification learners have hyperparameters we can set to change their behavior, and printing the learner object gives some basic information about it. Training a model and making predictions works in the same way as for regression:

```
splits = partition(task_penguins)
learner_rpart$train(task_penguins, splits$train)
learner_rpart$model
```

```
n= 231

node), split, n, loss, yval, (yprob)
      * denotes terminal node

1) root 231 129 Adelie (0.441558442 0.199134199 0.359307359)
  2) flipper_length< 206.5 143  43 Adelie (0.699300699 0.293706294 0.006993007)
    4) bill_length< 44.2 101   3 Adelie (0.970297030 0.029702970 0.000000000) *
    5) bill_length>=44.2 42   3 Chinstrap (0.047619048 0.928571429 0.023809524) *
  3) flipper_length>=206.5 88   6 Gentoo (0.022727273 0.045454545 0.931818182)
    6) bill_depth>=17.2 7   3 Chinstrap (0.285714286 0.571428571 0.142857143) *
    7) bill_depth< 17.2 81   0 Gentoo (0.000000000 0.000000000 1.000000000) *
```

```
predictions = learner_rpart$predict(task_penguins, splits$test)
predictions
```

```
<PredictionClassif> for 113 observations:
    row_ids     truth  response
          2    Adelie    Adelie
          3    Adelie    Adelie
         10    Adelie    Adelie
---
        332 Chinstrap Chinstrap
        335 Chinstrap Chinstrap
        341 Chinstrap    Adelie
```

Just like predictions of regression models, we can plot classification predictions with `autoplot()`:

```
library("mlr3viz")
autoplot(predictions)
```

Figure 2.6.: Comparing predicted and ground truth values for the penguins dataset.

2.4.2.1. Changing the Prediction Type

Classification problems support two types of predictions: the default "response", i.e. the class label, and "prob", which gives the probability for each class label. Not all learners support predicting probabilities.

The prediction type for a learner can be changed by setting `$predict_type`. After retraining the learner, all predictions have class probabilities (one for each class) in addition to the response, which is the class with the highest probability:

```
learner_rpart$predict_type = "prob"
learner_rpart$train(task_penguins, splits$train)
predictions = learner_rpart$predict(task_penguins, splits$test)
predictions
```

```
<PredictionClassif> for 113 observations:
    row_ids     truth  response prob.Adelie prob.Chinstrap prob.Gentoo
          2    Adelie    Adelie  0.97029703     0.02970297  0.00000000
          3    Adelie    Adelie  0.97029703     0.02970297  0.00000000
         10    Adelie    Adelie  0.97029703     0.02970297  0.00000000
---
        332 Chinstrap Chinstrap  0.04761905     0.92857143  0.02380952
        335 Chinstrap Chinstrap  0.04761905     0.92857143  0.02380952
        341 Chinstrap    Adelie  0.97029703     0.02970297  0.00000000
```

> **Tip**
>
> Section 2.6.1 shows how to list learners that support the probability prediction type.

2.4.3. Classification Evaluation

Evaluation measures for classification problems that are supported by `mlr3` can be found in the `mlr_measures` dictionary:

```
mlr_measures$keys("classif")
```

```
 [1] "classif.acc"         "classif.auc"         "classif.bacc"
 [4] "classif.bbrier"      "classif.ce"          "classif.costs"
 [7] "classif.dor"         "classif.fbeta"       "classif.fdr"
[10] "classif.fn"          "classif.fnr"         "classif.fomr"
[13] "classif.fp"          "classif.fpr"         "classif.logloss"
[16] "classif.mauc_au1p"   "classif.mauc_au1u"   "classif.mauc_aunp"
[19] "classif.mauc_aunu"   "classif.mbrier"      "classif.mcc"
[22] "classif.npv"         "classif.ppv"         "classif.prauc"
[25] "classif.precision"   "classif.recall"      "classif.sensitivity"
[28] "classif.specificity" "classif.tn"          "classif.tnr"
[31] "classif.tp"          "classif.tpr"
```

Some of these measures require the predictition type to be "prob" (e.g. `classif.auc`). As the default is "response", using those measures requires to change the prediction type, as shown above. You can check what prediction type a measure requires by looking at `$predict_type`.

```
measure = msr("classif.acc")
measure$predict_type
```

```
[1] "response"
```

Once we have created a classification measure, we can give it to the `$score()` method to compute its value for a given `PredictionClassif` object:

```
predictions$score(measure)
```

```
classif.acc
  0.9557522
```

2.4.3.1. Confusion Matrix

A popular way to show the quality of prediction of a classification model is a confusion matrix. It gives a quick overview of what observations are misclassified, and how they are misclassified. The rows in a confusion matrix are the predicted class and the columns are the true class. All off-diagonal entries are incorrectly classified observations, and all diagonal entries are correctly classified. More information on Wikipedia[2].

`mlr3` supports confusion matrices through the `$confusion` property of the `PredictionClassif` object:

```
predictions$confusion
```

```
           truth
response    Adelie Chinstrap Gentoo
  Adelie        49         3      0
  Chinstrap      1        19      1
  Gentoo         0         0     40
```

In this case, our classifier does fairly well classifying the penguins.

2.4.4. Binary Classification and Positive Classes

Classification problems with a two-class target are called binary classification tasks. Binary Classification is special in the sense that one of these classes is denoted *positive* and the other one *negative*. You can specify the *positive class* for a `classification task` object during task creation. If not explicitly set during construction, the positive class defaults to the first level of the target feature.

[2] https://en.wikipedia.org/wiki/Confusion_matrix

```
# during construction
data("Sonar", package = "mlbench")
task_sonar = as_task_classif(Sonar, target = "Class", positive = "R")

# switch positive class to level 'M'
task_sonar$positive = "M"
```

2.4.5. Thresholding

Models trained on binary classification tasks that predict the probability for the positive class usually use a simple rule to determine the predicted class label – if the probability is more than 50%, predict the positive label; otherwise, predict the negative label. In some cases, you may want to adjust this threshold, for example, if the classes are very unbalanced (i.e., one is much more prevalent than the other). For example, in the "german_credit" dataset, the credit risk is good for far more observations.

Training a classifier on this data overpredicts the majority class, i.e. the more prevalent class is more likely to be predicted for any given observation.

```
task_credit = tsk("german_credit")
splits = partition(task_credit)
learner = lrn("classif.rpart", predict_type = "prob")
learner$train(task_credit)
predictions = learner$predict(task_credit)
autoplot(predictions)
```

Figure 2.7.: Comparing predicted and ground truth values for the german_credit dataset.

Changing the prediction threshold allows to address this without having to adjust the hyperparameters of the learner or retrain the model.

```
predictions$set_threshold(0.7)
autoplot(predictions)
```

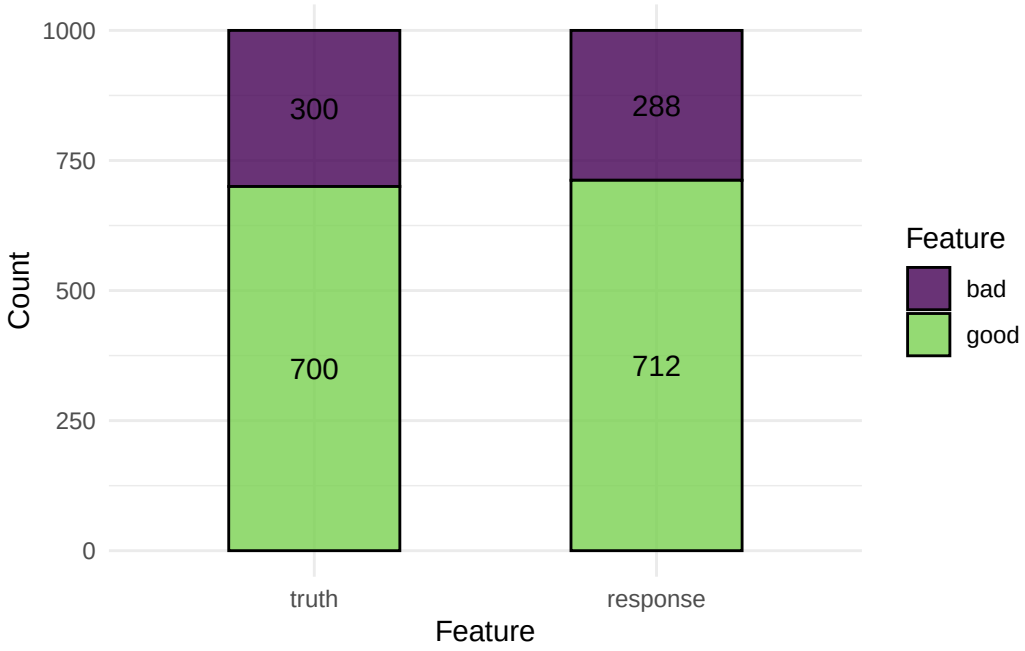


Figure 2.8.: Comparing predicted and ground truth values for the german_credit dataset with adjusted threshold.

> **Tip**
>
> Thresholds can be tuned automatically with respect to prediction performance with the `mlr3pipelines` package using `PipeOpTuneThreshold`. This is covered in Chapter 6.

Thresholding For Multiple Classes

For classification tasks with more than two classes you can also adjust the prediction threshold, which is 0.5 for each class by default. Thresholds work slightly differently with multiple classes:

- The probability for a data point is divided by each class threshold resulting in `n` ratios for `n` classes.
- The highest ratio is selected (ties are random by default).

Lowering the threshold for a class means that it is more likely to be predicted and raising it has the opposite effect. The `zoo` dataset illustrates this concept nicely.
When trained normally some classes are not predicted at all:

```r
task = tsk("zoo")
learner = lrn("classif.rpart", predict_type = "prob")
learner$train(task)
preds = learner$predict(task)

autoplot(preds)
```

Figure 2.9.: Comparing predicted and ground truth values for the zoo dataset.

The classes `amphibian` and `insect` are never predicted. On the other hand, the classes `mollusc` and `reptile` are predicted more often than they appear in the truth data. We can address this by lowering the threshold for `amphibian` and `insect`. `$set_threshold()` can be given a named list to set the threshold for all classes at once:

```r
# c("mammal", "bird", "reptile", "fish", "amphibian", "insect", "mollusc.et.al")
new_thresh = c(0.5, 0.5, 0.5, 0.5, 0.4, 0.4, 0.5)
names(new_thresh) = task$class_names

autoplot(preds$set_threshold(new_thresh))
```

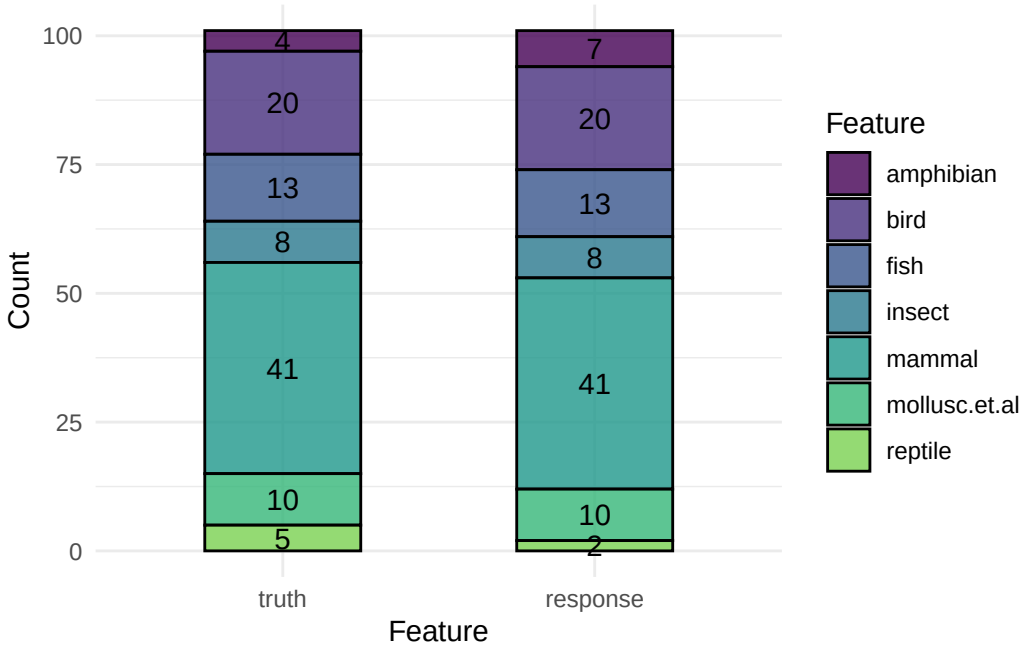


Figure 2.10.: Comparing predicted and ground truth values for the zoo dataset with adjusted thresholds.

We can again see that adjusting the thresholds results in better predictive performance, without having to retrain a model.

2.5. Additional Task Types

In addition to regression and classification, `mlr3` supports more types of tasks:

- Clustering (`mlr3cluster::TaskClust` in package `mlr3cluster`): An unsupervised task to identify similar groups within the feature space.
- Survival (`mlr3proba::TaskSurv` in package `mlr3proba`): The target is the (right-censored) time to an event.
- Density (`mlr3proba::TaskDens` in package `mlr3proba`): An unsupervised task to estimate the undetectable underlying probability distribution, based on observed data (as a numeric vector or a one-column matrix-like object).

Other task types that are less common are described in Chapter 8.

2.6. Additional Learners

As mentioned above, `mlr3` supports many learners. They can be accessed through three packages: the `mlr3` package, the `mlr3learners` package, and the `mlr3extralearners` package.

The list of learners included in the mlr3 package is dliberately small to avoid large sets of dependencies for this core package:

- Featureless classifier classif.featureless: Simple baseline classification learner. Predicts the label that is most frequent in the training set. It can be used as a "fallback learner" to make predictions if another, more sophisticated, learner fails for some reason.
- Featureless regressor regr.featureless: Simple baseline regression learner. Predicts the mean of the target values in the training set.
- Rpart decision tree learner classif.rpart: Tree learner from rpart.
- Rpart regression tree learner regr.rpart: Tree learner from rpart.

The mlr3learners package contains cherry-picked implementations of the most popular machine learning methods:

- Linear (regr.lm) and logistic (classif.log_reg) regression.
- Penalized Generalized Linear Models (regr.glmnet, classif.glmnet), possibly with built-in optimization of the penalization parameter (regr.cv_glmnet, classif.cv_glmnet).
- (Kernelized) k-Nearest Neighbors regression (regr.kknn) and classification (classif.kknn).
- Kriging / Gaussian Process Regression (regr.km).
- Linear (classif.lda) and Quadratic (classif.qda) Discriminant Analysis.
- Naïve Bayes Classification (classif.naive_bayes).
- Support-Vector machines (regr.svm, classif.svm).
- Gradient Boosting (regr.xgboost, classif.xgboost).
- Random Forests for regression and classification (regr.ranger, classif.ranger).

A complete list of supported learners across all mlr3 packages is hosted on our website[3].

The dictionary mlr_learners contains the supported learners and changes as packages are loaded. At the time of writing, mlr3 supports six learners, mlr3learners 21 learners, mlr3extralearners 88 learners, mlr3proba five learners, and mlr3cluster 19 learners.

2.6.1. Listing Learners

You can list all learners by converting the mlr_learners dictionary into a data.table:

```
1  as.data.table(mlr_learners)
```

```
                    key                          label task_type
  1:  classif.AdaBoostM1              Adaptive Boosting   classif
  2:         classif.C50               Tree-based Model   classif
  3:         classif.IBk              Nearest Neighbour   classif
  4:         classif.J48               Tree-based Model   classif
  5:        classif.JRip Propositional Rule Learner.    classif
 ---
136: surv.priority_lasso                 Priority Lasso      surv
137:         surv.ranger                  Random Forest      surv
```

[3] https://mlr-org.com/learners.html

```
138:          surv.rfsrc               Random Forest      surv
139:            surv.svm      Support Vector Machine      surv
140:        surv.xgboost           Gradient Boosting      surv
4 variables not shown: [feature_types, packages, properties, predict_types]
```

The resulting `data.table` contains a lot of meta-data that is useful for identifying learners that have particular properties. For example, we can list all learners that support regression problems:

```
as.data.table(mlr_learners)[task_type == "regr"]
```

```
             key                                     label task_type
 1:      regr.IBk                      K-nearest neighbour      regr
 2:  regr.M5Rules                     Rule-based Algorithm      regr
 3:    regr.abess Fast Best Subset Selection for Regression      regr
 4:     regr.bart        Bayesian Additive Regression Trees      regr
 5: regr.catboost                         Gradient Boosting      regr
---
35:    regr.rpart                           Regression Tree      regr
36:      regr.rsm                  Response Surface Model      regr
37:      regr.rvm                 Relevance Vector Machine      regr
38:      regr.svm                                     <NA>      regr
39:  regr.xgboost                                     <NA>      regr
4 variables not shown: [feature_types, packages, properties, predict_types]
```

We can check multiple conditions, to for example find all learners that support regression problems and can predict standard errors:

```
as.data.table(mlr_learners)[task_type == "regr" &
    sapply(predict_types, function(x) "se" %in% x)]
```

```
               key                                     label task_type
1:       regr.debug             Debug Learner for Regression      regr
2:       regr.earth Multivariate Adaptive Regression Splines      regr
3: regr.featureless           Featureless Regression Learner      regr
4:         regr.gam    Generalized Additive Regression Model      regr
5:         regr.glm            Generalized Linear Regression      regr
6:          regr.km                                     <NA>      regr
7:          regr.lm                                     <NA>      regr
8:         regr.mob       Model-based Recursive Partitioning      regr
9:      regr.ranger                                     <NA>      regr
4 variables not shown: [feature_types, packages, properties, predict_types]
```

Or we can list all learners that support classification problems and missing feature values:

```
as.data.table(mlr_learners)[task_type == "classif" &
    sapply(properties, function(x) "missings" %in% x)]
```

```
                       key                                label task_type
 1:              classif.C50                   Tree-based Model   classif
 2:              classif.J48                   Tree-based Model   classif
 3:             classif.PART                   Tree-based Model   classif
 4:         classif.catboost                  Gradient Boosting   classif
 5:            classif.debug   Debug Learner for Classification   classif
 6:      classif.featureless Featureless Classification Learner   classif
 7:              classif.gbm                  Gradient Boosting   classif
 8: classif.imbalanced_rfsrc           Imbalanced Random Forest   classif
 9:         classif.lightgbm                  Gradient Boosting   classif
10:            classif.rfsrc                      Random Forest   classif
11:            classif.rpart               Classification Tree   classif
12:          classif.xgboost                              <NA>   classif
4 variables not shown: [feature_types, packages, properties, predict_types]
```

2.7. Exercises

1. Using the Sonar dataset, measure the classification error (`classif.ce`) of a classification tree model (`classif.rpart`) trained with default hyperparameters on 80% of the data and tested on the remaining 20%.
2. Give the true positive, false positive, true negative, and false negative rates of the predictions made by the model in problem 1.
3. Change the threshold of the model from problem 1 such that the false positive rate is lower than the false negative rate. Give a reason why you might do this.

3. Evaluation, Resampling and Benchmarking

Estimating the generalization performance of a machine learning algorithm on a given task requires additional data not used during training. Resampling refers to the process of repeatedly splitting the available data into training and test sets to enable unbiased performance estimation. This chapter introduces common resampling strategies and illustrates their use with the `mlr3` ecosystem. Benchmarking builds upon resampling, encompassing the fair comparison of multiple machine learning algorithms on at least one task. We show how benchmarking can be performed within the `mlr3` ecosystem, from the construction of benchmark designs to the statistical analysis of the benchmark results.

In supervised machine learning, a model which is deployed in practice is expected to generalize well to new, unseen data. Accurate estimation of this so-called generalization performance is crucial for many aspects of machine learning application and research — whether we want to fairly compare a novel algorithm with established ones or to find the best algorithm for a particular task after tuning — we always rely on this performance estimate. Hence, performance estimation is a fundamental concept used for model selection, model comparison, and hyperparameter tuning (which will be discussed in depth in Chapter 4) in supervised machine learning. To properly assess the generalization performance of a model, we must first decide on a performance measure that is appropriate for our given task and evaluation goal. A performance measure typically computes a numeric score indicating, e.g., how well the model predictions match the ground truth. However, it may also reflect other qualities such as the time for training a model. An overview of some common performance measures implemented in `mlr3`, including a short description and a basic mathematical definition, can be found by following the link provided in the overview table under *Measures overview* in Appendix Appendix D.

Once we have decided on a performance measure, the next step is to adopt a strategy that defines how to use the available data to estimate the generalization performance. Unfortunately, using the same data to train and test a model is a bad strategy as it would lead to an overly optimistic performance estimate. For example, an overfitted model may perfectly fit the data on which it was trained, but may not generalize well to new data. Assessing its performance using the same data it was trained would misleadingly suggest a well-performing model. It is therefore common practice to test a model on independent data not used to train a model. However, we typically train a deployed model on all available data, which leaves no data to assess its generalization performance. To address this issue, existing performance estimation strategies withhold a subset of the available data for evaluation purposes. This so-called test set serves as unseen data and is used to estimate the generalization performance.

A common simple strategy is the holdout method, which randomly partitions the data into a single training and test set using a pre-defined splitting ratio. The training set is used to create an intermediate model, whose sole purpose is to estimate the performance using the test set. This

performance estimate is then used as a proxy for the performance of the final model trained on all available data and deployed in practice. Ideally, the training set should be as large as all available data so that the intermediate model represents the final model well. If the training data is much smaller, the intermediate model learns less complex relationships compared to the final model, resulting in a pessimistically biased performance estimate. On the other hand, we also want as much test data as possible to reliably estimate the generalization performance. However, both goals are not possible if we have only access to a limited amount of data.

To address this issue, resampling strategies (see Section 3.2) repeatedly split all available data into multiple training and test sets, with one repetition corresponding to what is called a resampling iteration in `mlr3`. An intermediate model is then trained on each training set and the remaining test set is used to measure the performance in each resampling iteration. The generalization performance is finally estimated by the averaged performance over multiple resampling iterations (see Figure 3.1 for an illustration). Resampling methods allow using more data points for testing, while keeping the training sets as large as possible. Specifically, repeating the data splitting process allows using all available data points to assess the performance, as each data point can be ensured to be part of the test set in at least one resampling iteration. A higher number of resampling iterations can reduce the variance and result in a more reliable performance estimate. It also reduces the risk of the performance estimate being strongly affected by an unlucky split that does not reflect the original data distribution well, which is a known issue of the holdout method. However, since resampling strategies create multiple intermediate models trained on different parts of the available data and average their performance, they evaluate the performance of the learning algorithm that induced these models, rather than the performance of the final model which is deployed in practice. It is therefore important to train the intermediate models on nearly all data points from the same distribution so that the intermediate models and the final model are similar. If we only have access to a limited amount of data, the best we can do is to use the performance of the learning algorithm as a proxy for the performance of the final model. In Section 3.2, we will learn how to estimate the generalization performance of a `Learner` using the `mlr3` package.

3.1. Quick Start

In the previous chapter, we have applied the holdout method by manually partitioning the data contained in a `Task` object into a single training set (to train the model) and a single test set (to estimate the generalization performance). As a quick start into resampling and benchmarking with the `mlr3` package, we show a short example of how to do this with the `resample()` and `benchmark()` convenience functions. Specifically, we show how to estimate the generalization performance of a learner on a given task by the holdout method using `resample()` and how to use `benchmark()` to compare two learners on a task.

We first define the corresponding `Task` and `Learner` objects used throughout this chapter as follows:

```
task = tsk("penguins")
learner = lrn("classif.rpart", predict_type = "prob")
```

The next obvious step is to select a suitable performance measure, which can be done as explained in Section 2.3 using the `mlr_measures` dictionary. Passing the dictionary to the `as.data.table`

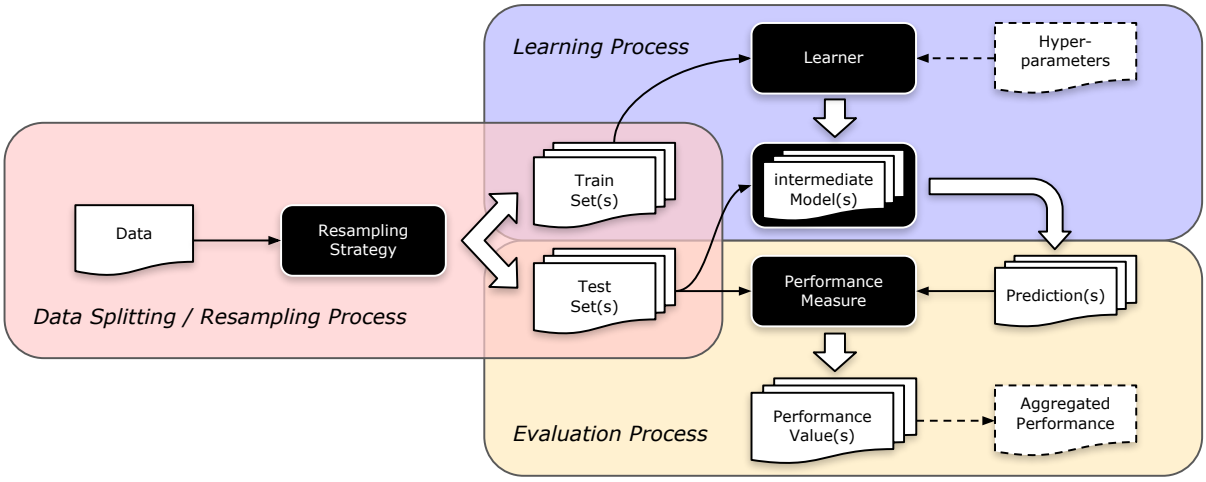


Figure 3.1.: A general abstraction of the performance estimation process: The available data is (repeatedly) split into (a set of) training data and test data (data splitting / resampling process). The learner is applied to each training data and produces intermediate models (learning process). Each intermediate model along with its associated test data produces predictions. The performance measure compares these predictions with the associated actual target values from each test data and computes a performance value for each test data. All performance values are aggregated into a scalar value to estimate the generalization performance (evaluation process).

function provides an overview of implemented measures with additional information from which we can select a suitable performance measure, which we print here in two parts for compactness:

```
msr_tbl = as.data.table(mlr_measures)
msr_tbl[1:5, .(key, label, task_type)]
```

```
            key                          label task_type
1:          aic   Akaika Information Criterion      <NA>
2:          bic Bayesian Information Criterion      <NA>
3:  classif.acc        Classification Accuracy   classif
4:  classif.auc       Area Under the ROC Curve   classif
5: classif.bacc              Balanced Accuracy   classif
```

```
msr_tbl[1:5, .(key, packages, predict_type, task_properties)]
```

```
            key          packages predict_type task_properties
1:          aic              mlr3     response
2:          bic              mlr3     response
3:  classif.acc mlr3,mlr3measures     response
4:  classif.auc mlr3,mlr3measures         prob        twoclass
5: classif.bacc mlr3,mlr3measures     response
```

Depending on our task at hand, we will look for a measure that fits our `"task_type"` (`"classif"` for `penguins`) and `"task_properties"`. The latter is important since measures like AUC `"classif.auc"` are only defined for binary tasks, which is indicated by `"twoclass"` in the `"task_properties"` column — multiclass-generalizations are available, but need to be selected explicitly. Similarly, some measures require the learner to predict probabilities, while others require class predictions. In our learner above, we have already selected `predict_type = "prob"`, which is often required for measures that are not defined on class labels, such as the aforementioned AUC.

> **Tip**
>
> More information about a performance measure, including its mathematical definition, can be obtained using the `$help()` method of a `Measure` object, which opens the help page of the corresponding measure, e.g., `msr("classif.acc")$help()` provides all information about the classification accuracy.

The code example below shows how to apply holdout (specified using `rsmp("holdout")`) on the previously specified `mlr_tasks_penguins` task to estimate classification accuracy (using `msr("classif.acc")`) of the previously defined decision tree learner from the `rpart` package:

```
resampling = rsmp("holdout")
rr = resample(task = task, learner = learner, resampling = resampling)
rr$aggregate(msr("classif.acc"))
```

```
classif.acc
  0.9391304
```

The `benchmark()` function internally uses the `resample()` function to estimate the performance based on a resampling strategy. For illustration, we show a minimal code example that compares the classification accuracy of the decision tree against a featureless learner which always predicts the majority class:

```
lrns = c(learner, lrn("classif.featureless"))
d = benchmark_grid(task = task, learner = lrns, resampling = resampling)
bmr = benchmark(design = d)
acc = bmr$aggregate(msr("classif.acc"))
acc[, .(task_id, learner_id, classif.acc)]
```

```
    task_id          learner_id classif.acc
1: penguins       classif.rpart   0.9565217
2: penguins classif.featureless   0.4695652
```

Further details on resampling and benchmarking can be found in Section 3.2 and Section 3.3.

3.2. Resampling

Existing resampling strategies differ in how they partition the available data into training and test set, and a comprehensive overview can be found in Japkowicz and Shah (2011). For example, the k-fold cross-validation method randomly partitions the data into k subsets, called folds (see Figure 3.2). Then k models are trained on training data consisting of $k-1$ of the folds, with the remaining fold being used as test data exactly once in each of the k iterations. The k performance estimates resulting from each fold are then averaged to obtain a more reliable performance estimate. This makes cross-validation a popular strategy, as each observation is guaranteed to be used in one of the test sets throughout the procedure, making efficient use of the available data for performance estimation. Several variations of cross-validation exist, including repeated k-fold cross-validation where the entire process illustrated in Figure 3.2 is repeated multiple times, and leave-one-out cross-validation where the test set in each fold consists of exactly one observation.

Other well-known resampling strategies include subsampling and bootstrapping. Subsampling — also known as repeated holdout — repeats the holdout method and creates multiple train-test splits, taking into account the ratio of observations to be included in the training sets. Bootstrapping creates training sets by randomly drawing observations from all available data with replacement. Some observations in the training sets may appear more than once, while the other observations that do not appear at all are used as test set. The choice of the resampling strategy usually depends on the specific task at hand and the goals of the performance assessment. Properties and pitfalls of different resampling techniques have been widely studied and discussed in the literature, see e.g., Bengio and Grandvalet (2003), Molinaro, Simon, and Pfeiffer (2005), Kim (2009), Bischl et al. (2012).

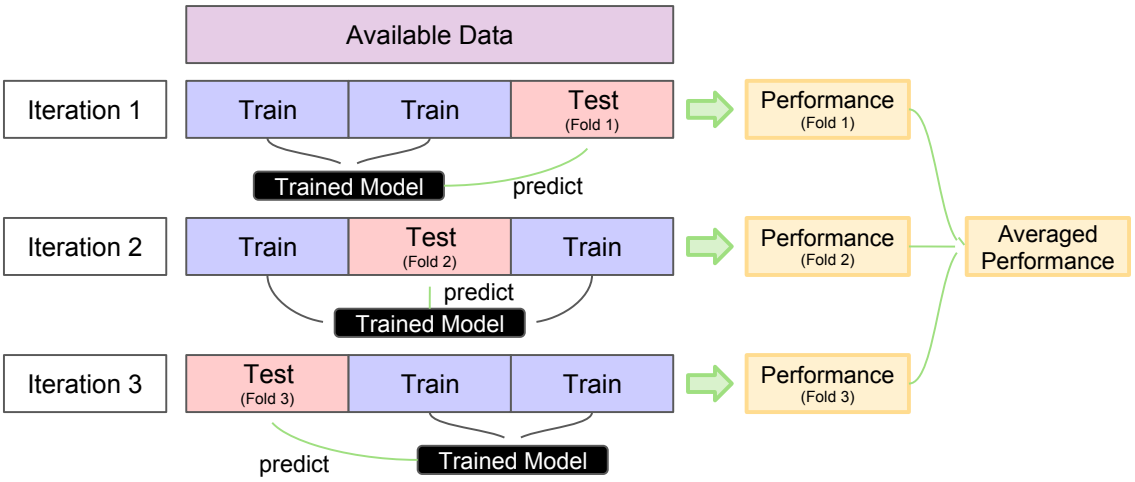


Figure 3.2.: Illustration of a 3-fold cross-validation.

In `mlr3`, many resampling strategies have already been implemented so that users do not have to implement them from scratch, which can be tedious and error-prone. In this section, we cover how to use `mlr3` to

- query (Section 3.2.1) implemented resampling strategies,
- construct (Section 3.2.2) resampling objects for a selected resampling strategy,

- instantiate (Section 3.2.3) the train-test splits of a resampling object on a given task, and
- execute (Section 3.2.4) the selected resampling strategy on a learning algorithm to obtain resampling results.

3.2.1. Query

All implemented resampling strategies can be queried by looking at the `mlr_resamplings` dictionary (also listed in Appendix Appendix D). Passing the dictionary to the `as.data.table` function provides a more structured output with additional information:

```
as.data.table(mlr_resamplings)
```

```
           key                         label        params iters
1:   bootstrap                     Bootstrap ratio,repeats    30
2:      custom                  Custom Splits                  NA
3:   custom_cv Custom Split Cross-Validation                  NA
4:          cv              Cross-Validation         folds    10
5:     holdout                      Holdout         ratio     1
6:    insample           Insample Resampling                   1
7:         loo                 Leave-One-Out                  NA
8: repeated_cv     Repeated Cross-Validation folds,repeats   100
9: subsampling                   Subsampling ratio,repeats    30
```

For example, the column `params` shows the parameters of each resampling strategy (e.g., the train-test splitting `ratio` or the number of `repeats`) and the column `iters` shows the default value for the number of performed resampling iterations (i.e., the number of model fits).

3.2.2. Construction

Once we have decided on a resampling strategy, we have to construct a `Resampling` object via the function `rsmp()` which will define the resampling strategy we want to employ. For example, to construct a `Resampling` object for holdout, we use the value of the `key` column from the `mlr_resamplings` dictionary and pass it to the convenience function `rsmp()`:

```
resampling = rsmp("holdout")
print(resampling)
```

```
<ResamplingHoldout>: Holdout
* Iterations: 1
* Instantiated: FALSE
* Parameters: ratio=0.6667
```

By default, the holdout method will use 2/3 of the data as training set and 1/3 as test set. We can adjust this by specifying the `ratio` parameter for holdout either during construction or by updating the `ratio` parameter afterwards. For example, we construct a `Resampling` object for holdout with a 80:20 split (see first line in the code below) then update to 50:50 (see second line in the code below):

```
resampling = rsmp("holdout", ratio = 0.8)
resampling$param_set$values = list(ratio = 0.5)
```

Holdout only estimates the generalization performance using a single test set. To obtain a more reliable performance estimate by making use of all available data, we may use other resampling strategies. For example, we could also set up a 10-fold cross-validation via

```
resampling = rsmp("cv", folds = 10)
```

By default, the `$is_instantiated` field of a `Resampling` object constructed as shown above is set to `FALSE`. This means that the resampling strategy is not yet applied to a task, i.e., the train-test splits are not contained in the `Resampling` object.

3.2.3. Instantiation

To generate the train-test splits for a given task, we need to instantiate a resampling strategy by calling the `$instantiate()` method of the previously constructed `Resampling` object on a `Task`. This will manifest a fixed partition and store the row indices for the training and test sets directly in the `Resampling` object. We can access these rows via the `$train_set()` and `$test_set()` methods:

```
resampling = rsmp("holdout", ratio = 0.8)
resampling$instantiate(task)
train_ids = resampling$train_set(1)
test_ids = resampling$test_set(1)
str(train_ids)
```

```
 int [1:275] 2 3 4 5 6 7 8 9 10 11 ...
```

```
str(test_ids)
```

```
 int [1:69] 1 12 16 22 26 28 30 32 37 38 ...
```

Instantiation is especially relevant is when the aim is to fairly compare multiple learners. Here, it is crucial to use the same train-test splits to obtain comparable results. That is, we need to ensure that all learners to be compared use the same training data to build a model and that they use the same test data to evaluate the model performance.

> **Tip**
>
> In Section 3.3, you will learn about the `ref ("benchmark()")` function, which automatically instantiates `Resampling` objects on all tasks to ensure a fair comparison by making use of the exact same training and test sets for learning and evaluating the fitted intermediate models.

3.2.4. Execution

Calling the function `resample()` on a task, learner, and constructed resampling object returns a `ResampleResult` object which contains all information needed to estimate the generalization performance. Specifically, the function will internally use the learner to train a model for each training set determined by the resampling strategy and store the model predictions of each test set. We can apply the `print` or `as.data.table` function to a `ResampleResult` object to obtain some basic information:

```
resampling = rsmp("cv", folds = 4)
rr = resample(task, learner, resampling)
print(rr)
```

```
<ResampleResult> of 4 iterations
* Task: penguins
* Learner: classif.rpart
* Warnings: 0 in 0 iterations
* Errors: 0 in 0 iterations
```

```
as.data.table(rr)
```

```
                task                    learner         resampling iteration
1: <TaskClassif[50]> <LearnerClassifRpart[38]> <ResamplingCV[20]>         1
2: <TaskClassif[50]> <LearnerClassifRpart[38]> <ResamplingCV[20]>         2
3: <TaskClassif[50]> <LearnerClassifRpart[38]> <ResamplingCV[20]>         3
4: <TaskClassif[50]> <LearnerClassifRpart[38]> <ResamplingCV[20]>         4
1 variable not shown: [prediction]
```

Here, we used 4-fold cross-validation as resampling strategy. The resulting `ResampleResult` object (stored as `rr`) provides various methods to access the stored information. The two most relevant methods for performance assessment are `$score()` and `$aggregate()`.

In Section 2.3, we learned that `Prediction` objects contain both model predictions and ground truth values, which are used to calculate the performance measure using the `$score()` method. Similarly, we can use the `$score()` method of a `ResampleResult` object to calculate the performance measure for each resampling iteration separately. This means that the `$score()` method produces one value per resampling iteration that reflects the performance estimate of the intermediate model trained in the corresponding iteration. By default, `$score()` uses the test set in each resampling iteration to calculate the performance measure.

> **Tip**
>
> We are not limited to scoring predictions on the test set — if we set the argument `predict_sets = "train"` within the `$score()` method, we calculate the performance measure of each resampling iteration based on the training set instead of the test set.

In the code example below, we explicitly use the classification accuracy (`classif.acc`) as performance measure and pass it to the `$score()` method to obtain the estimated performance of each resampling iteration separately:

```
acc = rr$score(msr("classif.acc"))
acc[, .(iteration, classif.acc)]
```

```
   iteration classif.acc
1:         1   0.9418605
2:         2   0.9767442
3:         3   0.9069767
4:         4   0.9534884
```

> **Tip**
>
> If we do not explicitly pass a `Measure` object to the `$score()` method, the classification error (`classif.ce`) and the mean squared error (`regr.mse`) are used as defaults for classification and regression tasks respectively.

Similarly, we can pass `Measure` objects to the `$aggregate()` method to calculate an aggregated score across all resampling iterations. The type of aggregation is usually determined by the `Measure` object (see also the fields `$average` and `$aggregator` the in help page of `Measure` for more details). There are two approaches for aggregating scores across resampling iterations: The first is referred to as the macro average, which first calculates the measure in each resampling iteration separately, and then averages these scores across all iterations. The second approach is the micro average, which pools all predictions across resampling iterations into one `Prediction` object and computes the measure on this directly. The classification accuracy `msr("classif.acc")` uses the macro-average by default, but the micro-average can be computed as well by specifying the `average` argument:

```
rr$aggregate(msr("classif.acc"))
```

```
classif.acc
  0.9447674
```

```
rr$aggregate(msr("classif.acc", average = "micro"))
```

```
classif.acc
  0.9447674
```

Tip

The classification accuracy compares the predicted class and the ground truth class of a single observation (point-wise loss) and calculates the proportion of correctly classified observations (average of point-wise loss). For performance measures that simply take the (unweighted) average of point-wise losses such as the classification accuracy, macro-averaging and micro-averaging will be equivalent unless the test sets in each resampling iteration have different sizes. For example, in the code example above, macro-averaging and micro-averaging yield the same classification accuracy because the `mlr_tasks_penguins` task (consisting of 344 observations) is split into 4 equally-sized test sets (consisting of 86 observations each) due to the 4-fold cross-validation. If we would use 5-fold cross-validation instead, macro-averaging and micro-averaging can lead to a (slightly) different performance estimate as the test sets can not have the exact same size:

```
rr5 = resample(task, learner, rsmp("cv", folds = 5))
rr5$aggregate(msr("classif.acc"))
```

```
classif.acc
  0.9415601
```

```
rr5$aggregate(msr("classif.acc", average = "micro"))
```

```
classif.acc
  0.9418605
```

For other performance measures that are not defined on observation level but rather on a set of observations such as the area under the ROC curve `msr("classif.auc")`, macro-averaging and micro-averaging will usually always lead to different values.

The aggregated score (as returned by `$aggregate()`) refers to the generalization performance of our selected learner on the given task estimated by the resampling strategy defined in the `Resampling` object. While we are usually interested in this aggregated score, it can be useful to look at the individual performance values of each resampling iteration (as returned by the `$score()` method) as well, e.g., to see if one (or more) of the iterations lead to very different performance results. Figure 3.3 visualizes the relationship between `$score()` and `$aggregate()` for a small example based on the `"penguins"` task.

3.2.5. Inspect ResampleResult Objects

In this section, we show how to inspect some important fields and methods of a `ResampleResult` object. We first take a glimpse at what is actually contained in the object by converting it to a `data.table`:

```
rrdt = as.data.table(rr)
rrdt
```

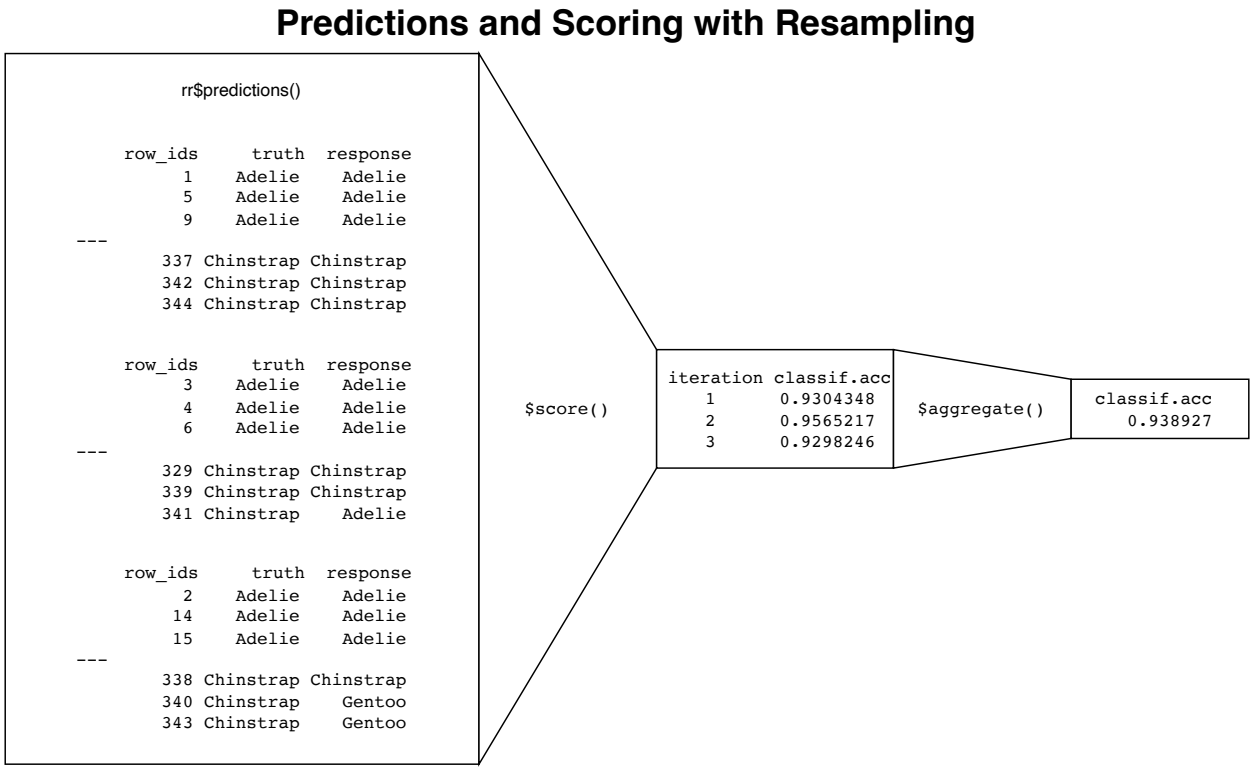


Figure 3.3.: An example of the difference between `$score()` and `$aggregate()`: The former aggregates predictions to a single score within each resampling iteration, and the former aggregates scores across all resampling folds

```
                task                    learner         resampling iteration
1: <TaskClassif[50]> <LearnerClassifRpart[38]> <ResamplingCV[20]>         1
2: <TaskClassif[50]> <LearnerClassifRpart[38]> <ResamplingCV[20]>         2
3: <TaskClassif[50]> <LearnerClassifRpart[38]> <ResamplingCV[20]>         3
4: <TaskClassif[50]> <LearnerClassifRpart[38]> <ResamplingCV[20]>         4
1 variable not shown: [prediction]
```

We can see that the task, learner and resampling strategy which we previously passed to the `resample()` function is stored in list columns of the `data.table`. In addition, we also have an integer column `iteration` that refers to the resampling iteration and another list column that contains the corresponding `Prediction` objects of each iteration. We can access the respective `prediction` column or directly use the `$predictions()` method of the `ResampleResult` object (without converting it to a `data.table` first) to obtain a list of `Prediction` objects of each resampling iteration:

```
rrdt$prediction
```

```
[[1]]
<PredictionClassif> for 86 observations:
    row_ids     truth  response prob.Adelie prob.Chinstrap prob.Gentoo
          4    Adelie    Adelie   0.9722222     0.02777778        0.00
          7    Adelie    Adelie   0.9722222     0.02777778        0.00
          8    Adelie    Adelie   0.9722222     0.02777778        0.00
---
        328 Chinstrap Chinstrap   0.0800000     0.90000000        0.02
        330 Chinstrap Chinstrap   0.0800000     0.90000000        0.02
        339 Chinstrap Chinstrap   0.0800000     0.90000000        0.02

[[2]]
<PredictionClassif> for 86 observations:
    row_ids     truth  response prob.Adelie prob.Chinstrap prob.Gentoo
          2    Adelie    Adelie  0.95575221     0.04424779  0.00000000
          3    Adelie    Adelie  0.95575221     0.04424779  0.00000000
         10    Adelie    Adelie  0.95575221     0.04424779  0.00000000
---
        326 Chinstrap Chinstrap  0.06818182     0.90909091  0.02272727
        329 Chinstrap Chinstrap  0.06818182     0.90909091  0.02272727
        333 Chinstrap Chinstrap  0.06818182     0.90909091  0.02272727

[[3]]
<PredictionClassif> for 86 observations:
    row_ids     truth  response prob.Adelie prob.Chinstrap prob.Gentoo
          1    Adelie    Adelie  0.97500000     0.02500000   0.0000000
          5    Adelie    Adelie  0.97500000     0.02500000   0.0000000
          6    Adelie    Adelie  0.97500000     0.02500000   0.0000000
---
        340 Chinstrap    Gentoo  0.02197802     0.03296703   0.9450549
```

```
        341 Chinstrap    Adelie  0.97500000     0.02500000   0.0000000
        342 Chinstrap Chinstrap  0.02127660     0.97872340   0.0000000

[[4]]
<PredictionClassif> for 86 observations:
    row_ids     truth  response prob.Adelie prob.Chinstrap prob.Gentoo
         11    Adelie    Adelie  0.97321429     0.02678571  0.00000000
         12    Adelie    Adelie  0.97321429     0.02678571  0.00000000
         13    Adelie    Adelie  0.97321429     0.02678571  0.00000000
---
        338 Chinstrap Chinstrap  0.06122449     0.91836735  0.02040816
        343 Chinstrap Chinstrap  0.14285714     0.57142857  0.28571429
        344 Chinstrap Chinstrap  0.06122449     0.91836735  0.02040816
```

```
all.equal(rrdt$prediction, rr$predictions())
```

```
[1] TRUE
```

This allows to analyze the predictions of individual intermediate models from each resampling iteration and, e.g., to manually compute a macro-averaged performance estimate. Instead, we can use the `$prediction()` method to extract a single `Prediction` object that combines the predictions of each intermediate model arcoss all resampling iterations. The combined prediction object can be used to manually compute a micro-averaged performance estimate, for example:

```
pred = rr$prediction()
pred
```

```
<PredictionClassif> for 344 observations:
    row_ids     truth  response prob.Adelie prob.Chinstrap prob.Gentoo
          4    Adelie    Adelie  0.97222222     0.02777778  0.00000000
          7    Adelie    Adelie  0.97222222     0.02777778  0.00000000
          8    Adelie    Adelie  0.97222222     0.02777778  0.00000000
---
        338 Chinstrap Chinstrap  0.06122449     0.91836735  0.02040816
        343 Chinstrap Chinstrap  0.14285714     0.57142857  0.28571429
        344 Chinstrap Chinstrap  0.06122449     0.91836735  0.02040816
```

```
pred$score(msr("classif.acc"))
```

```
classif.acc
  0.9447674
```

By default, the intermediate models produced at each resampling iteration are discarded after the prediction step to reduce memory consumption of the `ResampleResult` object and because only the predictions are required to calculate the performance measure. However, it can sometimes be useful to inspect, compare, or extract information from these intermediate models. To do so, we can configure the `resample()` function to keep the fitted intermediate models by setting the `store_models` argument to `TRUE`. Each model trained in a specific resampling iteration is then stored in the resulting `ResampleResult` object and can be accessed via `$learners[[i]]$model`, where `i` refers to the `i`-th resampling iteration:

```
rr = resample(task, learner, resampling, store_models = TRUE)
rr$learners[[1]]$model
```

```
n= 258

node), split, n, loss, yval, (yprob)
      * denotes terminal node

1) root 258 142 Adelie (0.449612403 0.189922481 0.360465116)
  2) flipper_length< 206.5 163  48 Adelie (0.705521472 0.288343558 0.006134969)
    4) bill_length< 43.35 116   4 Adelie (0.965517241 0.034482759 0.000000000) *
    5) bill_length>=43.35 47   4 Chinstrap (0.063829787 0.914893617 0.021276596) *
  3) flipper_length>=206.5 95   3 Gentoo (0.010526316 0.021052632 0.968421053) *
```

Here, we see the model output of a decision tree fitted by the `rpart` package. As models fitted by `rpart` provide information on how important features are, we can inspect if the importance varies across the resampling iterations:

```
lapply(rr$learners, function(x) x$model$variable.importance)
```

```
[[1]]
flipper_length    bill_length     bill_depth      body_mass         island
      98.05424       91.31166       73.88313       68.27175       51.43762

[[2]]
   bill_length flipper_length     bill_depth      body_mass         island
      97.11402       96.05475       76.89306       65.51456       57.70309

[[3]]
flipper_length    bill_length     bill_depth      body_mass         island
      94.82768       87.05866       77.18128       61.34559       49.95060

[[4]]
   bill_length flipper_length     bill_depth      body_mass         island
      92.44981       92.39868       74.20080       69.36664       57.28430
```

Each resampling iteration involves a training step and a prediction step. Learner-specific error or warning messages may occur at each of these two steps. If the learner passed to the `resample()` function runs in an encapsulated framework that allows logging (see the `$encapsulate` field of a `Learner` object), all potential warning or error messages will be stored in the `$warnings` and `$errors` fields of the `ResampleResult` object.

3.2.6. Custom Resampling

> **Some readers may want to skip this section of the book.**

Sometimes it is necessary to perform resampling with custom splits, e.g., to reproduce results reported in a study with pre-defined folds. A custom resampling strategy can be constructed using `rsmp("custom")`, where the row indices of the observations used for training and testing must be defined manually when instantiated in a task. In the example below, we construct a custom holdout resampling strategy by manually assigning row indices to the `$train` and `$test` fields.

```
resampling = rsmp("custom")
resampling$instantiate(task,
  train = list(c(1:50, 151:333)),
  test = list(51:150)
)
```

The resulting `Resampling` object can then be used like all other resampling strategies. To show that both sets contain the row indices we have defined, we can inspect the instantiated `Resampling` object:

```
str(resampling$train_set(1))
```

```
int [1:233] 1 2 3 4 5 6 7 8 9 10 ...
```

```
str(resampling$test_set(1))
```

```
int [1:100] 51 52 53 54 55 56 57 58 59 60 ...
```

The above is equivalent to a single custom train-test split analogous to the holdout strategy. A custom version of the cross-validation strategy can be constructed using `rsmp("custom_cv")`. The important difference is that we now have to specify either a custom `factor` variable (using the `f` argument of the `$instantiate()` method) or a `factor` column (using the `col` argument of the `$instantiate()` method) from the data to determine the folds.

In the example below, we instantiate a custom 4-fold cross-validation strategy using a `factor` variable called `folds` that contains 4 equally sized levels to define the 4 folds, each with one quarter of the total size of the `"penguin"` task:

```r
custom_cv = rsmp("custom_cv")
folds = as.factor(rep(1:4, each = task$nrow/4))
custom_cv$instantiate(task, f = folds)
custom_cv
```

```
<ResamplingCustomCV>: Custom Split Cross-Validation
* Iterations: 4
* Instantiated: TRUE
* Parameters: list()
```

3.2.7. Resampling with Stratification and Grouping

> **!** **This section of the book might be complex for some readers.**

In mlr3, we can assign a special role to a feature contained in the data by configuring the corresponding `$col_roles` field of a Task. The two relevant column roles that will affect behavior of a resampling strategy are `"group"` or `"stratum"`.

In some cases, it is desirable to keep observations together when the data is split into corresponding training and test sets, especially when a set of observations naturally belong to a group, e.g., when the data contains repeated measurements of individuals (longitudinal studies) or when dealing with spatial or temporal data. When observations belong to groups, we want to ensure that all observations of the same group belong to either the training set or the test set to prevent any potential leakage of information between training and testing sets. For example, in a longitudinal study, measurements of a person are usually taken at multiple time points. Grouping ensures that the model is tested on data from each person that it has not seen during training, while maintaining the integrity of the person's measurements across different time points. In this context, the leave-one-out cross-validation strategy can be coarsened to the "leave-one-object-out" cross-validation strategy, where not only a single observation is left out, but all observations associated with a certain group (see Figure 3.4 for an illustration).

In mlr3, the column role `"group"` allows to specify the column in the data that defines the group structure of the observations (see also the help page of Resampling for more information on the column role `"group"`). The column role can be specified by assigning a feature to the `$col_roles$group` field which will then determine the group structure. The following code performs leave-one-object-out cross-validation using the feature `year` of the `mlr_tasks_penguins` task to determine the grouping. Since the feature `year` contains only three distinct values (i.e., 2007, 2008, and 2009), the corresponding test sets consist of observations from only one year:

```r
task_grp = tsk("penguins")
task_grp$col_roles$group = "year"
r = rsmp("loo")
r$instantiate(task_grp)

table(task_grp$data(cols = "year"))
```

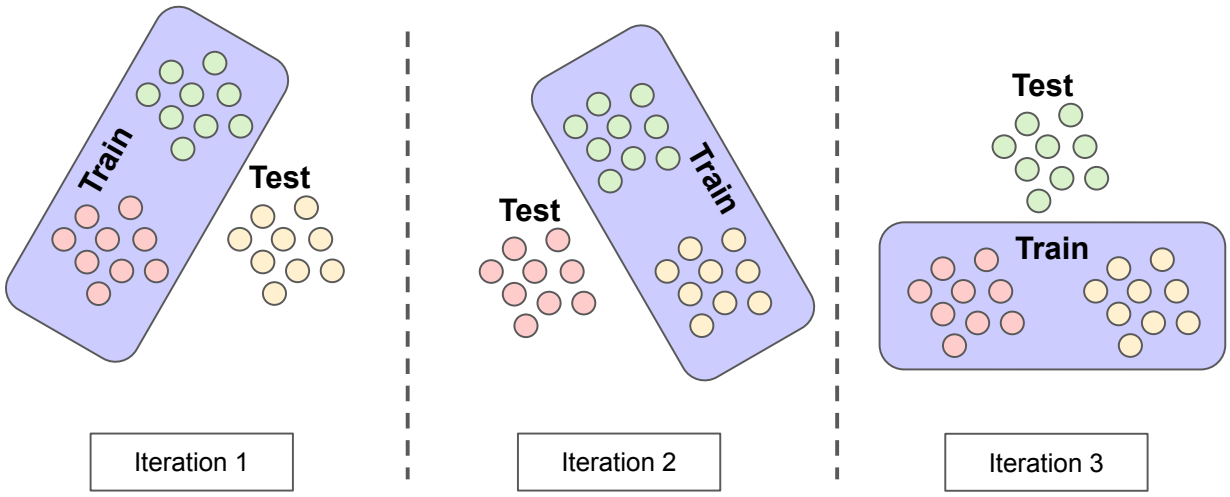


Figure 3.4.: Illustration of the train-test splits of a leave-one-object-out cross-validation with 3 groups of observations (highlighted by different colors).

```
year
2007 2008 2009
 110  114  120
```

```
table(task_grp$data(rows = r$test_set(1), cols = "year"))
```

```
year
2007
 110
```

```
table(task_grp$data(rows = r$test_set(2), cols = "year"))
```

```
year
2009
 120
```

```
table(task_grp$data(rows = r$test_set(3), cols = "year"))
```

```
year
2008
 114
```

> **Tip**
>
> If there are many groups, say 100 groups, we can limit the number of resampling iterations using k-fold cross-validation (or any other resampling strategy with a previously definable number of resampling iterations) instead of performing leave-one-object-out cross-validation. In this case, each group is considered as a single observation, so that the division into training and test sets is done as determined by the resampling strategy

Another column role available in `mlr3` is `"stratum"`, which implements stratified sampling. Stratified sampling ensures that one or more discrete features within the training and test sets will have a similar distribution as in the original task containing all observations. This is especially useful when a discrete feature is highly imbalanced and we want to make sure that the distribution of that feature is similar in each resampling iteration. Stratification is commonly used for imbalanced classification tasks where the classes of the target feature are imbalanced (see Figure 3.5 for an illustration). Stratification by the target feature ensures that each intermediate model is fit on training data where the class distribution of the target is representative of the actual task. Otherwise it could happen that target classes are severely under- or over represented in individual resampling iterations, skewing the estimation of the generalization performance.

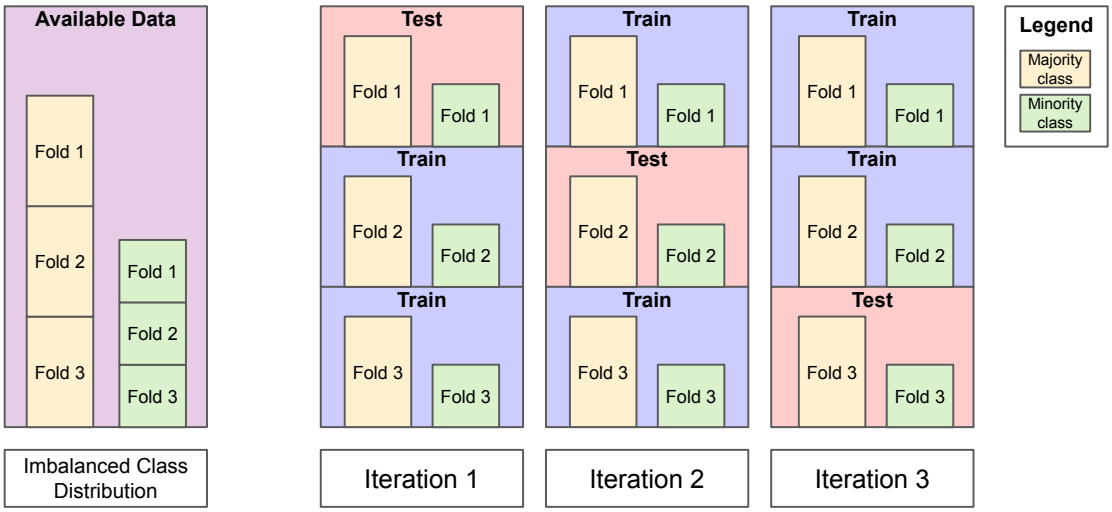


Figure 3.5.: Illustration of a 3-fold cross-validation with stratification for an imbalanced binary classification task with a majority class that is about twice as large as the minority class. In each resampling iteration, the class distribution from the available data is preserved (which is not necessarily the case for cross-validation without stratification).

The `$col_roles$stratum` field of a `Task` can be set to one or multiple features (including the target in case of classification tasks). In case of multiple features, each combination of the values of all stratification features will form a strata. For example, the target column `species` of the `mlr_tasks_penguins` task is imbalanced:

```
prop.table(table(task$data(cols = "species")))
```

```
species
```

```
   Adelie Chinstrap    Gentoo
0.4418605 0.1976744 0.3604651
```

Without specifying a `"stratum"` column role, the `species` column may have quite different class distributions across the training and test sets of a 3-fold cross-validation strategy:

```
r = rsmp("cv", folds = 3)
r$instantiate(task)
prop.table(table(task$data(rows = r$test_set(1), cols = "species")))
```

```
species
   Adelie Chinstrap    Gentoo
0.4000000 0.2086957 0.3913043
```

```
prop.table(table(task$data(rows = r$test_set(2), cols = "species")))
```

```
species
   Adelie Chinstrap    Gentoo
0.4695652 0.1913043 0.3391304
```

```
prop.table(table(task$data(rows = r$test_set(3), cols = "species")))
```

```
species
   Adelie Chinstrap    Gentoo
0.4561404 0.1929825 0.3508772
```

In the worst case, and especially for highly imbalanced classes, the minority class might be entirely left out of the training set in one or more resampling iterations. Consequently, the intermediate models within these resampling iterations will never predict the minority class, resulting in a misleading performance estimate for any resampling strategy without stratification. Relying on such a misleading performance estimate can have severe consequences for a deployed model, as it will perform poorly on the minority class in real-world scenarios. For example, misclassification of the minority class can have serious consequences in certain applications such as in medical diagnosis or fraud detection, where failing to identify the minority class may result in serious harm or financial losses. Therefore, it is important to be aware of the potential consequences of imbalanced class distributions in resampling and use stratification to mitigate highly unreliable performance estimates. The code below uses `species` as `"stratum"` column role to illustrate that the distribution of `species` in each test set will closely match the original distribution:

```
task_str = tsk("penguins")
task_str$col_roles$stratum = "species"
r = rsmp("cv", folds = 3)
r$instantiate(task_str)
```

```

prop.table(table(task_str$data(rows = r$test_set(1), cols = "species")))
```

```
species
   Adelie Chinstrap    Gentoo
0.4396552 0.1982759 0.3620690
```

```
prop.table(table(task_str$data(rows = r$test_set(2), cols = "species")))
```

```
species
   Adelie Chinstrap    Gentoo
0.4434783 0.2000000 0.3565217
```

```
prop.table(table(task_str$data(rows = r$test_set(3), cols = "species")))
```

```
species
   Adelie Chinstrap    Gentoo
0.4424779 0.1946903 0.3628319
```

Rather than assigning the `$col_roles$stratum` directly, it is also possible to use the `$set_col_roles()` method to add or remove columns to specific roles incrementally:

```
task_str$set_col_roles("species", remove_from = "stratum")
task_str$col_roles$stratum
```

```
character(0)
```

```
task_str$set_col_roles("species", add_to = "stratum")
task_str$col_roles$stratum
```

```
[1] "species"
```

We can further inspect the current stratification via the `$strata` field, which returns a `data.table` of the number of observations (`N`) and row indices (`row_id`) of each stratum. Since we stratified by the `species` column, we expect to see the same class frequencies as when we tabulate the task by the `species` column:

```
task_str$strata
```

```
     N                       row_id
1: 152             1,2,3,4,5,6,...
2: 124 153,154,155,156,157,158,...
3:  68 277,278,279,280,281,282,...
```

```
table(task$data(cols = "species"))
```

```
species
   Adelie Chinstrap    Gentoo
      152        68       124
```

Should we add another stratification column, the `$strata` field will show the same values as when we cross-tabulate the two variables of the task:

```
task_str$set_col_roles("year", add_to = "stratum")

task_str$strata
```

```
    N                      row_id
1: 50             1,2,3,4,5,6,...
2: 50       51,52,53,54,55,56,...
3: 52 101,102,103,104,105,106,...
4: 34 153,154,155,156,157,158,...
5: 46 187,188,189,190,191,192,...
6: 44 233,234,235,236,237,238,...
7: 26 277,278,279,280,281,282,...
8: 18 303,304,305,306,307,308,...
9: 24 321,322,323,324,325,326,...
```

```
table(task$data(cols = c("species", "year")))
```

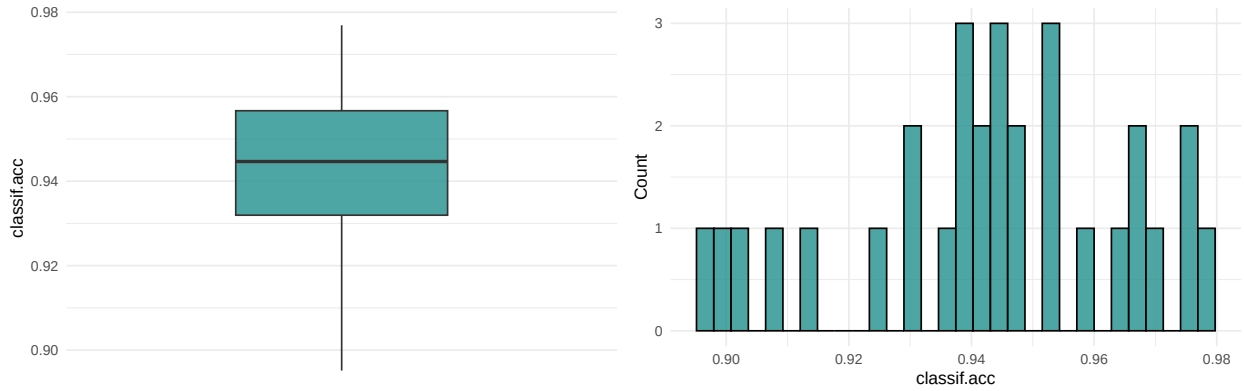
```
           year
species     2007 2008 2009
  Adelie      50   50   52
  Chinstrap   26   18   24
  Gentoo      34   46   44
```

3.2.8. Plotting Resample Results

mlr3viz provides a autoplot() method to automatically visualize the resampling results either in a boxplot or histogram:

```
resampling = rsmp("bootstrap")
rr = resample(task, learner, resampling)

library(mlr3viz)
autoplot(rr, measure = msr("classif.acc"), type = "boxplot")
autoplot(rr, measure = msr("classif.acc"), type = "histogram")
```

```
`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```

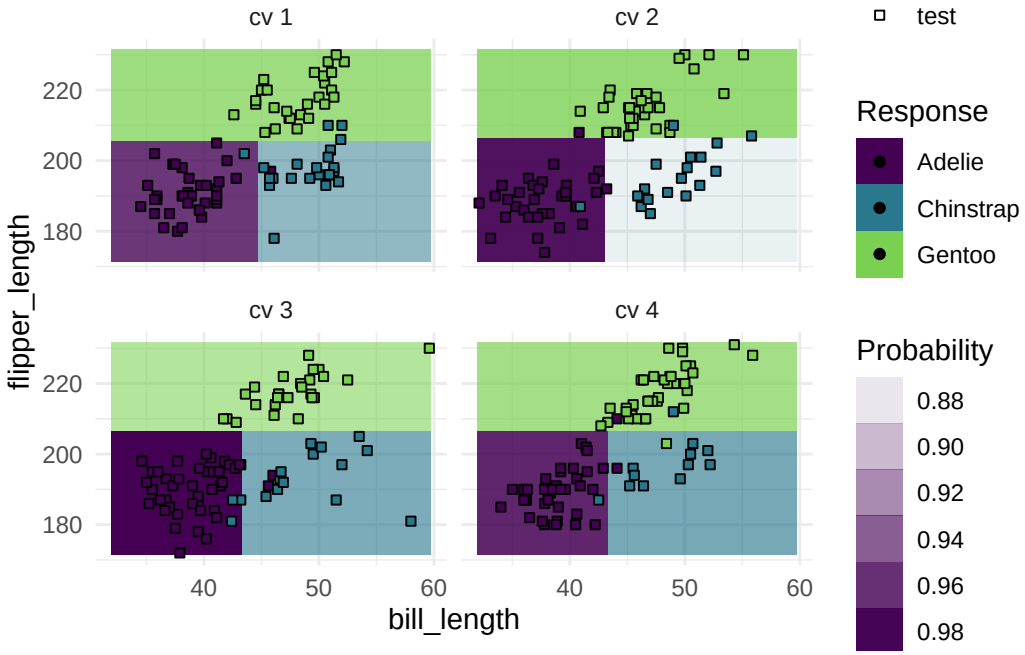


The histogram is useful to visually gauge the variance of the performance results across resampling iterations, whereas the boxplot is often used when multiple learners are compared side-by-side.

We can also visualize a 2-dimensional prediction surface of individual models in each resampling iteration if the task is restricted to two features:

```
task$select(c("bill_length", "flipper_length"))
resampling = rsmp("cv", folds = 4)
rr = resample(task, learner, resampling, store_models = TRUE)
autoplot(rr, type = "prediction")
```

```
Warning: Removed 2 rows containing missing values (`geom_point()`).
```



Prediction surfaces like this are a useful tool for model inspection, as they can help to identify the cause of unexpected performance result. Naturally, they are also popular for didactical purposes to illustrate the prediction behaviour of different learning algorithms, such as the classification tree in the example above with its characteristic orthogonal lines.

3.3. Benchmarking

Benchmarking in supervised machine learning refers to the comparison of different learners on a single task or multiple tasks. When comparing learners on a single task or on a domain consisting of multiple similar tasks, the main aim is often to rank the learners according to a pre-defined performance measure and to identify the best-performing learner for the considered task or domain. In an applied setting, benchmarking may be used to evaluate whether a deployed model used for a given task or domain can be replaced by a better alternative solution. When comparing multiple learners on multiple tasks, the main aim is often more of a scientific nature, e.g., to gain insights into how different learners perform in different data situations or whether there are certain data properties that heavily affect the performance of certain learners (or certain hyperparameter of learners). For example, it is common practice for algorithm designers to analyze the generalization performance or runtime of a newly proposed learning algorithm in a benchmark study where it has been compared with existing learners. In Section 3.3, we provide code examples for conducting benchmark studies and performing statistical analysis of benchmark results using the `mlr3` package.

The `mlr3` package offers the convenience function `benchmark()` to conduct a benchmark experiment. The function internally runs the `resample()` function on each task separately. The provided resampling strategy is instantiated on each task to ensure a fair comparison by training and evaluating multiple learners under the same conditions. This means that all provided learners use the same train-test splits for each task. In this section, we cover how to

- construct a benchmark design (Section 3.3.1) to define the benchmark experiments to be performed,
- run the benchmark experiments (Section 3.3.2) and aggregate their results, and
- convert benchmark objects (Section 3.3.3) to other types of objects that can be used for different purposes.

3.3.1. Constructing Benchmarking Designs

In `mlr3`, we can define a design to perform benchmark experiments via the `benchmark_grid()` convenience function. The design is essentially a table of scenarios to be evaluated and usually consists of unique combinations of `Task`, `Learner` and `Resampling` triplets.

The `benchmark_grid()` function constructs an exhaustive design to describe which combinations of learner, task and resampling should be used in a benchmark experiment. It properly instantiates the used resampling strategies so that all learners are evaluated on the same train-test splits for each task, ensuring a fair comparison. To construct a list of `Task`, `Learner` and `Resampling` objects, we can use the convenience functions `tsks()`, `lrns()`, and `rsmps()`.

We design an exemplary benchmark experiment and train a classification tree from the `rpart` package, a random forest from the `ranger` package and a featureless learner serving as a baseline

on four different binary classification tasks. The constructed benchmark design is a `data.table` containing the task, learner, and resampling combinations in each row that should be performed:

```
library("mlr3verse")

tsks = tsks(c("german_credit", "sonar", "breast_cancer"))
lrns = lrns(c("classif.ranger", "classif.rpart", "classif.featureless"),
  predict_type = "prob")
rsmp = rsmps("cv", folds = 5)

design = benchmark_grid(tsks, lrns, rsmp)
head(design)
```

```
                task                          learner         resampling
1: <TaskClassif[50]>      <LearnerClassifRanger[38]> <ResamplingCV[20]>
2: <TaskClassif[50]>       <LearnerClassifRpart[38]> <ResamplingCV[20]>
3: <TaskClassif[50]> <LearnerClassifFeatureless[38]> <ResamplingCV[20]>
4: <TaskClassif[50]>      <LearnerClassifRanger[38]> <ResamplingCV[20]>
5: <TaskClassif[50]>       <LearnerClassifRpart[38]> <ResamplingCV[20]>
6: <TaskClassif[50]> <LearnerClassifFeatureless[38]> <ResamplingCV[20]>
```

Since the `data.table` contains R6 columns within list-columns, we unfortunately can not infer too much about `task` column, but the `ids` utility function can be used for quick inspection or subsetting:

```
mlr3misc::ids(design$task)
```

```
[1] "german_credit" "german_credit" "german_credit" "sonar"
[5] "sonar"         "sonar"         "breast_cancer" "breast_cancer"
[9] "breast_cancer"
```

```
design[mlr3misc::ids(task) == "sonar", ]
```

```
                task                          learner         resampling
1: <TaskClassif[50]>      <LearnerClassifRanger[38]> <ResamplingCV[20]>
2: <TaskClassif[50]>       <LearnerClassifRpart[38]> <ResamplingCV[20]>
3: <TaskClassif[50]> <LearnerClassifFeatureless[38]> <ResamplingCV[20]>
```

It is also possible to subset the design, e.g., to exclude a specific task-learner combination by manually removing a certain row from the design which is a `data.table`. Alternatively, we can also construct a custom benchmark design by manually defining a `data.table` containing task, learner, and resampling objects (see also the examples section in the help page of `benchmark_grid()`).

3.3.2. Execution of Benchmark Experiments

To run the benchmark experiment, we can pass the constructed benchmark design to the `benchmark()` function, which will internally call `resample()` for all the combinations of task, learner, and resampling strategy in our benchmark design:

```
bmr = benchmark(design)
print(bmr)
```

```
<BenchmarkResult> of 45 rows with 9 resampling runs
 nr       task_id          learner_id resampling_id iters warnings errors
  1 german_credit      classif.ranger            cv     5        0      0
  2 german_credit       classif.rpart            cv     5        0      0
  3 german_credit classif.featureless            cv     5        0      0
  4         sonar      classif.ranger            cv     5        0      0
  5         sonar       classif.rpart            cv     5        0      0
  6         sonar classif.featureless            cv     5        0      0
  7 breast_cancer      classif.ranger            cv     5        0      0
  8 breast_cancer       classif.rpart            cv     5        0      0
  9 breast_cancer classif.featureless            cv     5        0      0
```

Once the benchmarking is finished (this can take some time, depending on the size of your design), we can aggregate the performance results with the `$aggregate()` method of the returned `BenchmarkResult`:

```
acc = bmr$aggregate(msr("classif.acc"))
acc[, .(task_id, learner_id, classif.acc)]
```

```
         task_id          learner_id classif.acc
1: german_credit      classif.ranger   0.7640000
2: german_credit       classif.rpart   0.7230000
3: german_credit classif.featureless   0.7000000
4:         sonar      classif.ranger   0.8082462
5:         sonar       classif.rpart   0.6535424
6:         sonar classif.featureless   0.5336818
7: breast_cancer      classif.ranger   0.9721662
8: breast_cancer       classif.rpart   0.9443431
9: breast_cancer classif.featureless   0.6500537
```

As the results are shown in a `data.table`, we can easily aggregate the results even further. For example, if we are interested in the learner that performed best across all tasks, we could average the performance of each individual learner across all tasks. Please note that averaging accuracy scores across multiple tasks as in this example is not always appropriate for comparison purposes. A more common alternative to compare the overall algorithm performance across multiple tasks is to first compute the ranks of each learner on each task separately and then compute the average

ranks. For illustration purposes, we show how to average the performance of each individual learner across all tasks:

```
acc[, list(mean_accuracy = mean(classif.acc)), by = "learner_id"]
```

```
           learner_id mean_accuracy
1:      classif.ranger     0.8481375
2:       classif.rpart     0.7736285
3: classif.featureless     0.6279118
```

Ranking the performance scores can either be done via standard `data.table` syntax, or more conveniently with the `mlr3benchmark` package. We first use `as.BenchmarkAggr` to aggregate the `BenchmarkResult` using our measure, after which we use the `$rank_data()` method to convert the performance scores to ranks. The `minimize` argument is used to indicate that the classification accuracy should not be minimized, i.e. a higher score is better.

```
library("mlr3benchmark")

bma = as.BenchmarkAggr(bmr, measures = msr("classif.acc"))
bma$rank_data(minimize = FALSE)
```

```
           german_credit sonar breast_cancer
ranger                 1     1             1
rpart                  2     2             2
featureless            3     3             3
```

This results in per-task rankings of the three learners. Unsurprisingly, the featureless learner ranks last, as it always predicts the majority class. However, it is common practice to include it as a baseline in benchmarking experiments to easily gauge the relative performance of other algorithms. In this simple benchmark experiment, the random forest ranked first, outperforming a single classification tree as one would expect.

3.3.3. Inspect BenchmarkResult Objects

A `BenchmarkResult` object is a collection of multiple `ResampleResult` objects. We can analogously use `as.data.table` to take a look at the contents and compare them to the `data.table` of the `ResampleResult` from the previous section (`rrdt`):

```
bmrdt = as.data.table(bmr)

names(bmrdt)
```

```
[1] "uhash"      "task"       "learner"    "resampling" "iteration"
[6] "prediction"
```

```
names(rrdt)
```

```
[1] "task"       "learner"    "resampling" "iteration"  "prediction"
```

By the column names alone, we see that the general contents of a BenchmarkResult and ResampleResult which we specified in Section 3.2.5 is very similar, with the additional unique identification column "uhash" in the former being the only difference.

The stored ResampleResults can be extracted via the $resample_result(i) method, where i is the index of the performed benchmark experiment. This allows us to investigate the extracted ResampleResult or individual resampling iterations as shown previously (see Section 3.2).

```
rr1 = bmr$resample_result(1)
rr2 = bmr$resample_result(2)
rr1
```

```
<ResampleResult> of 5 iterations
* Task: german_credit
* Learner: classif.ranger
* Warnings: 0 in 0 iterations
* Errors: 0 in 0 iterations
```

```
rr2
```

```
<ResampleResult> of 5 iterations
* Task: german_credit
* Learner: classif.rpart
* Warnings: 0 in 0 iterations
* Errors: 0 in 0 iterations
```

Multiple ResampleResult can be again converted to a BenchmarkResult with the function as_benchmark_result() and combined with c():

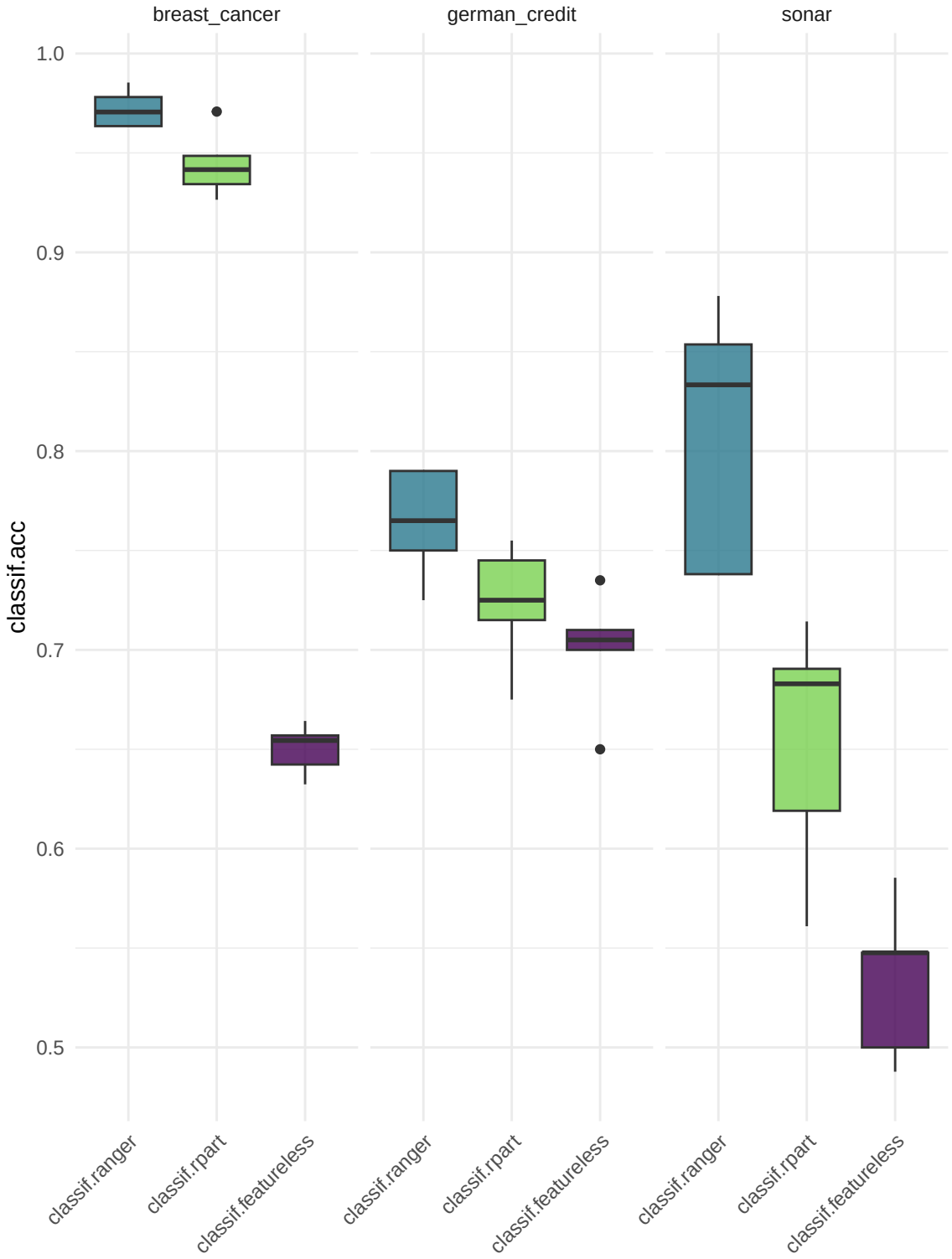
```
bmr1 = as_benchmark_result(rr1)
bmr2 = as_benchmark_result(rr2)

bmr_combined = c(bmr1, bmr2)
bmr_combined$aggregate(msr("classif.acc"))
```

```
   nr      resample_result       task_id     learner_id resampling_id iters
1:  1 <ResampleResult[21]> german_credit classif.ranger            cv     5
2:  2 <ResampleResult[21]> german_credit  classif.rpart            cv     5
1 variable not shown: [classif.acc]
```

Combining multiple `BenchmarkResult`s into a larger result object can be useful if related benchmarks where computed on different machines.

Similar to creating automated visualizations for tasks, predictions, or resample results, the `mlr3viz` package also provides a `autoplot()` method to visualize benchmark results, by default as a boxplot:

```
autoplot(bmr, measure = msr("classif.acc"))
```



Such a plot summarizes the benchmark experiment across all tasks and learners. Visualizing performance scores across all learners and tasks in a benchmark helps identifying potentially unexpected behavior, such as a learner performing reasonably well for most tasks, but yielding noticeably worse scores in one task. In the case of our example above, the three learners show consistent relative

performance to each other, in the order we would expect.

3.3.4. Statistical Tests

> **Some readers may want to skip this section of the book.**

The package `mlr3benchmark` we previously used for ranking also provides infrastructure for applying statistical significance tests on `BenchmarkResult` objects. Currently, Friedman tests and pairwise Friedman-Nemenyi tests (Demšar 2006) are supported to analyze benchmark experiments with at least two independent tasks and at least two learners.

`$friedman_posthoc()` can be used for a pairwise comparison:

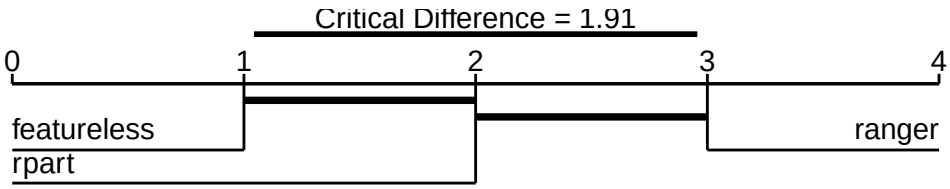
```
bma = as.BenchmarkAggr(bmr, measures = msr("classif.acc"))
bma$friedman_posthoc()
```

```
    Pairwise comparisons using Nemenyi-Wilcoxon-Wilcox all-pairs test for a two-way balanced co


data: acc and learner_id and task_id


            ranger rpart
rpart       0.438  -
featureless 0.038  0.438



P value adjustment method: single-step
```

These results would indicate a statistically significant difference between the `"featureless"` learner and `"ranger"`, assuming a 95% confidence level.

The results can be summarized in a critical difference plot which typically shows the mean rank of a learning algorithm on the x-axis along with a thick horizontal line that connects learners which are not significantly different:

```
autoplot(bma, type = "cd")
```



Similar to the test output before, this visualization leads to the conclusion that the `"featureless"` learner and `"ranger"` are significantly different, whereas the critical rank difference of 1.66 is not exceed for the comparison of the `"featureless"` learner, `"rpart"` and `"ranger"`, respectively.

3.4. ROC Analysis

ROC (Receiver Operating Characteristic) analysis is widely used to evaluate binary classifiers. Although extensions for multiclass classifiers exist (see e.g., Hand and Till (2001)), we will only cover the much easier binary classification case here. For binary classifiers that predict discrete classes, we can compute a confusion matrix which computes the following quantities (see also Figure 3.6):

- **True positives (TP)**: Instances that are actually positive and correctly classified as positive.
- **True negatives (TN)**: Instances that are actually negative and correctly classified as negative.
- **False positives (FP)**: Instances that are actually negative but incorrectly classified as positive.
- **False negatives (FN)**: Instances that are actually positive but incorrectly classified as negative.

There are a multitude of performance measures that can be derived from a confusion matrix. Unfortunately, many of them have different names for historical reasons, originating from different fields. For a good overview of common confusion matrix-based measures, see the comprehensive table on Wikipedia[1] which also provides many common aliases for each measure.

[1] https://en.wikipedia.org/wiki/Confusion_matrix#Table_of_confusion

3.4.1. Confusion Matrix-based Measures

Some common performance measures that are based on the confusion matrix and measure the ability of a classifier to separate the two classes (i.e., discrimination performance) include (see also Figure 3.6 for their definition based on TP, FP, TN and FN):

- **True Positive Rate (TPR)**, **Sensitivity** or **Recall**: How many of the true positives did we predict as positive?
- **True Negative Rate (TNR)** or **Specificity**: How many of the true negatives did we predict as negative?
- **False Positive Rate (FPR)**, or 1 - **Specificity**: How many of the true negatives did we predict as positive?
- **Positive Predictive Value (PPV)** or **Precision**: If we predict positive how likely is it a true positive?
- **Negative Predictive Value (NPV)**: If we predict negative how likely is it a true negative?
- **Accuracy (ACC)**: The proportion of correctly classified instances out of the total number of instances.
- **F1-score**: The harmonic mean of precision and recall, which balances the trade-off between precision and recall. It is calculated as $2 \times \frac{Precision \times Recall}{Precision + Recall}$.

		True Class y		
		$+$	$-$	
Predicted Class $\hat{y}$	$+$	TP	FP	$\text{PPV} = \frac{\text{TP}}{\text{TP+FP}}$
	$-$	FN	TN	$\text{NPV} = \frac{\text{TN}}{\text{FN+TN}}$
		$\text{TPR} = \frac{\text{TP}}{\text{TP+FN}}$	$\text{TNR} = \frac{\text{TN}}{\text{FP+TN}}$	$\text{ACC} = \frac{\text{TP+TN}}{\text{TP+FP+FN+TN}}$

Figure 3.6.: Binary confusion matrix of ground truth class vs. predicted class.

In the code example below, we first retrieve the `mlr_tasks_german_credit` task which is a binary classification task and construct a random forest learner using `classif.ranger` that predicts probabilities using the `predict_type = "prob"` option. Next, we use the `partition()` helper function which acts as a convenience shortcut function to the `"holdout"` resampling strategy to randomly partition the contained data into two disjoint set. We train the learner on the training set and use the trained model to generate predictions on the test set. Finally, we retrieve the confusion matrix from the resulting `Prediction` object by accessing the `$confusion` field (see also Section 2.4.3):

```
task = tsk("german_credit")
learner = lrn("classif.ranger", predict_type = "prob")
splits = partition(task, ratio = 0.8)

learner$train(task, splits$train)
pred = learner$predict(task, splits$test)
```

```
pred$confusion
```

```
        truth
response good bad
    good  125  31
    bad    15  29
```

The mlr3measures package allows to additionally compute several common confusion matrix-based measures using the confusion_matrix function:

```
mlr3measures::confusion_matrix(truth = pred$truth,
  response = pred$response, positive = task$positive)
```

```
        truth
response good bad
    good  125  31
    bad    15  29
acc :  0.7700; ce  :  0.2300; dor :  7.7957; f1  :  0.8446
fdr :  0.1987; fnr :  0.1071; fomr:  0.3409; fpr :  0.5167
mcc :  0.4162; npv :  0.6591; ppv :  0.8013; tnr :  0.4833
tpr :  0.8929
```

If a binary classifier predicts probabilities instead of discrete classes, we could arbitrarily set a threshold to cut-off the probabilities and assign them to the positive and negative class. When it comes to classification performance, it is generally difficult to achieve a high TPR and low FPR simultaneously because there is often a trade-off between the two rates. Increasing the threshold for identifying the positive cases, leads to a higher number of negative predictions and fewer positive predictions. As a consequence, the FPR is usually better (lower), but at the cost of a worse (lower) TPR. For example, in the special case where the threshold is set too high and no instance is predicted as positive, the confusion matrix shows zero true positives (no instances that are actually positive and correctly classified as positive) and zero false positives (no instances that are actually negative but incorrectly classified as positive). Therefore, the FPR and TPR are also zero since there are zero false positives and zero true positives. Conversely, lowering the threshold for identifying positive cases may never predict the negative class and can increase (improve) TPR, but at the cost of a worse (higher) FPR. For example, below we set the threshold to `0.99` and `0.01` for the mlr_tasks_german_credit task to illustrate the two special cases explained above where zero positives and where zero negatives are predicted and inspect the resulting confusion matrix-based measures (some measures can not be computed due to division by 0 and therefore will produce `NaN` values):

```
pred$set_threshold(0.99)
mlr3measures::confusion_matrix(pred$truth, pred$response, task$positive)
```

```
        truth
```

```
response good bad
    good    0   0
    bad   140  60
acc :  0.3000; ce  :  0.7000; dor :  NaN; f1  :  NaN
fdr :  NaN; fnr :  1.0000; fomr:  0.7000; fpr :  0.0000
mcc :  0.0000; npv :  0.3000; ppv :  NaN; tnr :  1.0000
tpr :  0.0000
```

```
pred$set_threshold(0.01)
mlr3measures::confusion_matrix(pred$truth, pred$response, task$positive)
```

```
        truth
response good bad
    good  140  60
    bad     0   0
acc :  0.7000; ce  :  0.3000; dor :  NaN; f1  :  0.8235
fdr :  0.3000; fnr :  0.0000; fomr:  NaN; fpr :  1.0000
mcc :  0.0000; npv :  NaN; ppv :  0.7000; tnr :  0.0000
tpr :  1.0000
```

3.4.2. ROC Space

ROC analysis aims at evaluating the performance of classifiers by visualizing the trade-off between the TPR and the FPR which can be obtained from a confusion matrix. Each classifier that predicts discrete classes, will be a single point in the ROC space (see Figure 3.7, panel (a)). The best classifier lies on the top-left corner where the TPR is 1 and the FPR is 0. Classifiers on the diagonal predict class labels randomly (possibly with different class proportions). For example, if each positive instance will be randomly classified with 25% as to the positive class, we get a TPR of 0.25. If we assign each negative instance randomly to the positive class, we get a FPR of 0.25. In practice, we should never obtain a classifier clearly below the diagonal. Swapping the predicted classes of a classifier would results in points in the ROC space being mirrored at the diagonal baseline. A point in the ROC space below the diagonal might indicate that the positive and negative class labels have been switched by the classifier.

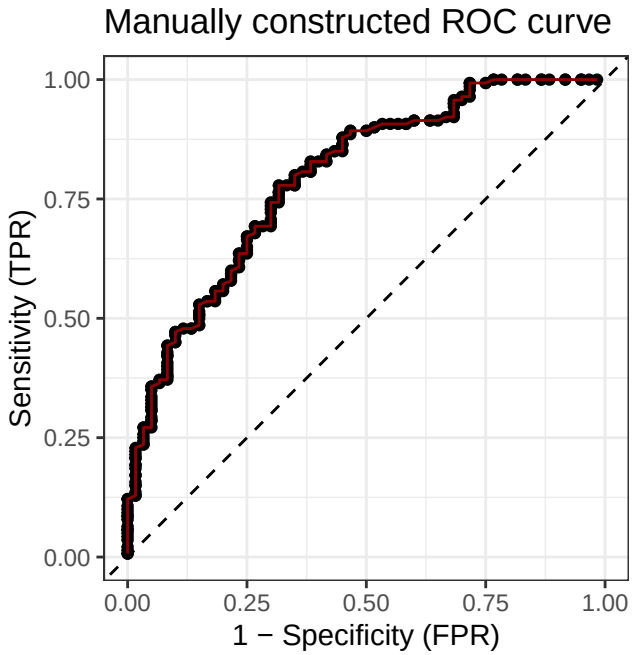
Using different thresholds to cut-off predicted probabilities and assign them to the positive and negative class may lead to different confusion matrices. In this case, we can characterize the behavior of a binary classifier for different thresholds by plotting the TPR and FPR values — this is the ROC curve. For example, we can use the previous `Prediction` object, compute all possible TPR and FPR combinations if we use all predicted probabilities as possible threshold, and visualize them to manually create a ROC curve:

```
thresholds = sort(pred$prob[,1])

rocvals = data.table::rbindlist(lapply(thresholds, function(t) {
  pred$set_threshold(t)
  data.frame(
```

```
    threshold = t,
    FPR = pred$score(msr("classif.fpr")),
    TPR = pred$score(msr("classif.tpr"))
  )
}))

head(rocvals)
```

```
   threshold       FPR TPR
1: 0.2351119 0.9833333   1
2: 0.2357222 0.9666667   1
3: 0.2404476 0.9500000   1
4: 0.2616540 0.9500000   1
5: 0.2799230 0.9166667   1
6: 0.2829881 0.9166667   1
```

```
library(ggplot2)
ggplot(rocvals, aes(FPR, TPR)) +
  geom_point() +
  geom_path(color = "darkred") +
  geom_abline(linetype = "dashed") +
  coord_fixed(xlim = c(0, 1), ylim = c(0, 1)) +
  labs(
    title = "Manually constructed ROC curve",
    x = "1 - Specificity (FPR)",
    y = "Sensitivity (TPR)"
  ) +
  theme_bw()
```



A natural performance measure that can be derived from the ROC curve is the area under the curve (AUC). The higher the AUC value, the better the performance, whereas a random classifier would result in an AUC of 0.5 (see Figure 3.7, panel (b) for an illustration). The AUC can be interpreted as the probability that a randomly chosen positive instance is ranked higher (in the sense that it gets a higher predicted probability of belonging to the positive class) by the classification model than a randomly chosen negative instance.

For `mlr3` prediction objects, the ROC curve can be constructed with the previously seen `autoplot.PredictionClassif` from `mlr3viz`. The x-axis showing the FPR is labelled "1 - Specificity" by convention, whereas the y-axis shows "Sensitivity" for the TPR.

```
autoplot(pred, type = "roc")
```

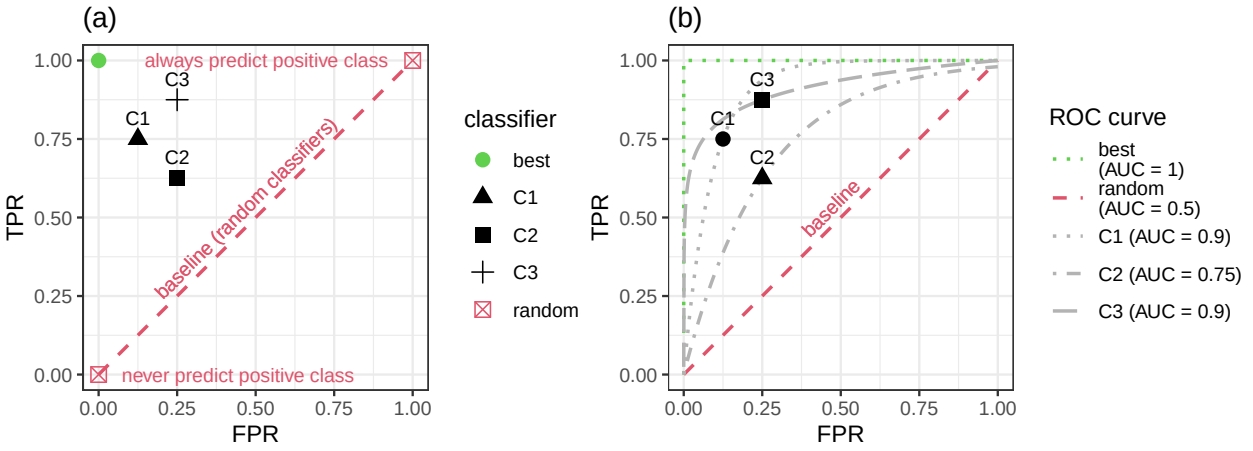
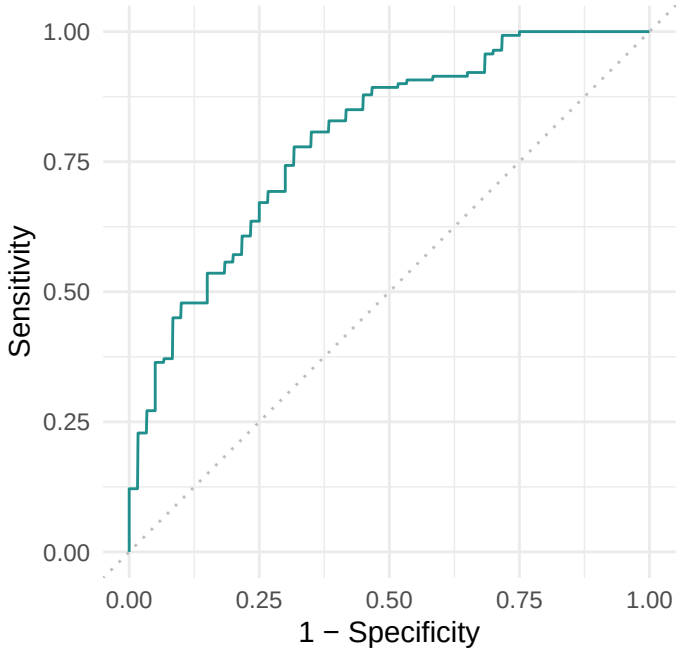


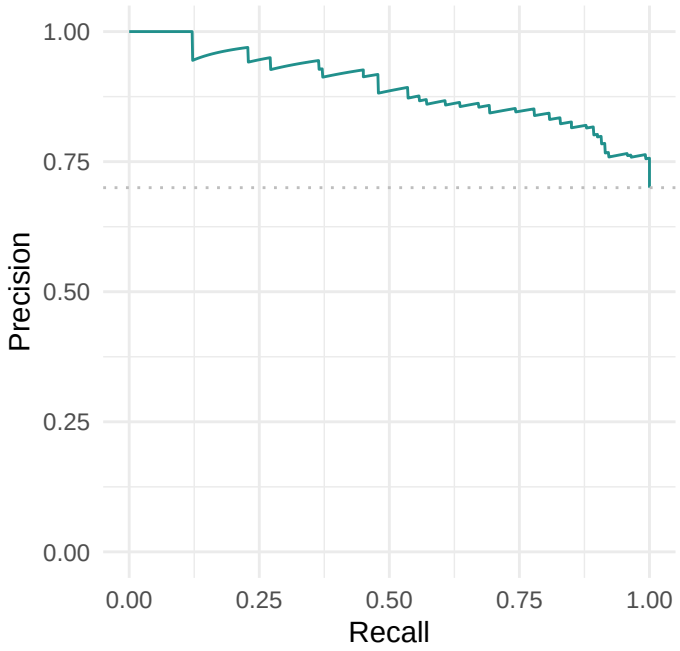
Figure 3.7.: Panel (a): ROC space with best discrete classifier, two random guessing classifiers lying on the diagonal line (baseline), one that always predicts the positive class and one that never predicts the positive class, and three classifiers C1, C2, C3. We cannot say if C1 or C3 is better as both lie on a parallel line to the baseline. C2 is clearly dominated by C1, C3 as it is further away from the best classifier at (TPR = 1, FPR = 0). Panel (b): ROC curves of the best classifier (AUC = 1), of a random guessing classifier (AUC = 0.5), and the classifiers C1, C3, and C2.



We can also plot the precision-recall (PR) curve which visualize the PPV vs. TPR. The main difference between ROC curves and PR curves is that the number of true-negatives are not used to produce a PR curve. PR curves are preferred over ROC curves for imbalanced populations. This is

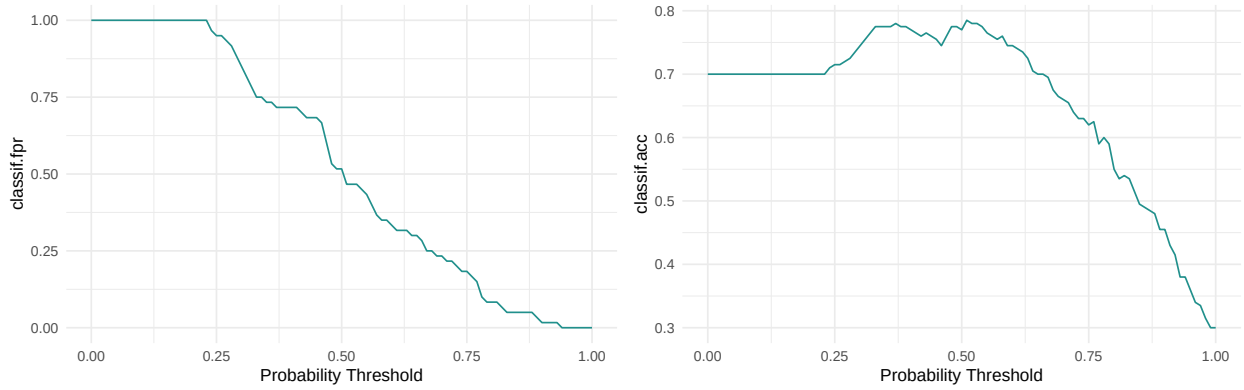
because the positive class is usually rare in imbalanced classification tasks. Hence, the FPR is often low even for a random classifier. As a result, the ROC curve may not provide a good assessment of the classifier's performance, because it does not capture the high rate of false negatives (i.e., misclassified positive observations). See also Davis and Goadrich (2006) for a detailed discussion about the relationship between the PRC and ROC curves.

```
autoplot(pred, type = "prc")
```



Another useful way to think about the performance of a classifier is to visualize the relationship of the set threshold with the performance metric at the given threshold. For example, if we want to see the FPR and accuracy across all possible thresholds:

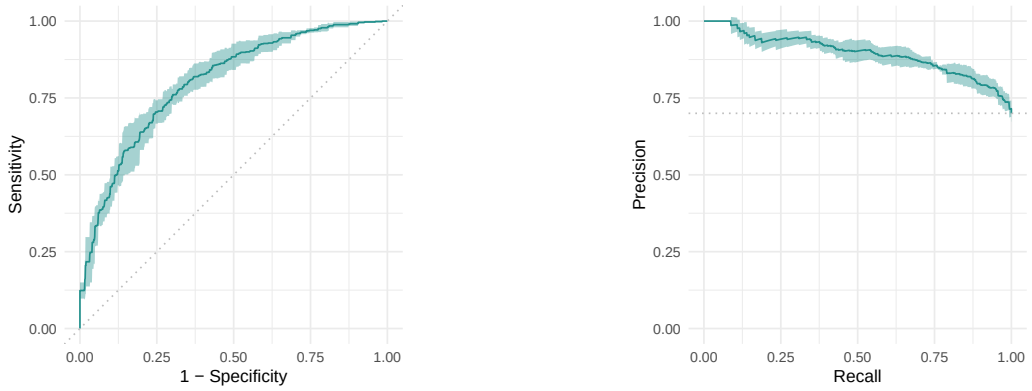
```
autoplot(pred, type = "threshold", measure = msr("classif.fpr"))
autoplot(pred, type = "threshold", measure = msr("classif.acc"))
```



This visualization would show us that it would not matter if we picked a threshold of 0.5 or 0.75, since neither FPR nor accuracy changes in that range.

These visualizations are also available for `ResampleResult`. Here, the predictions of individual resampling iterations are merged prior to calculating a ROC or PR curve (micro-averaged):

```
rr = resample(
  task = tsk("german_credit"),
  learner = lrn("classif.ranger", predict_type = "prob"),
  resampling = rsmp("cv", folds = 5)
)

autoplot(rr, type = "roc")
autoplot(rr, type = "prc")
```

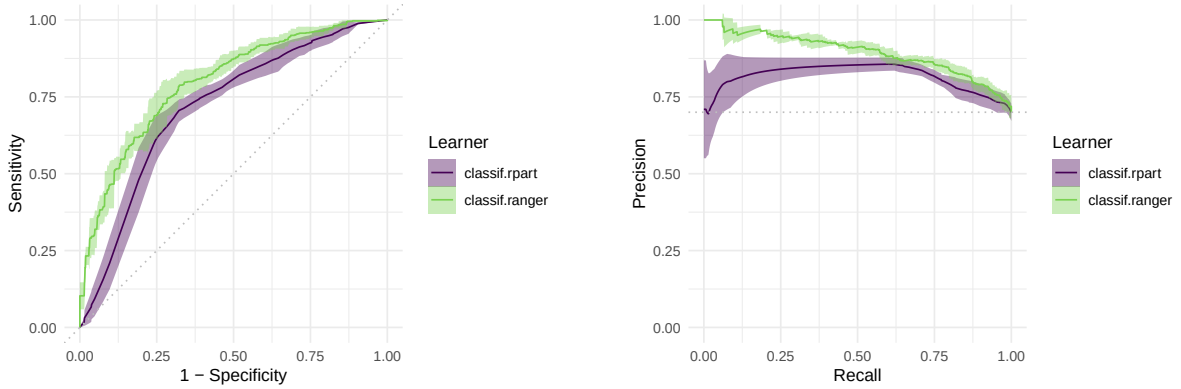


We can also visualize a `BenchmarkResult` to compare multiple learners on the same `Task`:

```
design = benchmark_grid(
  tasks = tsk("german_credit"),
  learners = lrns(c("classif.rpart", "classif.ranger"), predict_type = "prob"),
  resamplings = rsmp("cv", folds = 5)
)
bmr = benchmark(design)

autoplot(bmr, type = "roc")
autoplot(bmr, type = "prc")
```

3.5. Conclusion

In this chapter, we learned how to estimate the generalization performance of a model via resampling. We also learned about benchmarking to fairly compare the estimated generalization performance of different learners across multiple tasks. Performance calculations underpin these concepts, and we have seen some of them applied to classification tasks, with a more in-depth look



at the special case of binary classification and ROC analysis. We also learned how to visualize confusion matrix-based performance measures with regards to different thresholds as well as resampling and benchmark results with `mlr3viz`. The discussed topics belong to the fundamental concepts of supervised machine learning. Chapter 4 builds on these concepts and applies them for tuning (i.e., to automatically choose the optimal hyperparameters of a learner) through nested resampling (Section 4.5). In Chapter 8, we will also take a look at specialized tasks that require different resampling strategies. Finally, Table 3.1 provides an overview of some important `mlr3` functions and the corresponding R6 classes that were most frequently used throughout this chapter.

S3 function	R6 Class	Summary
`rsmp()`	`Resampling`	Assigns observations to train- and test sets
`resample()`	`ResampleResult`	Evaluates learners on given tasks using a resampling strategy
`benchmark_grid()`	-	Constructs a design grid of learners, tasks, and resamplings
`benchmark()`	`BenchmarkResult`	Evaluates learners on a given design grid

Table 3.1.: Core S3 'sugar' functions for resampling and benchmarking in mlr3 with the underlying R6 class that are constructed when these functions are called (if applicable) and a summary of the purpose of the functions.

Resources

- Learn more about advanced resampling techniques in: Resampling - Stratified, Blocked and Predefined[2].
- Check out the blog post mlr3 Basics on "Iris" - Hello World![3] to see minimal examples on using resampling and benchmarking on the iris dataset.
- Use resampling and benchmarking for the comparison of decision boundaries of classification learners[4].

[2] https://mlr-org.com/gallery/basic/2020-03-30-stratification-blocking/
[3] https://mlr-org.com/gallery/basic/2020-03-18-iris-mlr3-basics/
[4] https://mlr-org.com/gallery/basic/2020-08-14-comparison-of-decision-boundaries/

- Learn how to effectively pick thresholds by applying tuning and pipelines (Chapters 4 and 6) in this post on threshold tuning[5].

3.6. Exercises

1. Use the `spam` task and 5-fold cross-validation to benchmark Random Forest (`classif.ranger`), Logistic Regression (`classif.log_reg`), and XGBoost (`classif.xgboost`) with regards to AUC. Which learner appears to do best? How confident are you in your conclusion? How would you improve upon this?
2. A colleague claims to have achieved a 93.1% classification accuracy using the `classif.rpart` learner on the `penguins_simple` task. You want to reproduce their results and ask them about their resampling strategy. They said they used 3-fold cross-validation, and they assigned rows using the task's `row_id` modulo 3 to generate three evenly sized folds. Reproduce their results using the custom CV strategy.

[5] https://mlr-org.com/gallery/optimization/2020-10-14-threshold-tuning/index.html

4. Hyperparameter Optimization

Most machine learning algorithms are configurated by a set of hyperparameters. The goal of hyperparameter optimization is to find the optimal hyperparameter configuration of a machine learning algorithm for a given task. This chapter presents an introduction to hyperparameter optimization in the mlr3 ecosystem. As a practical example, we optimize the `cost` and `gamma` hyperparameters of a support vector machine on the sonar task. We introduce the tuning instance class that describes the tuning problem and the tuner class that wraps an optimization algorithm. After running the optimization, we show how to analyze the results and fit a final model. We also show how to run a multi-objective optimization with multiple measures. Then we move on to more advanced topics like search space transformations, fallback learners and encapsulation. Finally, we show how to use nested resampling to get an unbiased estimate of the performance of an optimized model.

```
set.seed(4)
```

Hyperparamete

Machine learning algorithms usually include parameters and hyperparameters. Parameters are what we might think of as model coefficients or weights, when fitting a model we are essentially just running algorithms that fit parameters. In contrast, hyperparameters, are configured by the user and determine how the model will fit its parameters. Examples include setting the number of trees in a random forest, penalty variables in SVMs, or the learning rate in a neural network. Building a neural network is sometimes referred to as an 'art' as there are so many hyperparameters to configure that strongly influence model performance, this is also true for other machine learning algorithms. So in this chapter, we will demonstrate how to make this into more of a science.

HPO: Hyperpa
Optimization

The goal of hyperparameter optimization (Section 4.1) or model tuning is to find the optimal configuration of hyperparameters of an ML algorithm for a given task. There is no closed-form mathematical representation (nor analytic gradient information) for model agnostic HPO, instead, we follow a numerical black-box optimization: an ML algorithm is configured with values chosen for one or more hyperparameters, this algorithm is then evaluated (optimally with a robust resampling method) and its performance measured, this is repeated with multiple configurations and the configuration with the best performance is selected. We could think of finding the optimal configuration in the same way as selecting a model from a benchmark experiment, where in this case each model uses the same underlying algorithm but with different hyperparameter configurations. For example, we could naively tune the number of trees in a random forest using basic mlr3 code:

```
bmr = benchmark(benchmark_grid(
  tasks = tsk("penguins_simple"),
  learners = list(
```

```
    lrn("classif.ranger", num.trees = 1, id = "1 tree"),
    lrn("classif.ranger", num.trees = 10, id = "10 trees"),
    lrn("classif.ranger", num.trees = 100, id = "100 trees")),
  resamplings = rsmp("cv", folds = 3)
))

autoplot(bmr)
```

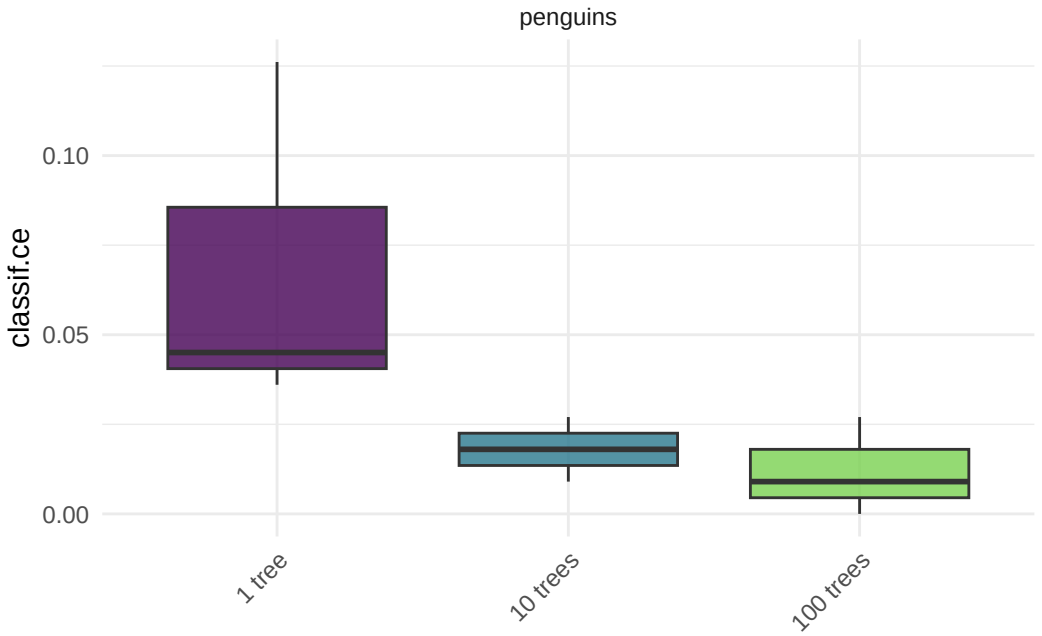


Figure 4.1.: In this code example we benchmark three random forest models with 1, 10, and 100 trees respectively, using 3-fold resampling, classification error loss, and tested on the simplified penguin dataset. The plot shows that the models with 10 and 100 trees are better performing across all three folds and 100 trees may be better than 10.

Human trial-and-error (which is essentially what we are doing above), is time-consuming, often biased, error-prone, and computationally irreproducible. Instead, many sophisticated HPO methods (Section 4.1.4) (or 'tuners') have been developed over the last few decades for robust and efficient HPO. Most HPO methods are iterative and propose different configurations until some termination criterion is met, at which point the optimal configuration is then returned (Figure 4.2). Popular, modern examples are given by algorithms based on evolutionary algorithms or Bayesian optimization methods. Recent HPO methods often also make use of evaluating a configuration at multiple so-called fidelity levels, e.g., a neural network can be trained for an increasing number of epochs, gradient boosting can be performed for an increasing number of boosting steps and training data can always be subsampled to only include a smaller fraction of all available data. The general idea of multi-fidelity HPO methods is that the performance of a model obtained by using computationally cheap lower fidelity evaluations (few numbers of epochs or boosting steps, only using a small sample of all available data for training) is predictive of the performance of the model obtained using computationally expensive higher fidelity evaluations and this concept can be leveraged to

make HPO more efficient (e.g., only continuing to evaluate those configurations on higher fidelities that appear to be promising). Another interesting direction of HPO is to optimize multiple metrics (Section 4.3) simultaneously, e.g., minimizing the generalization error along with the size of the model. This gives rise to multi-objective HPO. For more details on HPO in general, the reader is referred to Bischl et al. (2021) and Feurer and Hutter (2019).

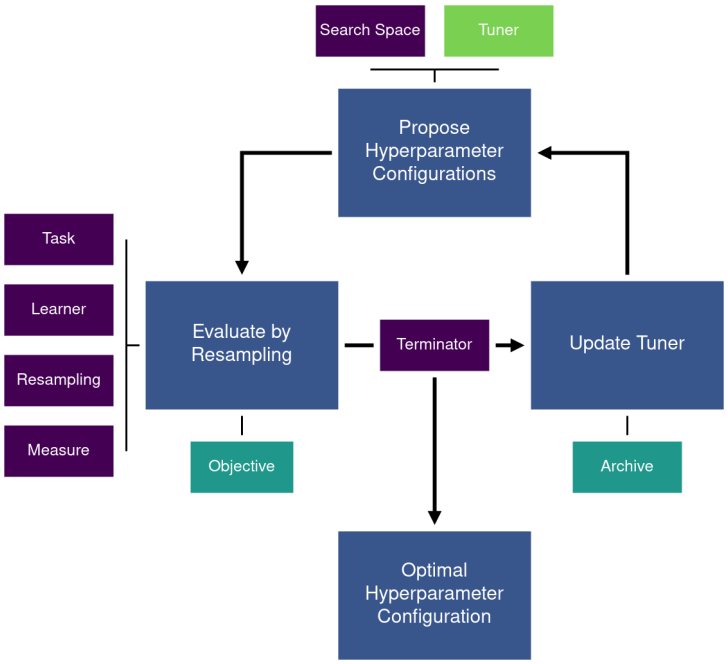


Figure 4.2.: Representation of the hyperparameter optimization loop in mlr3tuning. Blue - Hyperparameter optimization loop. Purple - Objects of the tuning instance supplied by the user. Blue-Green - Internally created objects of the tuning instance. Green - Optimization Algorithm.

4.1. Model Tuning

`mlr3tuning` is the hyperparameter optimization package of the mlr3 ecosystem. At the heart of the package (and indeed any optimization problem) are the R6 classes

- `TuningInstanceSingleCrit` and `TuningInstanceMultiCrit`, which are used to construct a tuning 'instance' which describes the optimization problem and stores the results; and
- `Tuner` which is used to get and set optimization algorithms.

In this section, we will cover these classes as well as other supporting functions and classes. Throughout this section, we will look at optimizing a support vector machine (SVM) on the `sonar` data set as a running example.

4.1.1. Learner and Search Space

We begin by constructing a support vector machine from the `e1071` with a radial kernel and specify we want to tune this using `"C-classification"` (the alternative is `"nu-classification"`, which

has the same underlying algorithm but with a `nu` parameter to tune over [0,1] instead of `cost` over $[0, \infty)$).

```
learner = lrn("classif.svm", type = "C-classification", kernel = "radial")
```

Learner hyperparameter information is stored in the `$param_set` field, including parameter name, class (e.g., discrete or numeric), levels it can be tuned over, tuning limits, and more.

```
as.data.table(learner$param_set)[, list(id, class, lower, upper, nlevels)]
```

```
                id    class lower upper nlevels
 1:       cachesize ParamDbl  -Inf   Inf     Inf
 2:   class.weights ParamUty    NA    NA     Inf
 3:            coef0 ParamDbl  -Inf   Inf     Inf
 4:             cost ParamDbl     0   Inf     Inf
 5:            cross ParamInt     0   Inf     Inf
 6: decision.values ParamLgl    NA    NA       2
 7:           degree ParamInt     1   Inf     Inf
 8:          epsilon ParamDbl     0   Inf     Inf
 9:           fitted ParamLgl    NA    NA       2
10:            gamma ParamDbl     0   Inf     Inf
11:           kernel ParamFct    NA    NA       4
12:               nu ParamDbl  -Inf   Inf     Inf
13:            scale ParamUty    NA    NA     Inf
14:       shrinking ParamLgl    NA    NA       2
15:       tolerance ParamDbl     0   Inf     Inf
16:            type ParamFct    NA    NA       2
```

Note that `$param_set` also displays non-tunable parameters. Detailed information about parameters can be found in the help pages of the underlying implementation, for this example see `e1071::svm()`.

Search Space

Given infinite resources, we could tune every single hyperparameter, but in reality that is not possible so instead only a subset of hyperparameters can be tuned. This subset is referred to as the search space or tuning space. In this example we will tune the regularization and influence hyperparameters, `cost` and `gamma`.

For numeric hyperparameters (we will explore others later) one must specify the bounds to tune over. We do this by constructing a learner and using `to_tune()` to set the lower and upper limits for the parameters we want to tune. This function allows us to construct a learner in the usual way but to leave the hyperparameters of interest to be unspecified within a set range. This is best demonstrated by example:

```
learner = lrn("classif.svm",
  cost  = to_tune(1e-5, 1e5),
  gamma = to_tune(1e-5, 1e5),
  type  = "C-classification",
  kernel = "radial"
```

```
)
learner
```

```
<LearnerClassifSVM:classif.svm>
* Model: -
* Parameters: cost=<RangeTuneToken>, gamma=<RangeTuneToken>,
  type=C-classification, kernel=radial
* Packages: mlr3, mlr3learners, e1071
* Predict Types:  [response], prob
* Feature Types: logical, integer, numeric
* Properties: multiclass, twoclass
```

Here we have constructed a classification SVM by setting the type to "C-classification", the kernel to "radial", and not fully specifying the `cost` and `gamma` hyperparameters but instead indicating that we will tune these parameters.

> **Note**
>
> The `cost` and `gamma` hyperparameters are usually tuned on the logarithmic scale. You can find out more in Section 4.2.2.

Search spaces are usually chosen by experience. In some cases these can be quite complex, Section 9.4 describes how to construct these. Section 4.2.3 introduces the `mlr3tuningspaces` extension package which allows loading of search spaces that have been established in published scientific articles.

4.1.2. Terminator

Theoretically, a tuner could search an entire search space exhaustively, however practically this is not possible and mathematically this is impossible for continuous hyperparameters. Therefore a core part of configuring tuning is to specify when to terminate the algorithm, this is also known as specifying the tuning budget. `mlr3tuning` includes many methods to specify when to terminate an algorithm, which are known as `Terminators`. Available terminators are listed in Table 4.1.

Tuning Budget
Terminators

Terminator	Function call and default parameters
Number of Evaluations	`trm("evals", n_evals = 500)`
Run Time	`trm("run_time", secs = 100)`
Performance Level	`trm("perf_reached", level = 0.1)`
Stagnation	`trm("stagnation", iters = 5, threshold = 1e-5)`

Terminator	Function call and default parameters
None	`trm("none")`
Clock Time	`trm("clock_time", stop_time = "2022-11-06 08:42:53 CET"`
Combo	`trm("combo", terminators = list(run_time_100, evals_200)`

Table 4.1.: Terminators available in `mlr3tuning`, their function call and default parameters.

The most commonly used terminators are those that stop the tuning after a certain time (`"run_time"`) or the number of evaluations (`"evals"`). Choosing a runtime is often based on practical considerations and intuition. Using a time limit can be important on clusters so that the tuning is finished before the account budget is exhausted. The `"perf_reached"` terminator stops the tuning when a certain performance level is reached, which can be helpful if a certain performance is seen as sufficient for the practical use of the model. However, one needs to be careful using this terminator as if the level is set too optimistically, the tuning might never terminate. The `"stagnation"` terminator stops when no progress is made in a certain amount of iterations. Note, this could result in the optimization being terminated too early if the search space is too complex. We use `"none"` when tuners, such as Grid Search and Hyperband, control the termination themselves. Terminators can be freely combined with the `"combo"` terminator, this is explored in the exercises at the end of this chapter. A complete and always up-to-date list of terminators can be found on our website at https://mlr-org.com/terminators.html.

4.1.3. Tuning Instance with `ti`

uning Instance

A tuning instance can be constructed manually (Section 4.1.3) with the `ti()` function or automated (Section 4.1.6) with the `tune()` function. We cover the manual approach first as this allows finer control of tuning and a more nuanced discussion about the design and use of `mlr3tuning`. The `ti` function constructs a tuning instance which collects together the information required to optimise a model.

Now continuing our example, we will construct a single-objective tuning problem (i.e., tuning over one measure) by using the `ti()` function to create a `TuningInstanceSingleCrit` (note: supplying two measures to `ti()` would result in `TuningInstanceMultiCrit` (Section 4.3)). For this example we will use three-fold resampling and will optimise the classification error measure. Note that we use `trm("none")` as we are using an exhaustive grid search.

```
resampling = rsmp("cv", folds = 3)

measure = msr("classif.ce")

```

```
learner = lrn("classif.svm",
  cost  = to_tune(1e-5, 1e5),
  gamma = to_tune(1e-5, 1e5),
  kernel = "radial",
  type = "C-classification"
)

instance = ti(
  task = tsk("sonar"),
  learner = learner,
  resampling = rsmp("cv", folds = 3),
  measures = msr("classif.ce"),
  terminator = trm("none")
)
instance
```

```
<TuningInstanceSingleCrit>
* State:  Not optimized
* Objective: <ObjectiveTuning:classif.svm_on_sonar>
* Search Space:
      id    class lower upper nlevels
1:  cost ParamDbl 1e-05 1e+05     Inf
2: gamma ParamDbl 1e-05 1e+05     Inf
* Terminator: <TerminatorNone>
```

4.1.4. Tuner

Tuners

After we created the tuning problem, we can look at *how* to tune. There are multiple `Tuners` in `mlr3tuning`, which implement different HPO algorithms.

Tuner	Function call	Method
Random Search	`tnr("random_search")`	Samples configurations from a uniform distribution randomly (Bergstra and Bengio 2012).
Grid Search	`tnr("grid_search")`	Discretizes the range of each configuration and exhaustively evaluates each combination.

Tuner	Function call	Method
Iterative Racing	`tnr("irace")`	Races down a random set of configurations and uses the surviving ones to initialize a new set of configurations which focus on a promising region of the search space (López-Ibáñez et al. 2016).
Bayesian Optimization	`tnr("mbo")`	Iterative algorithms that make use of a continuously updated surrogate model built for the objective function. By optimizing a (comparably cheap to evaluate) acquisition function defined on the surrogate prediction, the next candidate is chosen for evaluation, resulting in good sample efficiency.
Hyperband	`tnr("hyperband")`	Multi-fidelity algorithm that speeds up a random search with adaptive resource allocation and early stopping (Li et al. 2017).
Covariance Matrix Adaptation Evolution Strategy	`tnr("cmaes")`	Evolution strategy algorithm with sampling from a multivariate Gaussian who is updated with the success of the previous population (Hansen and Auger 2011).
Generalized Simulated Annealing	`tnr("gensa")`	Probabilistic algorithm for numeric search spaces (Xiang et al. 2013; Tsallis and Stariolo 1996).

Tuner	Function call	Method
Nonlinear Optimization	`tnr("nloptr")`	Several nonlinear optimization algorithms for numeric search spaces.

Table 4.2.: Tuning algorithms available in `mlr3tuning`, their function call and the methodology.

When selecting algorithms, grid search and random search are the most basic and are often selected first in initial experiments. They are 'naive' algorithms in that they try new configurations whilst ignoring performance from previous attempts. In contrast, more advanced algorithms such as Iterative Racing and CMA-ES learn from the previously evaluated configurations to find good configurations more quickly. Some advanced algorithms are included in extension packages, for example the package `mlr3mbo` implements Bayesian optimization (also called Model-Based Optimization), and `mlr3hyperband` implements algorithms of the hyperband family. A complete and up-to-date list of tuners can be found on the website.

For our SVM example, we will use a simple grid search with a resolution of 5, which is the distinct values to try *per hyperparameter*. For example for a search space $\{1, 2, 3, 4, 5, 6\}$ then a grid search with resolution 3 would pick three values evenly apart in this search space, i.e., $\{2, 4, 6\}$. The `batch_size` controls how many configurations are evaluated at the same time (see Section 9.1).

```
tuner = tnr("grid_search", resolution = 5, batch_size = 5)
tuner
```

```
<TunerGridSearch>: Grid Search
* Parameters: resolution=5, batch_size=5
* Parameter classes: ParamLgl, ParamInt, ParamDbl, ParamFct
* Properties: dependencies, single-crit, multi-crit
* Packages: mlr3tuning
```

In our example we are tuning over two numeric parameters, `TunerGridSearch` will create an equidistant grid between the respective upper and lower bounds. This means our two-dimensional grid of resolution 5 consists of $5^2 = 25$ configurations. Each configuration is a distinct set of hyperparameter values that is used to construct a model from the chosen learner, which is fit to the chosen task (Figure 4.2).

All configurations will be tried by the tuner (in random order) until either all configurations are evaluated or the terminator (Section 4.1.2) signals that the budget is exhausted.

Control Param

Just like learners, tuners also have parameters, known as control parameters, which (as the name suggests) controls the behavior of the tuners. Unlike learners, default values for control parameters usually give good results and these rarely need to be changed. Control parameters are stored in the `$param_set` field.

```
tuner$param_set
```

```
<ParamSet>
                  id    class lower upper nlevels        default value
1:        batch_size ParamInt     1   Inf     Inf <NoDefault[3]>     5
2:        resolution ParamInt     1   Inf     Inf <NoDefault[3]>     5
3: param_resolutions ParamUty    NA    NA     Inf <NoDefault[3]>
```

4.1.5. Trigger the Tuning

Now we have all our components, we are ready to start tuning! To do this we simply pass the constructed `TuningInstanceSingleCrit` to the `$optimize()` method of the initialized `Tuner`. The tuner then proceeds with the HPO loop we discussed at the beginning of the chapter (Figure 4.2).

```
tuner$optimize(instance)
```

```
   cost gamma learner_param_vals  x_domain classif.ce
1: 25000 1e-05          <list[4]> <list[2]>  0.2358178
```

The optimizer returns the best hyperparameter configuration and the corresponding measured performance. This information is also stored in `instance$result`.

> **Note**
>
> The column `x_domain` contains transformed values and `learner_param_vals` optional constants (none in this example). See section Section 4.2.2 for more information.

4.1.6. Quick Tuning with `tune`

In the previous section, we looked at creating a tuning instance manually using `ti()`, which offers more control over the tuning process. However, you can also simplify this (albeit with slightly less control) using the `tune()` sugar function. Internally this creates a `TuningInstanceSingleCrit`, starts the tuning and returns the result with the instance.

```
learner = lrn("classif.svm",
  cost  = to_tune(1e-5, 1e5),
  gamma = to_tune(1e-5, 1e5),
  kernel = "radial",
  type = "C-classification"
)

instance = tune(
  method = tnr("grid_search", resolution = 5, batch_size = 5),
  task = tsk("sonar"),
  learner = learner,
  resampling = rsmp("cv", folds = 3),
  measures = msr("classif.ce")
```

```
)

instance$result
```

```
    cost gamma learner_param_vals  x_domain classif.ce
1: 25000 1e-05          <list[4]> <list[2]>  0.2309179
```

4.1.7. Analyzing the Result

Whether you use `ti` or `tune` the output is the same and the 'archive' lists all evaluated hyperparameter configurations:

```
as.data.table(instance$archive)[, list(cost, gamma, classif.ce)]
```

```
       cost   gamma classif.ce
 1: 5.0e+04 5.0e+04  0.4661836
 2: 5.0e+04 1.0e+05  0.4661836
 3: 7.5e+04 7.5e+04  0.4661836
 4: 1.0e+05 1.0e-05  0.2499655
 5: 1.0e+05 7.5e+04  0.4661836
---
21: 1.0e-05 7.5e+04  0.4661836
22: 1.0e-05 1.0e+05  0.4661836
23: 2.5e+04 2.5e+04  0.4661836
24: 1.0e+05 2.5e+04  0.4661836
25: 1.0e+05 5.0e+04  0.4661836
```

Each row of the archive is a different evaluated configuration (there are 25 rows in total in the full `data.table`). The columns here show the tested configurations, the measure we optimize, the completed configuration time stamp, and the total train and predict times. If we only specify a single-objective criterium then the instance will return the configuration that optimizes this measure however we can manually inspect the archive to determine other important features. For example, how long did the model take to run? Were there any errors in running?

```
as.data.table(instance$archive)[,
  list(timestamp, runtime_learners, errors, warnings)]
```

```
             timestamp runtime_learners errors warnings
 1: 2023-03-03 13:16:18            0.066      0        0
 2: 2023-03-03 13:16:18            0.070      0        0
 3: 2023-03-03 13:16:18            0.079      0        0
 4: 2023-03-03 13:16:18            0.057      0        0
 5: 2023-03-03 13:16:18            0.076      0        0
---
```

```
21: 2023-03-03 13:16:21            0.077      0        0
22: 2023-03-03 13:16:21            0.073      0        0
23: 2023-03-03 13:16:21            0.068      0        0
24: 2023-03-03 13:16:21            0.078      0        0
25: 2023-03-03 13:16:21            0.069      0        0
```

Now we see not only was our optimal configuration the best performing with respect to classification error, but also it had the fastest runtime.

Another powerful feature of the instance is that we can score the internal ResampleResults on a different performance measure, for example looking at false negative rate (FNR) and false positive rate (FPR) as well as classification error:

```
as.data.table(instance$archive,
  measures = msrs(c("classif.fpr", "classif.fnr")))[,
  list(cost, gamma, classif.ce, classif.fpr, classif.fnr)]
```

```
       cost   gamma classif.ce classif.fpr classif.fnr
 1: 5.0e+04 5.0e+04  0.4661836   1.0000000    0.000000
 2: 5.0e+04 1.0e+05  0.4661836   1.0000000    0.000000
 3: 7.5e+04 7.5e+04  0.4661836   1.0000000    0.000000
 4: 1.0e+05 1.0e-05  0.2499655   0.2628968    0.232703
 5: 1.0e+05 7.5e+04  0.4661836   1.0000000    0.000000
---
21: 1.0e-05 7.5e+04  0.4661836   1.0000000    0.000000
22: 1.0e-05 1.0e+05  0.4661836   1.0000000    0.000000
23: 2.5e+04 2.5e+04  0.4661836   1.0000000    0.000000
24: 1.0e+05 2.5e+04  0.4661836   1.0000000    0.000000
25: 1.0e+05 5.0e+04  0.4661836   1.0000000    0.000000
```

Now we see our model is also the best performing with respect to FPR and FNR!

You can view all the resamplings in a BenchmarkResult object with `instance$archive$benchmark_result`.

Finally, for more visually appealing results you can use mlr3viz (Figure 4.3).

```
autoplot(instance, type = "surface")
```

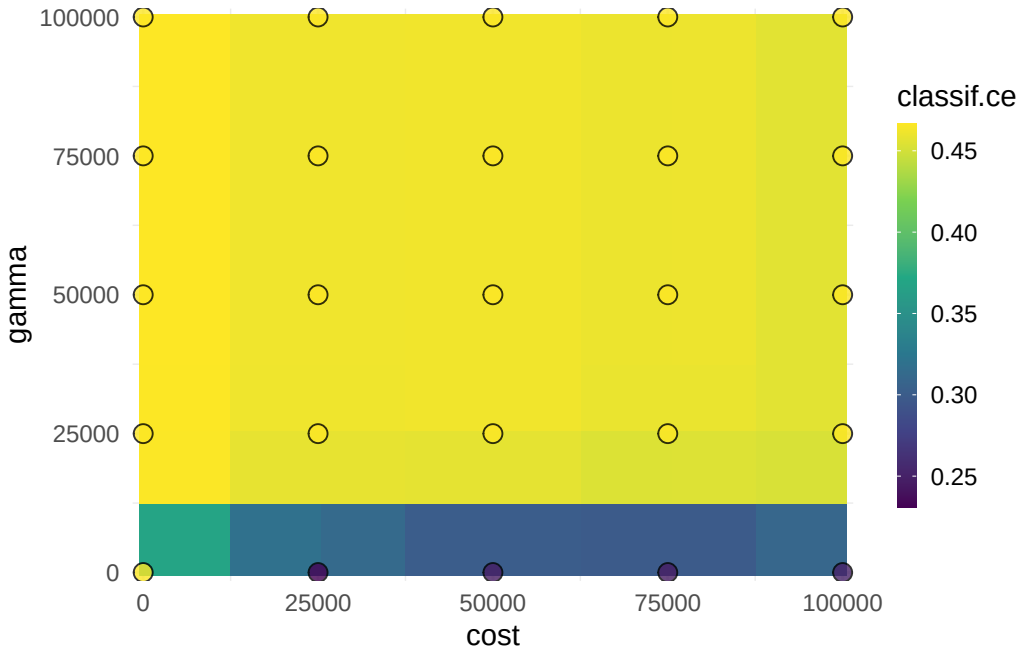


Figure 4.3.: Model performance with different configurations for cost and gamma. Bright yellow regions represent the model performing worse and dark blue performing better. We can see that high `cost` values and `gamma` values around `exp(-5)` achieve the best performance.

4.1.8. Using a tuned model

Once the learner has been tuned we can start to use it like any other model in the mlr3 universe. To do this we simply construct a new learner with the same underlying algorithm and set the learner hyperparameters with the optimal configurations:

```
svm_tuned = lrn("classif.svm", id = "SVM Tuned")
svm_tuned$param_set$values = instance$result_learner_param_vals
```

Now we can train the learner on the full dataset and we are ready to make predictions. The trained model can then be used to predict new, external data:

```
svm_tuned$train(tsk("sonar"))
svm_tuned$model
```

```
Call:
svm.default(x = data, y = task$truth(), type = "C-classification",
    kernel = "radial", gamma = 1e-05, cost = 25000.0000075, probability = (self$predict_type ==
        "prob"))
```

```
Parameters:
   SVM-Type:  C-classification
 SVM-Kernel:  radial
       cost:  25000

Number of Support Vectors:  89
```

> **Warning**
>
> A common mistake when tuning is to report the performance estimated on the resampling sets on which the tuning was performed (`instance$result$classif.ce`) as the model's performance. However, doing so would lead to bias and therefore nested resampling is required (Section 4.5). Therefore when tuning as above ensure that you do not make any statements about model performance without testing the model on more unseen data. We will come back to this in more detail in Section 4.4.

4.2. Advanced Tuning

4.2.1. Encapsulation and Fallback Learner

So far, we have only looked at the case where no issues occur. However, it often happens that learners with certain configurations do not converge, run out of memory, or terminate with an error. We can protect the tuning process from failing learners with encapsulation. The encapsulation separates the tuning from the training of the individual learner. The encapsulation method is set in the learner.

```
learner$encapsulate = c(train = "evaluate", predict = "evaluate")
```

The encapsulation can be set individually for training and predicting. There are currently two options for encapsulating a learner. The `evaluate` package and the `callr` package. The `callr` package comes with more overhead because the encapsulation spawns a separate R process. Both packages allow setting a timeout which is useful when a learner does not converge. We set a timeout of 30 seconds.

```
learner$timeout = c(train = 30, predict = 30)
```

With encapsulation, exceptions and timeouts do not stop the tuning. Instead, the error message is recorded and a fallback learner is fitted.

Fallback learners allow scoring a result when no model was fitted during training. A common approach is to predict a weak baseline e.g. predicting the mean of the data or just the majority class. See **?@sec-fallback-learner** for more detailed information.

The `featureless learner` predicts the most frequent label.

```
learner$fallback = lrn("classif.featureless")
```

Errors and warnings that occurred during tuning are stored in the archive.

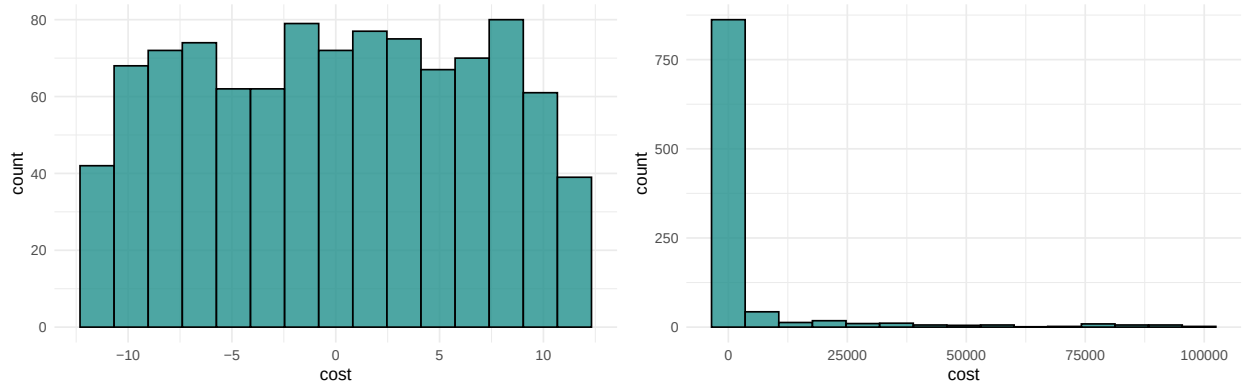
```
as.data.table(instance$archive)[, list(cost, gamma, classif.ce, errors, warnings)]
```

```
       cost   gamma classif.ce errors warnings
 1: 5.0e+04 5.0e+04  0.4661836      0        0
 2: 5.0e+04 1.0e+05  0.4661836      0        0
 3: 7.5e+04 7.5e+04  0.4661836      0        0
 4: 1.0e+05 1.0e-05  0.2499655      0        0
 5: 1.0e+05 7.5e+04  0.4661836      0        0
---
21: 1.0e-05 7.5e+04  0.4661836      0        0
22: 1.0e-05 1.0e+05  0.4661836      0        0
23: 2.5e+04 2.5e+04  0.4661836      0        0
24: 1.0e+05 2.5e+04  0.4661836      0        0
25: 1.0e+05 5.0e+04  0.4661836      0        0
```

4.2.2. Advanced Search Spaces

Usually, the `cost` and `gamma` hyperparameters are tuned on the logarithmic scale which means the optimization algorithm searches in $[log(1e-5), log(1e5)]$ but transforms the selected configuration with `exp()` before passing to the learner. Using the log transformation emphasizes smaller values but can also result in large values. The code below demonstrates this more clearly. The histograms show how the algorithm searches within a narrow range but exponentiating then results in the majority of points being relatively small but a few being very large.

```
cost = runif(1000, log(1e-5), log(1e5))
```



(a) `cost` values sampled by the optimization algorithm.

(b) `exp(cost)` values seen by the learner.

Figure 4.4.: Histogram of sampled `cost` values.

To add the `exp()` transformation to a hyperparameter, we pass `logscale = TRUE` to `to_tune()`.

```
learner = lrn("classif.svm",
  cost  = to_tune(1e-5, 1e5, logscale = TRUE),
  gamma = to_tune(1e-5, 1e5, logscale = TRUE),
  kernel = "radial",
  type = "C-classification"
)

instance = tune(
  method = tnr("grid_search", resolution = 5, batch_size = 5),
  task = tsk("sonar"),
  learner = learner,
  resampling = rsmp("cv", folds = 3),
  measures = msr("classif.ce")
)

instance$result
```

```
       cost     gamma learner_param_vals  x_domain classif.ce
1: 5.756463 -5.756463          <list[4]> <list[2]>  0.2014493
```

The column `x_domain` contains the hyperparameter values after the transformation i.e. `exp(5.76)` and `exp(-5.76)`:

```
instance$result$x_domain
```

```
[[1]]
[[1]]$cost
[1] 316.2278

[[1]]$gamma
[1] 0.003162278
```

4.2.3. Search Spaces Collection

Selected search spaces can require a lot of background knowledge or expertise. The package mlr3tuningspaces tries to make HPO more accessible by providing implementations of published search spaces for many popular machine learning algorithms. These search spaces should be applicable to a wide range of data sets, however, they may need to be adapted in specific situations. The search spaces are stored in the dictionary mlr_tuning_spaces.

```
as.data.table(mlr_tuning_spaces)
```

```
                       key                                label        learner
1: classif.glmnet.default    Classification GLM with Default classif.glmnet
```

```
 2:    classif.glmnet.rbv2  Classification GLM with RandomBot classif.glmnet
 3:   classif.kknn.default   Classification KKNN with Default   classif.kknn
 4:      classif.kknn.rbv2 Classification KKNN with RandomBot   classif.kknn
 5: classif.ranger.default Classification Ranger with Default classif.ranger
---
20:        regr.rpart.rbv2    Regression Rpart with RandomBot     regr.rpart
21:       regr.svm.default        Regression SVM with Default       regr.svm
22:          regr.svm.rbv2      Regression SVM with RandomBot       regr.svm
23:   regr.xgboost.default    Regression XGBoost with Default   regr.xgboost
24:      regr.xgboost.rbv2  Regression XGBoost with RandomBot   regr.xgboost
1 variable not shown: [n_values]
```

The tuning spaces are named according to the scheme `{learner-id}.{publication}`. The sugar function `lts()` is used to retrieve a `TuningSpace`.

```
lts("classif.rpart.default")
```

```
<TuningSpace:classif.rpart.default>: Classification Rpart with Default
          id lower upper levels logscale
1:  minsplit 2e+00 128.0            TRUE
2: minbucket 1e+00  64.0            TRUE
3:        cp 1e-04   0.1            TRUE
```

A tuning space can be passed to `ti()` as the `search_space`.

```
instance = ti(
  task = tsk("sonar"),
  learner = lrn("classif.rpart"),
  resampling = rsmp("cv", folds = 3),
  measures = msr("classif.ce"),
  terminator = trm("evals", n_evals = 20),
  search_space = lts("classif.rpart.rbv2")
)
instance
```

```
<TuningInstanceSingleCrit>
* State:  Not optimized
* Objective: <ObjectiveTuning:classif.rpart_on_sonar>
* Search Space:
          id    class    lower upper nlevels
1:        cp ParamDbl -9.21034     0     Inf
2:  maxdepth ParamInt  1.00000    30      30
3: minbucket ParamInt  1.00000   100     100
4:  minsplit ParamInt  1.00000   100     100
* Terminator: <TerminatorEvals>
```

Alternatively, we can explicitly set the search space of a learner with `TuneTokens`

```
vals = lts("classif.rpart.default")$values
vals
```

```
$minsplit
Tuning over:
range [2, 128] (log scale)


$minbucket
Tuning over:
range [1, 64] (log scale)


$cp
Tuning over:
range [1e-04, 0.1] (log scale)
```

```
learner = lrn("classif.rpart")
learner$param_set$set_values(.values = vals)
learner
```

```
<LearnerClassifRpart:classif.rpart>: Classification Tree
* Model: -
* Parameters: xval=0, minsplit=<RangeTuneToken>,
  minbucket=<RangeTuneToken>, cp=<RangeTuneToken>
* Packages: mlr3, rpart
* Predict Types:  [response], prob
* Feature Types: logical, integer, numeric, factor, ordered
* Properties: importance, missings, multiclass, selected_features,
  twoclass, weights
```

When passing a learner to `lts()`, the default search space from the Bischl et al. (2021) article is applied.

```
lts(lrn("classif.rpart"))
```

```
<LearnerClassifRpart:classif.rpart>: Classification Tree
* Model: -
* Parameters: xval=0, minsplit=<RangeTuneToken>,
  minbucket=<RangeTuneToken>, cp=<RangeTuneToken>
* Packages: mlr3, rpart
* Predict Types:  [response], prob
* Feature Types: logical, integer, numeric, factor, ordered
```

```
* Properties: importance, missings, multiclass, selected_features,
  twoclass, weights
```

It is possible to simply overwrite a predefined tuning space in construction, for example here we change the range of the `nrounds` hyperparameter in XGBoost:

```
lts("classif.xgboost.rbv2", nrounds = to_tune(1, 1024))
```

```
<TuningSpace:classif.xgboost.rbv2>: Classification XGBoost with RandomBot
                  id lower upper               levels logscale
 1:           booster    NA    NA gblinear,gbtree,dart    FALSE
 2:           nrounds 1e+00  1024                       FALSE
 3:               eta 1e-04     1                        TRUE
 4:             gamma 1e-05     7                        TRUE
 5:            lambda 1e-04  1000                        TRUE
 6:             alpha 1e-04  1000                        TRUE
 7:         subsample 1e-01     1                       FALSE
 8:         max_depth 1e+00    15                       FALSE
 9:  min_child_weight 1e+00   100                        TRUE
10:  colsample_bytree 1e-02     1                       FALSE
11: colsample_bylevel 1e-02     1                       FALSE
12:         rate_drop 0e+00     1                       FALSE
13:         skip_drop 0e+00     1                       FALSE
```

4.3. Multi-Objective Tuning

So far we have considered optimizing a model with respect to one metric but multi-metric, or multi-objective optimization is also possible. A simple example of multi-objective optimization might be optimizing a classifier to minimize false positive and false negative predictions. In a more complex example, consider the problem of deploying a classifier in a healthcare setting, there is clearly an ethical argument to tune the model to make the best possible predictions, however in machine learning this can often lead to models that are harder to interpret (think about deep neural networks!). In this case, we may be interested in minimizing *both* classification error (for example) and complexity.

Multi-objective

In general, when optimizing multiple metrics, these will be in competition (if they were not we would only need to optimize with respect to one of them!) and so no single configuration exists that optimizes all metrics. Focus is therefore given to the concept of Pareto optimality. One hyperparameter configuration is said to Pareto-dominate another one if the resulting model is equal or better in all metrics and strictly better in at least one metric. All configurations that are not Pareto-dominated are referred to as Pareto efficient and the set of all these configurations is referred to as the Pareto front (Figure 4.5).

Pareto Front

The goal of multi-objective HPO is to approximate the true, unknown Pareto front. More methodological details on multi-objective HPO can be found in Karl et al. (2022).

We will now demonstrate multi-objective HPO by tuning a decision tree on the Spam data set with respect to the classification error, as a measure of model performance, and the number of selected features, as a measure of model complexity (in a decision tree the number of selected features is straightforward to obtain by simply counting the number of unique splitting variables). We will tune

- The complexity hyperparameter `cp` that controls when the learner considers introducing another branch.
- The `minsplit` hyperparameter that controls how many observations must be present in a leaf for another split to be attempted.
- The `maxdepth` hyperparameter that limits the depth of the tree.

```
learner = lrn("classif.rpart",
  cp = to_tune(1e-04, 1e-1, logscale = TRUE),
  minsplit = to_tune(2, 128, logscale = TRUE),
  maxdepth = to_tune(1, 30)
)

measures = msrs(c("classif.ce", "selected_features"))
```

Note that as we tune with respect to multiple measures, the function `ti` creates a TuningInstanceMultiCrit instead of a TuningInstanceSingleCrit.

```
instance = ti(
  task = tsk("spam"),
  learner = learner,
  resampling = rsmp("cv", folds = 3),
  measures = measures,
  terminator = trm("evals", n_evals = 20),
  store_models = TRUE  # required to inspect selected_features
)
instance
```

```
<TuningInstanceMultiCrit>
* State:  Not optimized
* Objective: <ObjectiveTuning:classif.rpart_on_spam>
* Search Space:
         id    class      lower     upper nlevels
1:       cp ParamDbl -9.2103404 -2.302585     Inf
2: minsplit ParamDbl  0.6931472  4.859812     Inf
3: maxdepth ParamInt  1.0000000 30.000000      30
* Terminator: <TerminatorEvals>
```

As before we will then select and run a tuning algorithm, here we use random search:

```
tuner = tnr("random_search", batch_size = 20)
tuner$optimize(instance)
```

Finally, we inspect the best-performing configurations, i.e., the Pareto set. And then inspect the estimated Pareto set and visualize the estimated Pareto front:

```
instance$archive$best()[, list(cp, minsplit, maxdepth, classif.ce, selected_features)]
```

```
           cp minsplit maxdepth classif.ce selected_features
 1: -4.897655 3.338026       17 0.10302293          7.666667
 2: -7.051424 3.896918       12 0.10041637         12.333333
 3: -4.245193 1.541127        8 0.10780375          5.666667
 4: -2.774911 3.148014       30 0.16387611          2.333333
 5: -4.807622 1.987267       11 0.10432672          7.333333
 6: -4.853549 4.375677       19 0.10671726          6.000000
 7: -3.739909 1.772185       26 0.11193239          5.000000
 8: -4.937744 1.286328       29 0.10302293          7.666667
 9: -4.553218 2.750349       22 0.10563050          6.666667
10: -3.714380 2.555973       25 0.11193239          5.000000
11: -5.076189 2.735166       11 0.10085053          9.333333
12: -4.519566 4.470367       30 0.10845564          5.333333
13: -5.445322 1.663845       23 0.08715871         13.000000
14: -6.465093 1.536021       16 0.07759311         29.000000
15: -6.528747 2.155507        6 0.08585422         16.333333
```

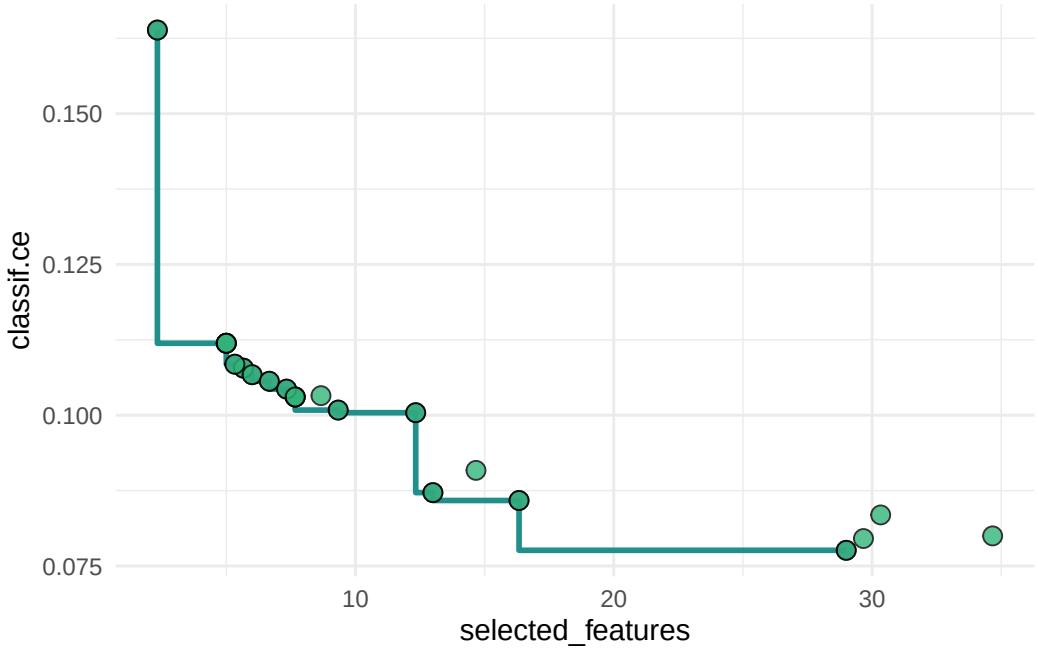


Figure 4.5.: Pareto front of selected features and classification error. Black dots represent tested configurations, each red dot individually represents a Pareto-optimal configuration and all red dots together represent the Pareto front.

4.4. Automated Tuning with `AutoTuner`

One of the most powerful classes in mlr3 is the `AutoTuner`. The `AutoTuner` wraps a learner and augments it with an automatic tuning process for a given set of hyperparameters – this allows transparent tuning of any learner, without the need to extract information on the best hyperparameter settings at the end. As the `AutoTuner` itself inherits from the `Learner` base class, it can be used like any other learner!

Let us see this in practice. We will run the exact same example as above but this time using the `AutoTuner` for automated tuning:

```
learner = lrn("classif.svm",
  cost  = to_tune(1e-5, 1e5, logscale = TRUE),
  gamma = to_tune(1e-5, 1e5, logscale = TRUE),
  kernel = "radial",
  type = "C-classification"
)

at = auto_tuner(
  method = tnr("grid_search", resolution = 5, batch_size = 5),
  learner = learner,
  resampling = rsmp("cv", folds = 3),
  measure = msr("classif.ce")
)

at
```

```
<AutoTuner:classif.svm.tuned>
* Model: list
* Search Space:
<ParamSet>
      id    class     lower    upper nlevels        default value
1:  cost ParamDbl -11.51293 11.51293     Inf <NoDefault[3]>
2: gamma ParamDbl -11.51293 11.51293     Inf <NoDefault[3]>
Trafo is set.
* Packages: mlr3, mlr3tuning, mlr3learners, e1071
* Predict Type: response
* Feature Types: logical, integer, numeric
* Properties: multiclass, twoclass
```

We can now use this like any other learner, calling the `$train()` and `$predict()` methods. The key difference to a normal learner, is that calling `$train()` also tunes the model.

```
task = tsk("sonar")
split = partition(task)
at$train(task, row_ids = split$train)
at$predict(task, row_ids = split$test)$score()
```

```
classif.ce
 0.2608696
```

We could also pass the `AutoTuner` to `resample()` and `benchmark()`, which would result in a nested resampling (Section 4.5), discussed next.

4.5. Nested Resampling

Hyperparameter optimization generally requires an additional layer or resampling to prevent bias in tuning. If the same data is used for determining the optimal configuration and the evaluation of the resulting model itself, the actual performance estimate of the model might be severely biased (Simon 2007). This is analogous to optimism of the training error described in (James et al. 2014), which occurs when training error is taken as an estimate of out-of-sample performance. This bias is represented in Figure 4.6 which shows an algorithm being tuned on data that has been split intro training and testing data, and then the same data is used to estimate the model performance after selecting the best configuration after HPO.

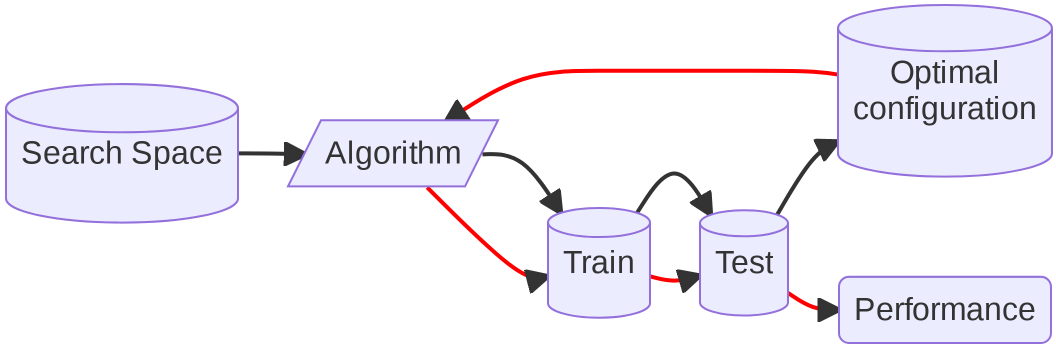


Figure 4.6.: Illustration of biased tuning. An algorithm is tuned by training on the `Train` dataset and then the optimal configuration is selected by evaluation on the `Test` data. The model's performance is then evaluated with the optimal configuration on the same data.

Nested resampling separates model optimization from the process of estimating the performance of the model by adding an additional layer of resampling, i.e., whilst model performance is estimated using a resampling method in the 'usual way', tuning is then performed by resampling the resampled data (Figure 4.7). For more details and a formal introduction to nested resampling the reader is referred to Bischl et al. (2021). Nested Resamp

A common confusion is how and when to use nested resampling. In the rest of this section we will answer the 'how' question but first the 'when'. A common mistake is to confuse nested resampling for model evaluation and comparison, with tuning for model deployment. To put it differently, nested resampling is a statistical procedure to estimate the predictive performance of the model trained on the full dataset, it is *not* a procedure to select optimal hyperparameters. Nested resampling

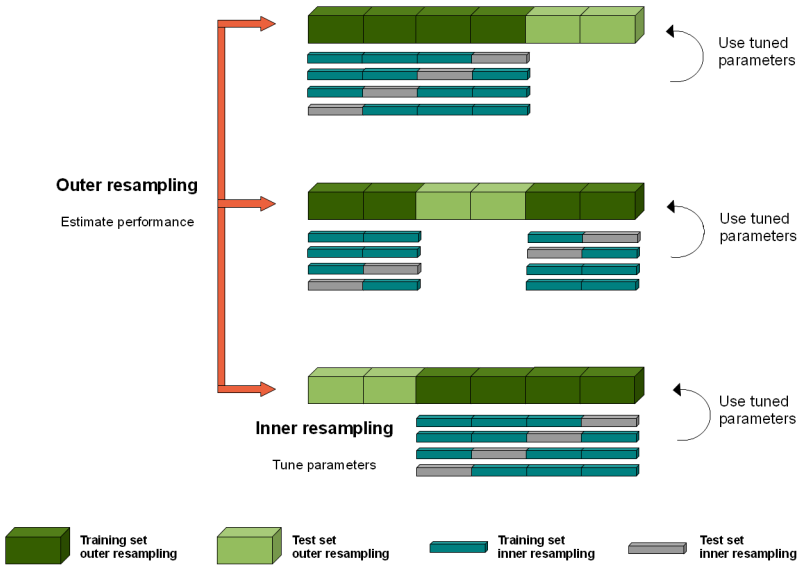


Figure 4.7.: An illustration of nested resampling. The green blocks represent 3-fold coss-validation for the outer resampling for model evaluation and the blue and gray blocks represent 4-fold cross-validation for the inner resampling for HPO.

produces many hyperparameter configurations which should not be used to construct a final model (Simon 2007).

In words this process runs as follows:

1. Outer resampling – Instantiate 3-fold cross-validation to create different testing and training data sets.
2. Inner resampling – Within the training data instantiate 4-fold cross-validation to create different inner testing and training data sets.
3. HPO – Tune the hyperparameters using the inner data splits (blue and gray blocks).
4. Training – Fit the learner on the outer training data set using the optimal hyperparameter configuration obtained from the inner resampling (dark green blocks).
5. Evaluation – Evaluate the performance of the learner on the outer testing data (light green blocks).
6. Cross-validation – Repeat (2)-(5) for each of the three folds.
7. Aggregation – Take the sample mean of the three performance values for an unbiased performance estimate.

That is enough theory for now, let us take a look at how this works in mlr3.

4.5.1. Nested Resampling with `AutoTuner`

Nested resampling in mlr3 becomes quite simple with the `AutoTuner` (Section 4.4). We simply specify the inner-resampling and tuning setup with the `AutoTuner` and then pass this to `resample()` or `benchmark()`. Continuing with our previous example we will use the auto-tuner to resample

a support vector classifier with 3-fold cross-validation in the outer-resampling and 4-fold cross-validation in the inner resampling.

```
learner = lrn("classif.svm",
  cost  = to_tune(1e-5, 1e5, logscale = TRUE),
  gamma = to_tune(1e-5, 1e5, logscale = TRUE),
  kernel = "radial",
  type = "C-classification"
)

at = auto_tuner(
  method = tnr("grid_search", resolution = 5, batch_size = 5),
  learner = learner,
  resampling = rsmp("cv", folds = 4),
  measure = msr("classif.ce"),
  term_evals = 20,
)

task = tsk("sonar")
outer_resampling = rsmp("cv", folds = 3)

rr = resample(task, at, outer_resampling, store_models = TRUE)

rr
```

```
<ResampleResult> of 3 iterations
* Task: sonar
* Learner: classif.svm.tuned
* Warnings: 0 in 0 iterations
* Errors: 0 in 0 iterations
```

Note we set `store_models = TRUE` so that the `AutoTuner` models are stored to investigate the inner tuning. In this example, we utilized the same resampling strategy (K-fold cross-validation) but the mlr3 infrastructure is not limited to this, you can freely combine different inner and outer resampling strategies as you choose. You can also mix-and-match parallelization methods for controlling the process (Section 9.1.4).

There are some special functions for nested resampling available in addition to the methods described in Section 3.2.

The `extract_inner_tuning_results()` and `extract_inner_tuning_archives()` functions return the optimal configurations (across all outer folds) and full tuning archives respectively.

```
extract_inner_tuning_results(rr)[,
  list(iteration, cost, gamma, classif.ce)]
```

```
   iteration      cost     gamma classif.ce
```

```
1:         1 11.512925 -5.756463  0.1663866
2:         2  5.756463 -5.756463  0.2090336
3:         3  5.756463 -5.756463  0.1941176
```

```
extract_inner_tuning_archives(rr)[,
  list(iteration, cost, gamma, classif.ce)]
```

```
    iteration       cost      gamma classif.ce
 1:         1 -11.512925 -11.512925  0.4567227
 2:         1 -11.512925   5.756463  0.4567227
 3:         1  -5.756463 -11.512925  0.4567227
 4:         1   0.000000   5.756463  0.4567227
 5:         1   5.756463 -11.512925  0.2747899
---
56:         3   0.000000 -11.512925  0.4678571
57:         3   0.000000  -5.756463  0.2151261
58:         3   0.000000   5.756463  0.4678571
59:         3   5.756463   0.000000  0.4678571
60:         3  11.512925  -5.756463  0.1941176
```

From the optimal results, we observe a trend toward larger `cost` and smaller `gamma` values. However, as we discussed earlier, these values should not be used to fit a final model as the selected hyperparameters might differ greatly between the resampling iterations. On the one hand, this could be due to the optimization algorithm used, for example, with simple algorithms like random search, we do not expect stability of hyperparameters. On the other hand, more advanced methods like irace converge to an optimal hyperparameter configuration. Another reason for instability in hyperparameters could be due to small data sets and/or a low number of resampling iterations (i.e., the usual small data high variance problem).

4.5.2. Performance comparison

Finally, we will compare the predictive performances estimated on the outer resampling to the inner resampling to gain an understanding of model overfitting and general performance.

```
extract_inner_tuning_results(rr)[,
  list(iteration, cost, gamma, classif.ce)]
```

```
   iteration      cost     gamma classif.ce
1:         1 11.512925 -5.756463  0.1663866
2:         2  5.756463 -5.756463  0.2090336
3:         3  5.756463 -5.756463  0.1941176
```

```
rr$score()[,
  list(iteration, classif.ce)]
```

```
   iteration classif.ce
1:         1  0.1285714
2:         2  0.1014493
3:         3  0.1884058
```

Significantly lower predictive performances on the outer resampling indicate that the models with the optimized hyperparameters overfit the data.

It is therefore important to ensure that the performance of a tuned model is *always* reported as the aggregated performance of all outer resampling iterations, which is an unbiased estimate of future model performance. Note here we use the term *unbiased* to refer only to the statistical procedure of the performance estimation. The underlying prediction of the model could still be biased e.g. due to a bias in the data set.

```
rr$aggregate()
```

```
classif.ce
 0.1394755
```

As a final note, nested resampling is computationally expensive, as a simple example using five outer folds and three inner folds with a grid search of resolution 5 used to tune 2 parameters, results in $5 3 5 * 5 = 375$ iterations of model training/testing. In practice, you may often see closer to three folds used in inner resampling or even holdout, or if you have the resources then we recommend parallelization (Section 9.1).

4.6. Conclusion

In this chapter, we learned how to optimize a model using tuning instances, about different tuners and terminators, how to make use of the automated methods for quicker implementation in larger experiments, and the importance of nested resampling. The most important functions and classes we learned about are in Table 4.3 alongside their R6 classes. If you are interested in learning more about the underlying R6 classes to gain finer control of these methods, then take a look at the online API.

S3 function	R6 Class	Summary
`tnr()`	`Tuner`	Determines an optimisation algorithm
`trm()`	`Terminator`	Controls when to terminate the tuning algorithm
`ti()`	`TuningInstanceSingleCrit` or `TuningInstanceMultiCrit`	Stores tuning settings and save results
`paradox::to_tune()`	`paradox::TuneToken`	Sets which parameters in a learner to tune and over what search space
`auto_tuner()`	`AutoTuner`	Automates the tuning process

S3 function	R6 Class	Summary
`extract_inner_tuning_results()`	-	Extracts inner results from nested resampling
`extract_inner_tuning_archives()`	-	Extracts inner archives from nested resampling

Table 4.3.: Core S3 'sugar' functions for model optimization in mlr3 with the underlying R6 class that are constructed when these functions are called (if applicable) and a summary of the purpose of the functions.

Resources

The mlr3tuning cheatsheet[1] summarizes the most important functions of mlr3tuning and the mlr3 gallery[2] features a collection of case studies and demonstrations about optimization, most notably learn how to:

- Apply advanced methods in the practical tuning series[3].
- Optimize an rpart classification tree with only a few lines of code[4].
- Tune an XGBoost model with early stopping[5].
- Quickly load and tune over search spaces that have been published in literature with mlr3tuningspaces[6].

4.7. Exercises

1. Tune the `mtry`, `sample.fraction`, `num.trees` hyperparameters of a random forest model (`regr.ranger`) on the `Motor Trend` data set (`mtcars`). Use a simple random search with 50 evaluations and select a suitable batch size. Evaluate with a 3-fold cross-validation and the root mean squared error.
2. Evaluate the performance of the model created in Question 1 with nested resampling. Use a holdout validation for the inner resampling and a 3-fold cross-validation for the outer resampling. Print the unbiased performance estimate of the model.
3. Tune and benchmark an XGBoost model against a logistic regression and determine which has the best Brier score. Use mlr3tuningspaces and nested resampling.

[1] https://cheatsheets.mlr-org.com/mlr3tuning.pdf
[2] https://mlr-org.com/gallery.html#category:tuning
[3] https://mlr-org.com/gallery.html#category:practical_tuning_series
[4] https://mlr-org.com/gallery/2022-11-10-hyperparameter-optimization-on-the-palmer-penguins/
[5] https://mlr-org.com/gallery/2022-11-04-early-stopping-with-xgboost/
[6] https://mlr-org.com/gallery/2021-07-06-introduction-to-mlr3tuningspaces/

5. Feature Selection

Feature selection is a key component of data analysis and is part of most machine learning applications. This chapter introduces two concepts of feature selection and how to use them in mlr3. Filter methods are preprocessing steps that are independent of the model to be fitted, whereas wrapper methods work by fitting models on feature subsets and evaluating their performance. We start with simple examples such as univariate filters and sequential forward selection but also cover more advanced topics such as optimizing multiple performance measures simultaneously. To integrate feature selection into complex machine learning pipelines and the mlr3 ecosystem, we show how to combine feature selection with mlr3 pipelines and how to automate feature selection by wrapping it in mlr3 learners.

Feature selection, also known as variable or descriptor selection, is the process of finding a subset of features to use with a given task and learner. Using an *optimal set* of features can have several benefits:

- improved predictive performance, since we reduce overfitting on irrelevant features,
- robust models that do not rely on noisy features,
- simpler models that are easier to interpret,
- faster model fitting, e.g. for model updates,
- faster prediction, and
- no need to collect potentially expensive features.

However, these objectives will not necessarily be optimized by the same *optimal set* of features and thus feature selection is inherently multi-objective. In this chapter, we mostly focus on feature selection as a means of improving predictive performance, but also briefly cover optimization of multiple criteria (Section 5.2.5).

Reducing the amount of features can improve models across many scenarios, but it can be especially helpful in datasets that have a high number of features in comparison to the number of datapoints. Many learners perform implicit, also called embedded, feature selection, e.g. via the choice of variables used for splitting in a decision tree. Most other feature selection methods are model agnostic, i.e. they can be used together with any learner. Of the many different approaches to identifying relevant features, we will focus on two general concepts, which are described in detail below: Filter and Wrapper methods (Guyon and Elisseeff 2003; Chandrashekar and Sahin 2014).

For this chapter, the reader should know the basic concepts of mlr3 (Chapter 2), i.e. know about tasks (Appendix C) and learners (Section 2.2). Basics about performance evaluation (Chapter 3), i.e. resampling (Section 3.2) and benchmarking (Section 3.3) are helpful but not strictly necessary.

5.1. Filters

Filter methods are preprocessing steps that can be applied before training a model. A very simple filter approach could look like this:

1. calculate the correlation coefficient ρ between each feature and a numeric target variable, and
2. select all features with $\rho > 0.2$ for further modelling steps.

This approach is a *univariate* filter because it only considers the univariate relationship between each feature and the target variable. Further, it can only be applied to regression tasks with continuous features and the threshold of $\rho > 0.2$ is quite arbitrary. Thus, more advanced filter methods, e.g. *multivariate* filters based on feature importance, usually perform better (Bommert et al. 2020). On the other hand, a benefit of univariate filters is that they are usually computationally cheaper than more complex filter or wrapper methods. In the following, it is described how to calculate univariate, multivariate and feature importance filters, how to access implicitly selected features, how to integrate filters in a machine learning pipeline and how to optimize filter thresholds.

Filter algorithms select features by assigning numeric scores to each feature, e.g. correlation between feature and target variables, use these to rank the features and select a feature subset based on the ranking. Features that are assigned lower scores can then be omitted in subsequent modeling steps. All filters are implemented via the package `mlr3filters`. Below, we cover how to

- instantiate a `Filter` object,
- calculate scores for a given task, and
- use calculated scores to select or drop features.

One special case of filters are feature importance filters (Section 5.1.2). They select features that are important according to the model induced by a selected `Learner`. Feature importance filters rely on the learner to extract information on feature importance from a trained model, for example, by inspecting a learned decision tree and returning the features that are used as split variables, or by computing model-agnostic feature importance (Chapter 10) values for each feature.

Many filter methods are implemented in `mlr3filters`, for example:

- Correlation, calculating Pearson or Spearman correlation between numeric features and numeric targets (`FilterCorrelation`)
- Information gain, i.e. mutual information of the feature and the target or the reduction of uncertainty of the target due to a feature (`FilterInformationGain`)
- Minimal joint mutual information maximization, minimizing the joint information between selected features to avoid redundancy (`FilterJMIM`)
- Permutation score, which calculates permutation feature importance (see Chapter 10) with a given learner for each feature (`FilterPermutation`)
- Area under the ROC curve calculated for each feature separately (`FilterAUC`)

Most of the filter methods have some limitations, e.g. the correlation filter can only be calculated for regression tasks with numeric features. For a full list of all implemented filter methods we refer the reader to the mlr3filters website[1], which also shows the supported task and features types. A benchmark of filter methods was performed by Bommert et al. (2020), who recommend to not

[1] https://mlr3filters.mlr-org.com

rely on a single filter method but try several ones if the available computational resources allow. If only a single filter method is to be used, the authors recommend to use a feature importance filter using random forest permutation importance (see Section 5.1.2), similar to the permutation method described above, but also the JMIM and AUC filters performed well in their comparison.

5.1.1. Calculating Filter Values

The first step is to create a new R object using the class of the desired filter method. Similar to other instances in `mlr3`, these are registered in a dictionary (`mlr_filters`) with an associated shortcut function `flt()`. Each object of class `Filter` has a `$calculate()` method which computes the filter values and ranks them in a descending order. For example, we can use the information gain filter described above:

```
library("mlr3verse")
filter = flt("information_gain")
```

Such a `Filter` object can now be used to calculate the filter on the penguins data and get the results:

```
task = tsk("penguins")
filter$calculate(task)

as.data.table(filter)
```

```
          feature       score
1: flipper_length 0.581167901
2:    bill_length 0.544896584
3:     bill_depth 0.538718879
4:         island 0.520157171
5:      body_mass 0.442879511
6:            sex 0.007244168
7:           year 0.000000000
```

Some filters have hyperparameters, which can be changed similar to setting hyperparameters of a `Learner` using `$param_set$values`. For example, to calculate `"spearman"` instead of `"pearson"` correlation with the correlation filter:

```
filter_cor = flt("correlation")
filter_cor$param_set$values = list(method = "spearman")
filter_cor$param_set
```

```
<ParamSet>
       id    class lower upper nlevels    default    value
1:    use ParamFct    NA    NA       5 everything
2: method ParamFct    NA    NA       3    pearson spearman
```

5.1.2. Feature Importance Filters

To use feature importance filters, we can use a learner with integrated feature importance methods. All learners with the property "importance" have this functionality. A list of all learners with this property can be found with

```
as.data.table(mlr_learners)[sapply(properties, function(x) "importance" %in% x)]
```

```
                        key                                label task_type
 1:         classif.catboost                    Gradient Boosting   classif
 2:      classif.featureless Featureless Classification Learner   classif
 3:              classif.gbm                    Gradient Boosting   classif
 4: classif.imbalanced_rfsrc            Imbalanced Random Forest   classif
 5:         classif.lightgbm                    Gradient Boosting   classif
---
22:                surv.gbm                    Gradient Boosting      surv
23:             surv.mboost Boosted Generalized Additive Model      surv
24:             surv.ranger                        Random Forest      surv
25:              surv.rfsrc                        Random Forest      surv
26:            surv.xgboost                    Gradient Boosting      surv
4 variables not shown: [feature_types, packages, properties, predict_types]
```

or on the mlr3 website[2].

For some learners, the desired filter method needs to be set during learner creation. For example, learner `classif.ranger` comes with multiple integrated methods, c.f. the help page of `ranger::ranger()`. To use the feature importance method "impurity", select it during learner construction:

```
lrn = lrn("classif.ranger", importance = "impurity")
```

Now we can use the `FilterImportance` filter class:

```
task = tsk("penguins")

# Remove observations with missing data
task$filter(which(complete.cases(task$data())))

filter = flt("importance", learner = lrn)
filter$calculate(task)
as.data.table(filter)
```

```
          feature     score
1:    bill_length 76.374739
2: flipper_length 45.348924
```

[2] https://mlr-org.com/learners.html

```
3:     bill_depth 36.305939
4:      body_mass 26.457564
5:         island 24.077990
6:            sex  1.597289
7:           year  1.215536
```

5.1.3. Embedded Methods

Many learners internally select a subset of the features which they find helpful for prediction, but ignore other features. For example, a decision tree might never select some features for splitting. These subsets can be used for feature selection, which we call embedded methods because the feature selection is embedded in the learner. The selected features (and those not selected) can be queried if the learner has the `"selected_features"` property, as the following example demonstrates:

```
task = tsk("penguins")
learner = lrn("classif.rpart")

# ensure that the learner selects features
stopifnot("selected_features" %in% learner$properties)

learner = learner$train(task)
learner$selected_features()
```

```
[1] "flipper_length" "bill_length"    "island"
```

The features selected by the model can be extracted by a `Filter` object, where `$calculate()` corresponds to training the learner on the given task:

```
filter = flt("selected_features", learner = learner)
filter$calculate(task)
as.data.table(filter)
```

```
          feature score
1:         island     1
2: flipper_length     1
3:    bill_length     1
4:     bill_depth     0
5:            sex     0
6:           year     0
7:      body_mass     0
```

Contrary to other filter methods, embedded methods just return value of 1 (selected features) and 0 (dropped feature).

5.1.4. Filter-based Feature Selection

After calculating a score for each feature, one has to select the features to be kept or those to be dropped from further modelling steps. For the `"selected_features"` filter described in embedded methods (Section 5.1.3), this step is straight-forward since the methods assigns either a value of 1 for a feature to be kept or 0 for a feature to be dropped. With `task$select()` the features with a value of 1 can be selected:

```
task = tsk("penguins")
learner = lrn("classif.rpart")
filter = flt("selected_features", learner = learner)
filter$calculate(task)

# select all features used by rpart
keep = names(which(filter$scores == 1))
task$select(keep)
task$feature_names
```

```
[1] "bill_length"    "flipper_length" "island"
```

> **Tip**
>
> To select features, we use the function `task$select()` and not `task$filter()`, which is used to filter rows (not columns) of the data matrix, see task mutators (Section 2.1.3).

For filter methods which assign continuous scores, there are essentially two ways to select features:

- select the top k features, or
- select all features with a score above a threshold τ.

Where the first option is equivalent to dropping the bottom $p - k$ features. For both options, one has to decide on a threshold, which is often quite arbitrary. For example, to implement the first option with the information gain filter:

```
task = tsk("penguins")
filter = flt("information_gain")
filter$calculate(task)

# select top 3 features from information gain filter
keep = names(head(filter$scores, 3))
task$select(keep)
task$feature_names
```

```
[1] "bill_depth"     "bill_length"    "flipper_length"
```

Or, the second option with $\tau = 0.5$:

```
task = tsk("penguins")
filter = flt("information_gain")
filter$calculate(task)

# select all features with score >0.5 from information gain filter
keep = names(which(filter$scores > 0.5))
task$select(keep)
task$feature_names
```

```
[1] "bill_depth"     "bill_length"    "flipper_length" "island"
```

Filters can be integrated into pipelines. While pipelines are described in detail in Chapter 6, here is a brief preview:

```
library(mlr3pipelines)
task = tsk("penguins")

# combine filter (keep top 3 features) with learner
graph = po("filter", filter = flt("information_gain"), filter.nfeat = 3) %>>%
  po("learner", lrn("classif.rpart"))

# now it can be used as any learner, but it includes the feature selection
learner = as_learner(graph)
learner$train(task)
```

Pipelines can also be used to apply hyperparameter optimization (Chapter 4) to the filter, i.e. tune the filter threshold to optimize the feature selection regarding prediction performance. We first combine a filter with a learner,

```
graph = po("filter", filter = flt("information_gain")) %>>%
  po("learner", lrn("classif.rpart"))
learner = as_learner(graph)
```

and tune how many feature to include

```
library("mlr3tuning")
ps = ps(information_gain.filter.nfeat = p_int(lower = 1, upper = 7))
instance = TuningInstanceSingleCrit$new(
  task = task,
  learner = learner,
  resampling = rsmp("holdout"),
  measure = msr("classif.acc"),
  search_space = ps,
  terminator = trm("none")
)
tuner = tnr("grid_search")
```

```
12 tuner$optimize(instance)
```

```
   information_gain.filter.nfeat learner_param_vals  x_domain classif.acc
1:                             5          <list[2]> <list[1]>   0.9391304
```

The output above shows only the best result. To show the results of all tuning steps, retrieve them from the archive of the tuning instance:

```
1 as.data.table(instance$archive)
```

```
   information_gain.filter.nfeat classif.acc
1:                             2   0.9304348
2:                             5   0.9391304
3:                             1   0.7478261
4:                             7   0.9391304
5:                             3   0.9391304
6:                             6   0.9391304
7:                             4   0.9391304
7 variables not shown: [x_domain_information_gain.filter.nfeat, runtime_learners, timestamp, ba
```

We can also plot the tuning results:

```
1 autoplot(instance)
```

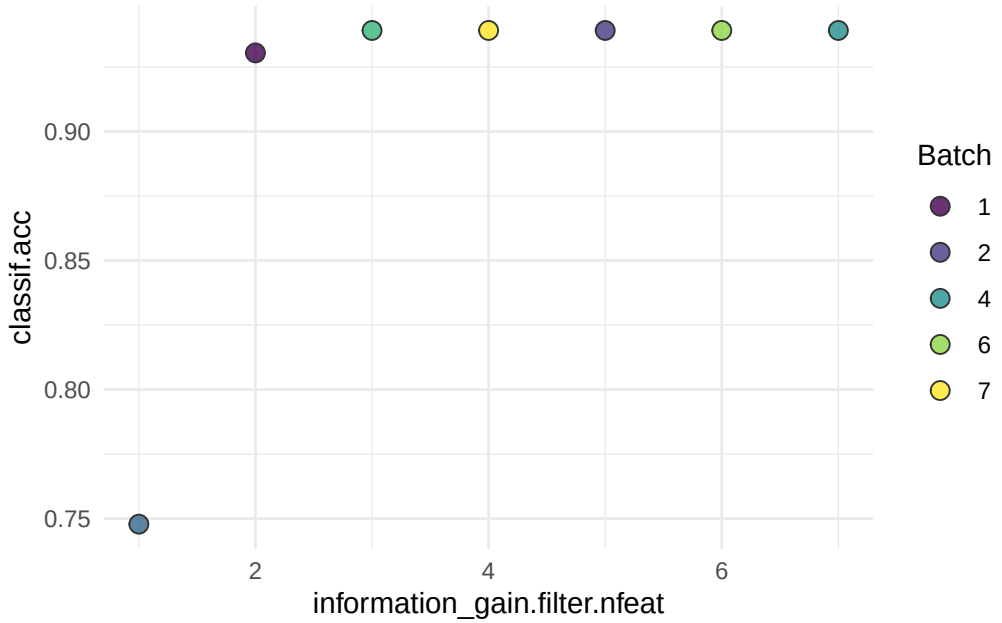


Figure 5.1.: Model performance with different numbers of features, selected by an information gain filter.

For more details, see Pipelines (Chapter 6) and Hyperparameter Optimization (Chapter 4).

5.2. Wrapper Methods

Wrapper methods work by fitting models on selected feature subsets and evaluating their performance. This can be done in a sequential fashion, e.g. by iteratively adding features to the model in the so-called sequential forward selection, or in a parallel fashion, e.g. by evaluating random feature subsets in a random search. Below, the use of these simple approaches is described in a common framework along with more advanced methods such as genetic search. It is further shown how to select features by optimizing multiple performance measures and how to wrap a learner with feature selection to use it in pipelines or benchmarks.

In more detail, wrapper methods iteratively select features that optimize a performance measure. Instead of ranking features, a model is fit on a selected subset of features in each iteration and evaluated in resampling with respect to a selected performance measure. The strategy that determines which feature subset is used in each iteration is given by the `FSelector` object. A simple example is the sequential forward selection that starts with computing each single-feature model, selects the best one, and then iteratively adds the feature that leads to the largest performance improvement. Wrapper methods can be used with any learner but need to train the learner potentially many times, leading to a computationally intensive method. All wrapper methods are implemented via the package `mlr3fselect`. In this chapter, we cover how to

- instantiate an `FSelector` object,
- configure it, to e.g. respect a runtime limit or for different objectives,
- run it or fuse it with a `Learner` via an `AutoFSelector`.

> **Note**
>
> Wrapper-based feature selection is very similar to hyperparameter optimization (Chapter 4). The major difference is that we search for well-performing feature subsets instead of hyperparameter configurations. We will see below, that we can even use the same terminators, that some feature selection algorithms are similar to tuners and that we can also optimize multiple performance measures with feature selection.

5.2.1. Simple Forward Selection Example

We start with the simple example from above and do sequential forward selection with the penguins data:

```
library("mlr3fselect")

# subset features to ease visualization
task = tsk("penguins")
task$select(c("bill_depth", "bill_length", "body_mass", "flipper_length"))

instance = fselect(
```

```
  method = "sequential",
  task =  task,
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msr("classif.acc")
)
```

To show all analyzed feature subsets and the corresponding performance, we use `as.data.table(instance$archiv`

```
dt = as.data.table(instance$archive)
dt[batch_nr == 1, 1:5]
```

```
   bill_depth bill_length body_mass flipper_length classif.acc
1:       TRUE       FALSE     FALSE          FALSE   0.6956522
2:      FALSE        TRUE     FALSE          FALSE   0.7652174
3:      FALSE       FALSE      TRUE          FALSE   0.7043478
4:      FALSE       FALSE     FALSE           TRUE   0.7913043
```

We see that the feature `flipper_length` achieved the highest prediction performance in the first iteration and is thus selected. In the second round, adding `bill_length` improves performance to over 90%:

```
dt[batch_nr == 2, 1:5]
```

```
   bill_depth bill_length body_mass flipper_length classif.acc
1:       TRUE       FALSE     FALSE           TRUE   0.7652174
2:      FALSE        TRUE     FALSE           TRUE   0.9391304
3:      FALSE       FALSE      TRUE           TRUE   0.8173913
```

However, adding a third feature does not improve performance

```
dt[batch_nr == 3, 1:5]
```

```
   bill_depth bill_length body_mass flipper_length classif.acc
1:       TRUE        TRUE     FALSE           TRUE   0.9391304
2:      FALSE        TRUE      TRUE           TRUE   0.9391304
```

and the algorithm terminates. To directly show the best feature set, we can use:

```
instance$result_feature_set
```

```
[1] "bill_length"    "flipper_length"
```

> **Note**
>
> `instance$result_feature_set` shows features in alphabetical order and not in the order selected.

Internally, the `fselect` function creates an `FSelectInstanceSingleCrit` object and executes the feature selection with an `FSelector` object, based on the selected method, in this example an `FSelectorSequential` object. It uses the supplied resampling and measure to evaluate all feature subsets provided by the `FSelector` on the task.

At the heart of `mlr3fselect` are the R6 classes:

- `FSelectInstanceSingleCrit`, `FSelectInstanceMultiCrit`: These two classes describe the feature selection problem and store the results.
- `FSelector`: This class is the base class for implementations of feature selection algorithms.

In the following two sections, these classes will be created manually, to learn more about the `mlr3fselect` package.

5.2.2. The `FSelectInstance` Classes

To create an `FSelectInstanceSingleCrit` object, we use the sugar function `fsi`, which is short for `FSelectInstanceSingleCrit$new()` or `FSelectInstanceMultiCrit$new()`, depending on the selected measure(s):

```
instance = fsi(
  task = tsk("penguins"),
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msr("classif.acc"),
  terminator = trm("evals", n_evals = 20)
)
```

Note that we have not selected a feature selection algorithm and thus did not select any features, yet. We have also supplied a so-called `Terminator`, which is used to stop the feature selection. For the forward selection in the example above, we did not need a terminator because we simply tried all remaining features until the full model or no further performance improvement. However, for other feature selection algorithms such as `random search`, a terminator is required. The following terminator are available:

- Terminate after a given time (`TerminatorClockTime`)
- Terminate after a given amount of iterations (`TerminatorEvals`)
- Terminate after a specific performance is reached (`TerminatorPerfReached`)
- Terminate when feature selection does not improve (`TerminatorStagnation`)
- A combination of the above in an *ALL* or *ANY* fashion (`TerminatorCombo`)

Above we used the sugar function `trm` to select `TerminatorEvals` with 20 evaluations.

To start the feature selection, we still need to select an algorithm which are defined via the `FSelector` class, described in the next section.

5.2.3. The `FSelector` Class

The `FSelector` class is the base class for different feature selection algorithms. The following algorithms are currently implemented in `mlr3fselect`:

- Random search, trying random feature subsets until termination (`FSelectorRandomSearch`)
- Exhaustive search, trying all possible feature subsets (`FSelectorExhaustiveSearch`)
- Sequential search, i.e. sequential forward or backward selection (`FSelectorSequential`)
- Recursive feature elimination, which uses learner's importance scores to iteratively remove features with low feature importance (`FSelectorRFE`)
- Design points, trying all user-supplied feature sets (`FSelectorDesignPoints`)
- Genetic search, implementing a genetic algorithm which treats the features as a binary sequence and tries to find the best subset with mutations (`FSelectorGeneticSearch`)
- Shadow variable search, which adds permuted copies of all features (shadow variables) and stops when a shadow variable is selected (`FSelectorShadowVariableSearch`)

In this example, we will use a simple random search and retrieve it from the dictionary `mlr_fselectors` with the `fs()` sugar function, which is short for `FSelectorRandomSearch$new()`:

```
fselector = fs("random_search")
```

5.2.4. Starting the Feature Selection

To start the feature selection, we pass the `FSelectInstanceSingleCrit` object to the `$optimize()` method of the initialized `FSelector` object:

```
fselector$optimize(instance)
```

The algorithm proceeds as follows

1. The `FSelector` proposes at least one feature subset and may propose multiple subsets to improve parallelization, which can be controlled via the setting `batch_size`.
2. For each feature subset, the given learner is fitted on the task using the provided resampling and evaluated with the given measure.
3. All evaluations are stored in the archive of the `FSelectInstanceSingleCrit` object.
4. The terminator is queried if the budget is exhausted. If the budget is not exhausted, restart with 1) until it is.
5. Determine the feature subset with the best observed performance.
6. Store the best feature subset as the result in the instance object.

The best feature subset and the corresponding measured performance can be accessed from the instance:

```
as.data.table(instance$result)[, .(features, classif.acc)]
```

```
                                                          features classif.acc
1: bill_depth,bill_length,body_mass,flipper_length,island,sex,...   0.9391304
```

As in the forward selection example above, one can investigate all resamplings which were undertaken, as they are stored in the archive of the `FSelectInstanceSingleCrit` object and can be accessed by using `as.data.table()`:

```
as.data.table(instance$archive)[, .(bill_depth, bill_length, body_mass, classif.acc)]
```

```
    bill_depth bill_length body_mass classif.acc
 1:       TRUE        TRUE      TRUE   0.9391304
 2:      FALSE       FALSE      TRUE   0.7391304
 3:       TRUE        TRUE      TRUE   0.9391304
 4:       TRUE        TRUE      TRUE   0.9391304
 5:       TRUE        TRUE      TRUE   0.9391304
 6:      FALSE       FALSE     FALSE   0.6869565
 7:       TRUE       FALSE      TRUE   0.8086957
 8:      FALSE       FALSE      TRUE   0.7391304
 9:       TRUE       FALSE     FALSE   0.7739130
10:       TRUE       FALSE     FALSE   0.8000000
11:      FALSE       FALSE     FALSE   0.8086957
12:      FALSE       FALSE      TRUE   0.6869565
13:       TRUE        TRUE      TRUE   0.9391304
14:      FALSE       FALSE     FALSE   0.6173913
15:       TRUE        TRUE      TRUE   0.9217391
16:       TRUE        TRUE      TRUE   0.9391304
17:       TRUE        TRUE      TRUE   0.9043478
18:      FALSE       FALSE      TRUE   0.7391304
19:      FALSE       FALSE     FALSE   0.7739130
20:      FALSE       FALSE     FALSE   0.8086957
```

Now the optimized feature subset can be used to subset the task and fit the model on all observations:

```
task = tsk("penguins")
learner = lrn("classif.rpart")

task$select(instance$result_feature_set)
learner$train(task)
```

The trained model can now be used to make a prediction on external data.

> ⚠ Warning
>
> Predicting on observations present in the task used for feature selection should be avoided. The model has seen these observations already during feature selection and therefore performance evaluation results would be over-optimistic. Instead, to get unbiased performance estimates for the current task, nested resampling (see Section 5.2.6 and Section 4.5) is required.

5.2.5. Optimizing Multiple Performance Measures

You might want to use multiple criteria to evaluate the performance of the feature subsets. For example, you might want to select the subset with the highest classification accuracy and lowest time to train the model. However, these two subsets will generally not coincide, i.e. the subset with highest classification accuracy will probably be another subset than that with lowest training time. With `mlr3fselect`, the result is the pareto-optimal solution, i.e. the best feature subset for each of the criteria that is not dominated by another subset. For the example with classification accuracy and training time, a feature subset that is best in accuracy *and* training time will dominate all other subsets and thus will be the only pareto-optimal solution. If, however, different subsets are best in the two criteria, both subsets are pareto-optimal.

We will expand the previous example and perform feature selection on the penguins dataset, however, this time we will use `FSelectInstanceMultiCrit` to select the subset of features that has the highest classification accuracy and the one with the lowest time to train the model.

The feature selection process with multiple criteria is similar to that with a single criterion, except that we select two measures to be optimized:

```
instance = fsi(
  task = tsk("penguins"),
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msrs(c("classif.acc", "time_train")),
  terminator = trm("evals", n_evals = 5)
)
```

The function `fsi` creates an instance of `FSelectInstanceMultiCrit` if more than one measure is selected. We now create an `FSelector` and call the `$optimize()` function of the `FSelector` with the `FSelectInstanceMultiCrit` object, to search for the subset of features with the best classification accuracy and time to train the model. This time, we use `design points` to manually specify two feature sets to try: one with only the feature `sex` and one with all features except `island`, `sex` and `year`. We expect the sex-only model to train fast and the model including many features to be accurate.

```
design = mlr3misc::rowwise_table(
  ~bill_depth, ~bill_length, ~body_mass, ~flipper_length, ~island, ~sex, ~year,
  FALSE, FALSE, FALSE, FALSE, FALSE, TRUE, FALSE,
  TRUE, TRUE, TRUE, TRUE, FALSE, FALSE, FALSE
)
```

```

fselector = fs("design_points", design = design)
fselector$optimize(instance)
```

As above, the best feature subset and the corresponding measured performance can be accessed from the instance. However, in this simple case, if the fastest subset is not also the best performing subset, the result consists of two subsets: one with the lowest training time and one with the best classification accuracy:

```
as.data.table(instance$result)[, .(features, classif.acc, time_train)]
```

```
                                          features classif.acc time_train
1:                                             sex   0.4347826      0.004
2: bill_depth,bill_length,body_mass,flipper_length   0.9304348      0.005
```

As explained above, the result is the pareto-optimal solution.

5.2.6. Automating the Feature Selection

The `AutoFSelector` class wraps a learner and augments it with an automatic feature selection for a given task. Because the `AutoFSelector` itself inherits from the `Learner` base class, it can be used like any other learner. Below, a new learner is created. This learner is then wrapped in a random search feature selector, which automatically starts a feature selection on the given task using an inner resampling, as soon as the wrapped learner is trained. Here, the function `auto_fselector` creates an instance of `AutoFSelector`, i.e. it is short for `AutoFSelector$new()`.

```
at = auto_fselector(
  method = fs("random_search"),
  learner = lrn("classif.log_reg"),
  resampling = rsmp("holdout"),
  measure = msr("classif.acc"),
  terminator = trm("evals", n_evals = 10)
)
at
```

```
<AutoFSelector:classif.log_reg.fselector>
* Model: list
* Packages: mlr3, mlr3fselect, mlr3learners, stats
* Predict Type: response
* Feature Types: logical, integer, numeric, character, factor, ordered
* Properties: loglik, twoclass
```

We can now, as with any other learner, call the `$train()` and `$predict()` method. This time however, we pass it to `benchmark()` to compare the optimized feature subset to the complete feature set. This way, the `AutoFSelector` will do its resampling for feature selection on the training set

of the respective split of the outer resampling. The learner then undertakes predictions using the test set of the outer resampling. Here, the outer resampling refers to the resampling specified in `benchmark()`, whereas the inner resampling is that specified in `auto_fselector()`. This is called nested resampling (Section 4.5) and yields unbiased performance measures, as the observations in the test set have not been used during feature selection or fitting of the respective learner.

In the call to `benchmark()`, we compare our wrapped learner `at` with a normal logistic regression `lrn("classif.log_reg")`. For that, we create a benchmark grid with the task, the learners and a 3-fold cross validation on the `sonar` data.

```
grid = benchmark_grid(
  task = tsk("sonar"),
  learner = list(at, lrn("classif.log_reg")),
  resampling = rsmp("cv", folds = 3)
)

bmr = benchmark(grid)
```

Now, we compare those two learners regarding classification accuracy and training time:

```
aggr = bmr$aggregate(msrs(c("classif.acc", "time_train")))
as.data.table(aggr)[, .(learner_id, classif.acc, time_train)]
```

```
                learner_id classif.acc time_train
1: classif.log_reg.fselector   0.7351967 1.25166667
2:           classif.log_reg   0.6585231 0.03833333
```

We can see that, in this example, the feature selection improves prediction performance but also drastically increases the training time, since the feature selection (including resampling and random search) is part of the model training of the wrapped learner.

5.3. Conclusion

In this chapter, we learned how to perform feature selection with mlr3. We introduced filter and wrapper methods, combined feature selection with pipelines, learned how to automate the feature selection and covered the optimization of multiple performance measures. Table 5.1 gives an overview of the most important functions (S3) and classes (R6) used in this chapter.

S3 function	R6 Class	Summary
`flt()`	`Filter`	Selects features by calculating a score for each feature
`Filter$calculate()`	`Filter`	Calculates scores on a given task

S3 function	R6 Class	Summary
`fselect()`	`FSelectInstanceSingleCrit` or `FSelectInstanceMultiCrit`	Specifies a feature selection problem and stores the results
`fs()`	`FSelector`	Specifies a feature selection algorithm
`FSelector$optimize()`	`FSelector`	Executes the features selection specified by the `FSelectInstance` with the algorithm specified by the `FSelector`
`auto_fselector()`	`AutoFSelector`	Defines a learner that includes feature selection

Table 5.1.: Core S3 'sugar' functions for feature selection in mlr3 with the underlying R6 class that are constructed when these functions are called (if applicable) and a summary of the purpose of the functions.

Resources

- A list of implemented filters in the `mlr3filters` package is provided on the mlr3filters website[3].
- A summary of wrapper-based feature selection with the `mlr3fselect` package is provided in the mlr3fselect cheatsheet[4].
- An overview of feature selection methods is provided by Chandrashekar and Sahin (2014).
- A more formal and detailed introduction to filters and wrappers is given in Guyon and Elisseeff (2003).
- Bommert et al. (2020) perform a benchmark of filter methods.
- Filters can be used as part of a machine learning pipeline (Chapter 6).
- Filters can be optimized with hyperparameter optimization (Chapter 4).

5.4. Exercises

1. Calculate a correlation filter on the `Motor Trend` data set (`mtcars`).
2. Use the filter from the first exercise to select the five best features in the `mtcars` data set.
3. Apply a backward selection to the `penguins` data set with a classification tree learner `"classif.rpart"` and holdout resampling by the measure classification accuracy. Compare the results with those in Section 5.2.1. Answer the following questions:
   a. Do the selected features differ?
   b. Which feature selection method achieves a higher classification accuracy?
   c. Are the accuracy values in b) directly comparable? If not, what has to be changed to make them comparable?

[3] https://mlr3filters.mlr-org.com
[4] https://cheatsheets.mlr-org.com/mlr3fselect.pdf

4. Automate the feature selection as in Section 5.2.6 with the `spam` data set and a logistic regression learner (`"classif.log_reg"`). Hint: Remember to call `library("mlr3learners")` for the logistic regression learner.

6. Pipelines

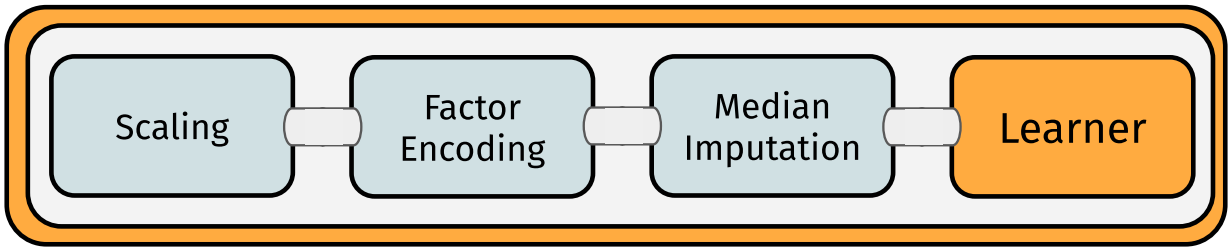
TODO (150-200 WORDS)

> **Note**
>
> This chapter is currently being re-written, in this PR. You can continue reading here if you want to learn about `mlr3pipelines`, but you currently don't need to bother checking this chapter for typos etc.

`mlr3pipelines` (Binder et al. 2021) is a dataflow programming toolkit. This chapter focuses on the applicant's side of the package. A more in-depth and technically oriented guide can be found in the In-depth look into mlr3pipelines chapter.

Machine learning workflows can be written as directed "Graphs"/"Pipelines" that represent data flows between preprocessing, model fitting, and ensemble learning units in an expressive and intuitive language. We will most often use the term "Graph" in this manual but it can interchangeably be used with "pipeline" or "workflow".

Below you can examine an example for such a graph:



Single computational steps can be represented as so-called PipeOps, which can then be connected with directed edges in a Graph. The scope of `mlr3pipelines` is still growing. Currently supported features are:

- Data manipulation and preprocessing operations, e.g. PCA, feature filtering, imputation
- Task subsampling for speed and outcome class imbalance handling
- `mlr3` Learner operations for prediction and stacking
- Ensemble methods and aggregation of predictions

Additionally, we implement several meta operators that can be used to construct powerful pipelines:

- Simultaneous path branching (data going both ways)

- Alternative path branching (data going one specific way, controlled by hyperparameters)

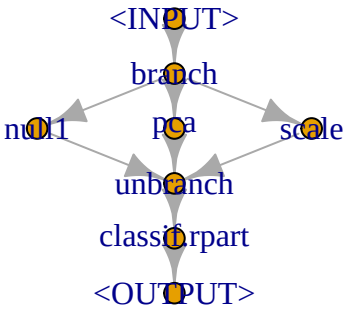
An extensive introduction to creating custom **PipeOps** (PO's) can be found in the technical introduction.

Using methods from `mlr3tuning`, it is even possible to simultaneously optimize parameters of multiple processing units.

A predecessor to this package is the `mlrCPO` package, which works with `mlr` 2.x. Other packages that provide, to varying degree, some preprocessing functionality or machine learning domain specific language, are:

- the `caret` package and the related `recipes` project
- the `dplyr` package

An example for a Pipeline that can be constructed using `mlr3pipelines` is depicted below:



6.1. The Building Blocks: PipeOps

The building blocks of `mlr3pipelines` are **PipeOp**-objects (PO). They can be constructed directly using `PipeOp<NAME>$new()`, but the recommended way is to retrieve them from the `mlr_pipeops` dictionary:

```
1 library("mlr3pipelines")
2 as.data.table(mlr_pipeops)
```

```
              key                                                label
 1:         boxcox          Box-Cox Transformation of Numeric Features
 2:         branch                                    Path Branching
 3:          chunk                 Chunk Input into Multiple Outputs
 4: classbalancing                                    Class Balancing
 5:     classifavg                          Majority Vote Prediction
---
60:      threshold Change the Threshold of a Classification Prediction
61:  tunethreshold   Tune the Threshold of a Classification Prediction
62:       unbranch                          Unbranch Different Paths
63:         vtreat                    Interface to the vtreat Package
64:     yeojohnson      Yeo-Johnson Transformation of Numeric Features
9 variables not shown: [packages, tags, feature_types, input.num, output.num, input.type.train
```

Single POs can be created using the dictionary:

```
pca = mlr_pipeops$get("pca")
```

or using **syntactic sugar** `po(<name>)`:

```
pca = po("pca")
```

Some POs require additional arguments for construction:

```
learner = po("learner")

# Error in as_learner(learner) : argument "learner" is missing, with no default argument "le
```

```
learner = mlr_pipeops$get("learner", lrn("classif.rpart"))
```

or in short `po("learner", lrn("classif.rpart"))`.

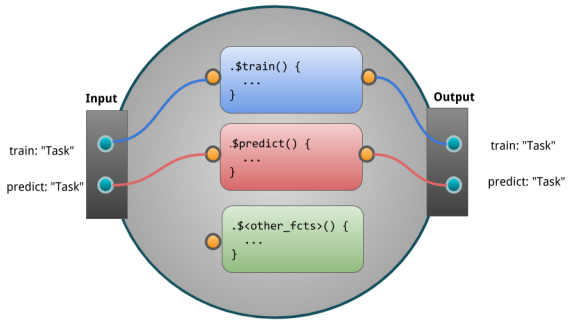
Hyperparameters of POs can be set through the `param_vals` argument. Here we set the fraction of features for a filter:

```
filter = po("filter",
  filter = mlr3filters::flt("variance"),
  param_vals = list(filter.frac = 0.5))
```

or in short notation:

```
po("filter", mlr3filters::flt("variance"), filter.frac = 0.5)
```

The figure below shows an exemplary `PipeOp`. It takes an input, transforms it during `.$train` and `.$predict` and returns data:

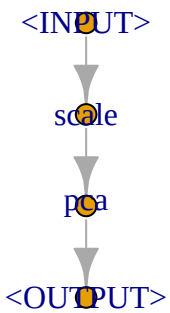


6.2. The Pipeline Operator: %>>%

It is possible to create intricate `Graphs` with edges going all over the place (as long as no loops are introduced). Irrespective, there is usually a clear direction of flow between "layers" in the `Graph`. It is therefore convenient to build up a `Graph` from layers.

This can be done using the **%>>%** ("double-arrow") operator. It takes either a `PipeOp` or a `Graph` on each of its sides and connects all of the outputs of its left-hand side to one of the inputs each of its right-hand side. The number of inputs therefore must match the number of outputs.

```
library("magrittr")

gr = po("scale") %>>% po("pca")
gr$plot(html = FALSE)
```



6.3. Nodes, Edges and Graphs

POs are combined into `Graph`s.

POs are identified by their `$id`. Note that the operations all modify the object in-place and return the object itself. Therefore, multiple modifications can be chained.

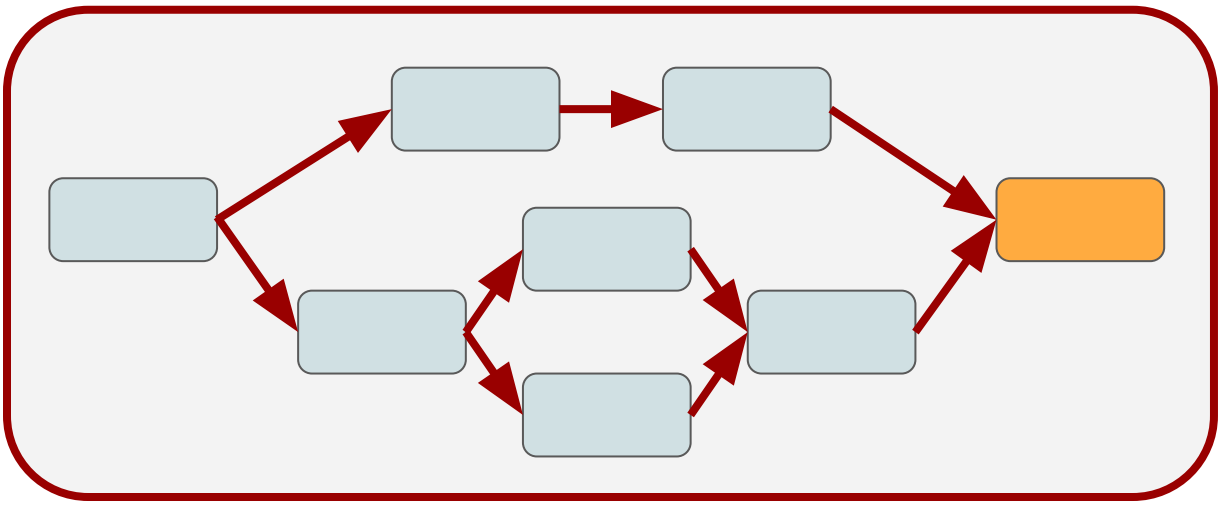
For this example we use the `pca` PO defined above and a new PO named "mutate". The latter creates a new feature from existing variables. Additionally, we use the filter PO again.

```
mutate = po("mutate")

filter = po("filter",
  filter = mlr3filters::flt("variance"),
  param_vals = list(filter.frac = 0.5))
```

The recommended way to construct a graph is to use the `%>>%` operator to chain POs or `Graph`s.

```
graph = mutate %>>% filter
```

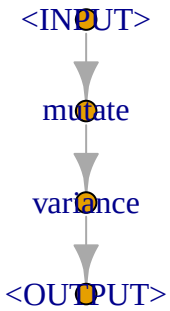
To illustrate how this sugar operator works under the surface we will include an example of the manual way (= hard way) to construct a `Graph`. This is done by creating an empty graph first. Then one fills the empty graph with POs, and connects edges between the POs. Conceptually, this may look like this:



```
graph = Graph$new()$
  add_pipeop(mutate)$
  add_pipeop(filter)$
  add_edge("mutate", "variance") # add connection mutate -> filter
```

The constructed `Graph` can be inspected using its `$plot()` function:

```
graph$plot()
```



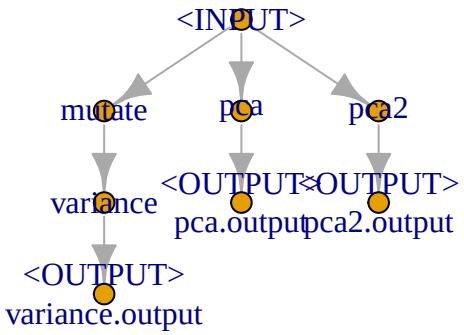
Chaining multiple POs of the same kind

If multiple POs of the same kind should be chained, it is necessary to change the `id` to avoid name clashes. This can be done by either accessing the `$id` slot or during construction:

```
graph$plot()
```

```
graph$add_pipeop(po("pca", id = "pca2"))
```

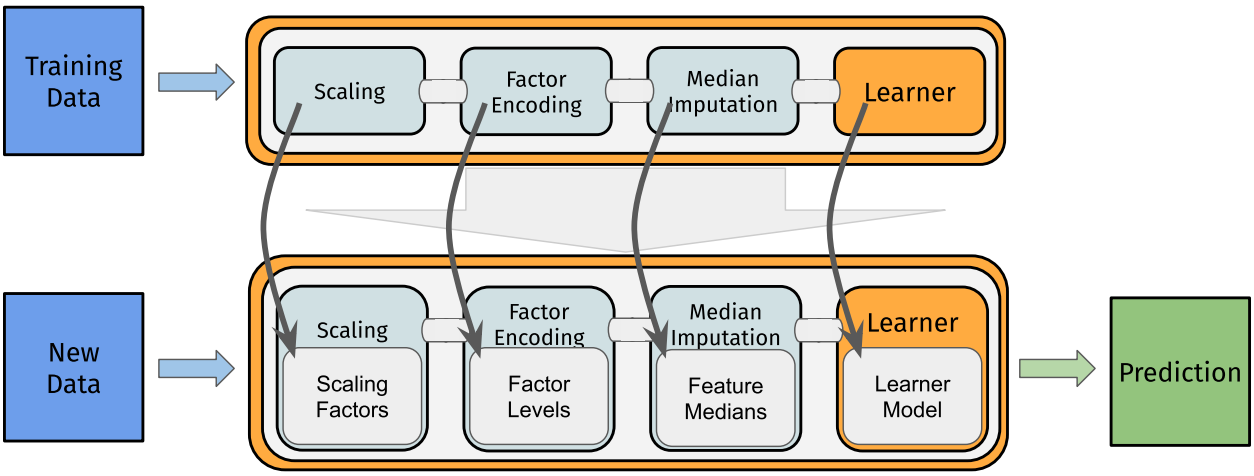
```
graph$add_pipeop(po("pca"))
```



6.4. Modeling

The main purpose of a `Graph` is to build combined preprocessing and model fitting pipelines that can be used as `mlr3 Learner`.

Conceptually, the process may be summarized as follows:



In the following we chain two preprocessing tasks:

- mutate (creation of a new feature)
- filter (filtering the dataset)

Subsequently one can chain a PO learner to train and predict on the modified dataset.

```
mutate = po("mutate")
filter = po("filter",
  filter = mlr3filters::flt("variance"),
  param_vals = list(filter.frac = 0.5))

graph = mutate %>>%
  filter %>>%
  po("learner",
    learner = lrn("classif.rpart"))
```

Until here we defined the main pipeline stored in `Graph`. Now we can train and predict the pipeline:

```
task = tsk("iris")
graph$train(task)
```

```
$classif.rpart.output
NULL
```

```
graph$predict(task)
```

```
$classif.rpart.output
<PredictionClassif> for 150 observations:
    row_ids     truth  response
          1    setosa    setosa
          2    setosa    setosa
          3    setosa    setosa
---
        148 virginica virginica
        149 virginica virginica
        150 virginica virginica
```

Rather than calling `$train()` and `$predict()` manually, we can put the pipeline `Graph` into a `GraphLearner` object. A `GraphLearner` encapsulates the whole pipeline (including the preprocessing steps) and can be put into `resample()` or `benchmark()` . If you are familiar with the old *mlr* package, this is the equivalent of all the `make*Wrapper()` functions. The pipeline being encapsulated (here `Graph`) must always produce a `Prediction` with its `$predict()` call, so it will probably contain at least one `PipeOpLearner` .

```
glrn = as_learner(graph)
```

This learner can be used for model fitting, resampling, benchmarking, and tuning:

```
cv3 = rsmp("cv", folds = 3)
resample(task, glrn, cv3)
```

```
<ResampleResult> of 3 iterations
* Task: iris
* Learner: mutate.variance.classif.rpart
* Warnings: 0 in 0 iterations
* Errors: 0 in 0 iterations
```

6.4.1. Setting Hyperparameters

Individual POs offer hyperparameters because they contain `$param_set` slots that can be read and written from `$param_set$values` (via the `paradox` package). The parameters get passed down to the `Graph`, and finally to the `GraphLearner` . This makes it not only possible to easily change the behavior of a `Graph` / `GraphLearner` and try different settings manually, but also to perform tuning using the `mlr3tuning` package.

```
glrn$param_set$values$variance.filter.frac = 0.25
cv3 = rsmp("cv", folds = 3)
resample(task, glrn, cv3)
```

```
<ResampleResult> of 3 iterations
* Task: iris
* Learner: mutate.variance.classif.rpart
* Warnings: 0 in 0 iterations
* Errors: 0 in 0 iterations
```

6.4.2. Tuning

If you are unfamiliar with tuning in `mlr3`, we recommend to take a look at the section about tuning first. Here we define a `ParamSet` for the "rpart" learner and the "variance" filter which should be optimized during the tuning process.

```
library("paradox")
ps = ps(
  classif.rpart.cp = p_dbl(lower = 0, upper = 0.05),
  variance.filter.frac = p_dbl(lower = 0.25, upper = 1)
)
```

After having defined the `Tuner`, a random search with 10 iterations is created. For the inner resampling, we are simply using holdout (single split into train/test) to keep the runtimes reasonable.

```
library("mlr3tuning")
instance = TuningInstanceSingleCrit$new(
  task = task,
  learner = glrn,
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
```

```
  search_space = ps,
  terminator = trm("evals", n_evals = 20)
)
```

```
tuner = tnr("random_search")
tuner$optimize(instance)
```

```
   classif.rpart.cp variance.filter.frac learner_param_vals  x_domain
1:       0.04886918            0.6870548          <list[5]> <list[2]>
1 variable not shown: [classif.ce]
```

The tuning result can be found in the respective `result` slots.

```
instance$result_learner_param_vals
```

```
$mutate.mutation
list()

$mutate.delete_originals
[1] FALSE

$variance.filter.frac
[1] 0.6870548

$classif.rpart.xval
[1] 0

$classif.rpart.cp
[1] 0.04886918
```

```
instance$result_y
```

```
classif.ce
      0.02
```

6.5. Non-Linear Graphs

The Graphs seen so far all have a linear structure. Some POs may have multiple input or output channels. These channels make it possible to create non-linear Graphs with alternative paths taken by the data.

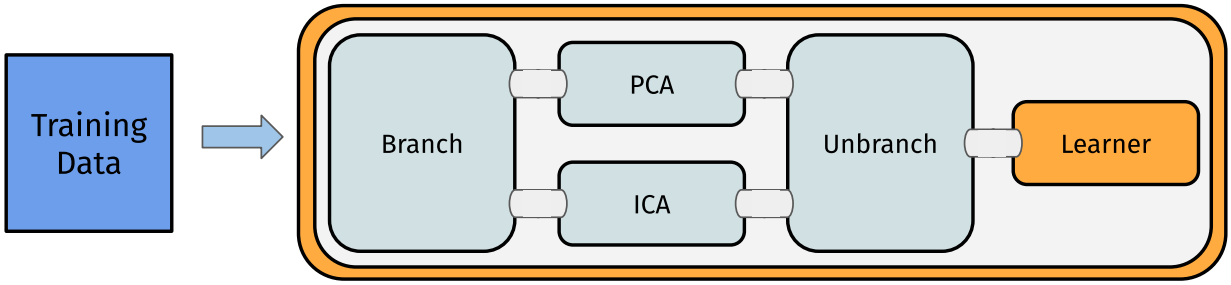
Possible types are:

- Branching: Splitting of a node into several paths, e.g. useful when comparing multiple feature-selection methods (pca, filters). Only one path will be executed.
- Copying: Splitting of a node into several paths, all paths will be executed (sequentially). Parallel execution is not yet supported.
- Stacking: Single graphs are stacked onto each other, i.e. the output of one `Graph` is the input for another. In machine learning this means that the prediction of one `Graph` is used as input for another `Graph`

6.5.1. Branching & Copying

The `PipeOpBranch` and `PipeOpUnbranch` POs make it possible to specify multiple alternative paths. Only one path is actually executed, the others are ignored. The active path is determined by a hyperparameter. This concept makes it possible to tune alternative preprocessing paths (or learner models).

Below a conceptual visualization of branching:



`PipeOp(Un)Branch` is initialized either with the number of branches, or with a `character`-vector indicating the names of the branches. If names are given, the "branch-choosing" hyperparameter becomes more readable. In the following, we set three options:

1. Doing nothing ("nop")
2. Applying a PCA
3. Scaling the data

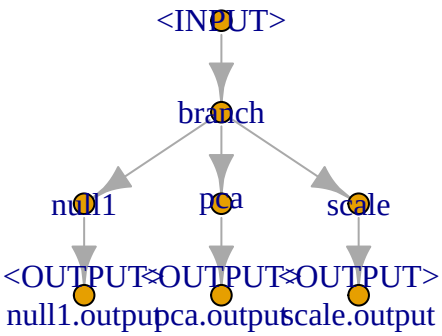
It is important to "unbranch" again after "branching", so that the outputs are merged into one result objects.

In the following we first create the branched graph and then show what happens if the "unbranching" is not applied:

```
graph = po("branch", c("nop", "pca", "scale")) %>>%
  gunion(list(
    po("nop", id = "null1"),
    po("pca"),
    po("scale")
  ))
```

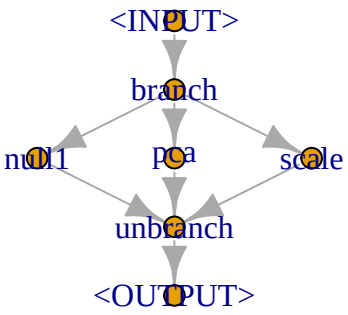
Without "unbranching" one creates the following graph:

```
graph$plot(html = FALSE)
```



Now when "unbranching", we obtain the following results:

```
(graph %>>% po("unbranch", c("nop", "pca", "scale")))$plot(html = FALSE)
```



The same can be achieved using a shorter notation:

```
# List of pipeops
opts = list(po("nop", "no_op"), po("pca"), po("scale"))
# List of po ids
opt_ids = mlr3misc::map_chr(opts, `[[`, "id")
po("branch", options = opt_ids) %>>%
  gunion(opts) %>>%
  po("unbranch", options = opt_ids)
```

```
Graph with 5 PipeOps:
       ID         State        sccssors       prdcssors
   branch <<UNTRAINED>> no_op,pca,scale
    no_op <<UNTRAINED>>        unbranch          branch
      pca <<UNTRAINED>>        unbranch          branch
    scale <<UNTRAINED>>        unbranch          branch
 unbranch <<UNTRAINED>>                 no_op,pca,scale
```

6.5.2. Model Ensembles

We can leverage the different operations presented to connect POs. This allows us to form powerful graphs.

Before we go into details, we split the task into train and test indices.

```
task = tsk("iris")
train.idx = sample(seq_len(task$nrow), 120)
test.idx = setdiff(seq_len(task$nrow), train.idx)
```

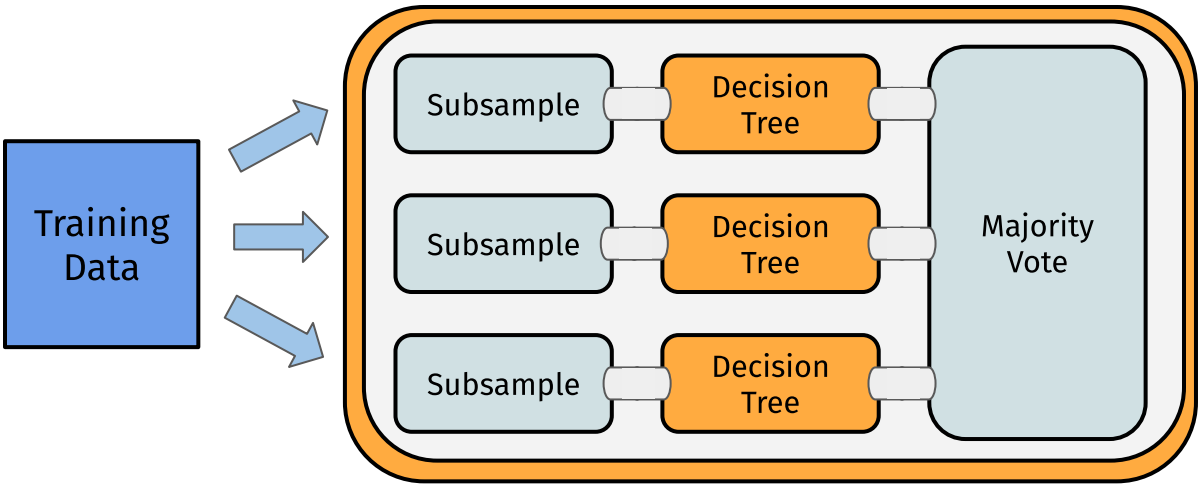
6.5.2.1. Bagging

We first examine Bagging introduced by (Breiman 1996). The basic idea is to create multiple predictors and then aggregate those to a single, more powerful predictor.

> "... multiple versions are formed by making bootstrap replicates of the learning set and using these as new learning sets" (Breiman 1996)

Bagging then aggregates a set of predictors by averaging (regression) or majority vote (classification). The idea behind bagging is, that a set of weak, but different predictors can be combined in order to arrive at a single, better predictor.

We can achieve this by downsampling our data before training a learner, repeating this e.g. 10 times and then performing a majority vote on the predictions. Graphically, it may be summarized as follows:



First, we create a simple pipeline, that uses `PipeOpSubsample` before a `PipeOpLearner` is trained:

```
single_pred = po("subsample", frac = 0.7) %>>%
  po("learner", lrn("classif.rpart"))
```

We can now copy this operation 10 times using `pipeline_greplicate`. The `pipeline_greplicate` allows us to parallelize many copies of an operation by creating a Graph containing `n` copies of the input Graph. We can also create it using **syntactic sugar** via `ppl()`:

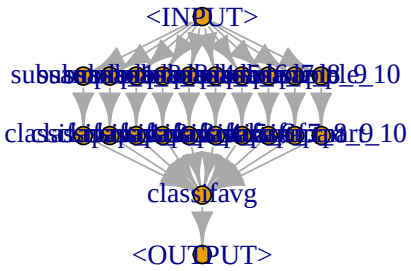
```
pred_set = ppl("greplicate", single_pred, 10L)
```

Afterwards we need to aggregate the 10 pipelines to form a single model:

```
bagging = pred_set %>>%
  po("classifavg", innum = 10)
```

Now we can plot again to see what happens:

```
bagging$plot(html = FALSE)
```



This pipeline can again be used in conjunction with `GraphLearner` in order for Bagging to be used like a `Learner`:

```
baglrn = as_learner(bagging)
baglrn$train(task, train.idx)
baglrn$predict(task, test.idx)
```

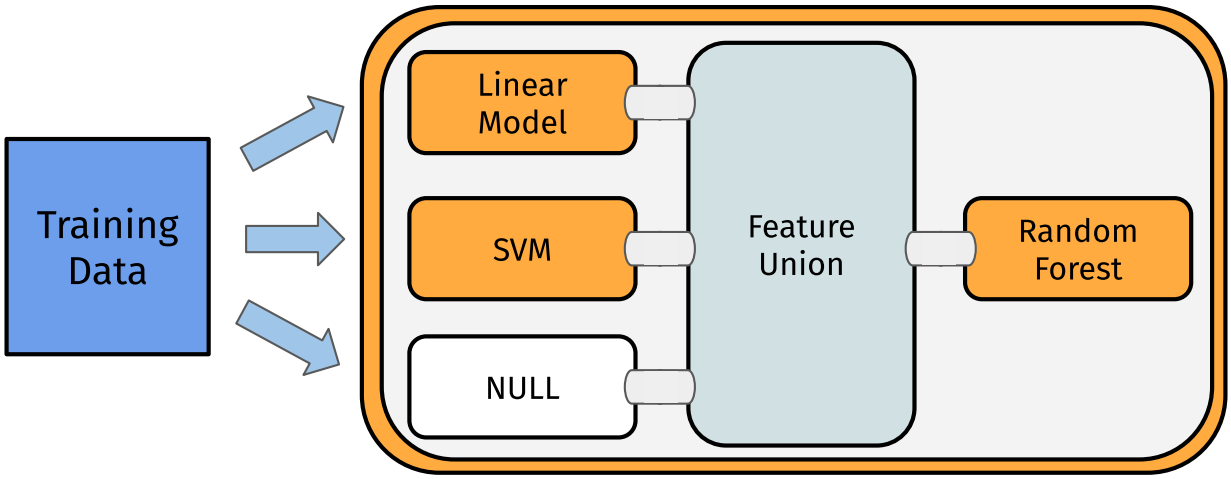
```
<PredictionClassif> for 30 observations:
    row_ids     truth   response prob.setosa prob.versicolor prob.virginica
         16    setosa     setosa           1             0.0            0.0
         18    setosa     setosa           1             0.0            0.0
         21    setosa     setosa           1             0.0            0.0
---
        129 virginica  virginica           0             0.0            1.0
        134 virginica versicolor           0             0.5            0.5
        149 virginica  virginica           0             0.0            1.0
```

In conjunction with different `Backends`, this can be a very powerful tool. In cases when the data does not fully fit in memory, one can obtain a fraction of the data for each learner from a `DataBackend` and then aggregate predictions over all learners.

6.5.2.2. Stacking

Stacking (Wolpert 1992) is another technique that can improve model performance. The basic idea behind stacking is the use of predictions from one model as features for a subsequent model to possibly improve performance.

Below an conceptual illustration of stacking:



As an example we can train a decision tree and use the predictions from this model in conjunction with the original features in order to train an additional model on top.

To limit overfitting, we additionally do not predict on the original predictions of the learner. Instead, we predict on out-of-bag predictions. To do all this, we can use `PipeOpLearnerCV` .

`PipeOpLearnerCV` performs nested cross-validation on the training data, fitting a model in each fold. Each of the models is then used to predict on the out-of-fold data. As a result, we obtain predictions for every data point in our input data.

We first create a "level 0" learner, which is used to extract a lower level prediction. Additionally, we `$clone()` the learner object to obtain a copy of the learner. Subsequently, one sets a custom id for the `PipeOp` .

```
lrn = lrn("classif.rpart")
lrn_0 = po("learner_cv", lrn$clone())
lrn_0$id = "rpart_cv"
```

We use `PipeOpNOP` in combination with `gunion`, in order to send the unchanged Task to the next level. There it is combined with the predictions from our decision tree learner.

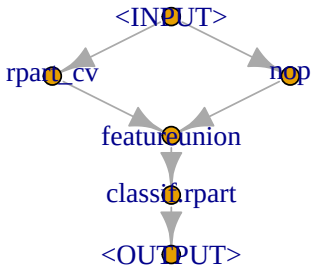
```
level_0 = gunion(list(lrn_0, po("nop")))
```

Afterwards, we want to concatenate the predictions from `PipeOpLearnerCV` and the original Task using `PipeOpFeatureUnion` :

```
combined = level_0 %>>% po("featureunion", 2)
```

Now we can train another learner on top of the combined features:

```
stack = combined %>>% po("learner", lrn$clone())
stack$plot(html = FALSE)
```




```
stacklrn = as_learner(stack)
stacklrn$train(task, train.idx)
stacklrn$predict(task, test.idx)
```

```
<PredictionClassif> for 30 observations:
    row_ids     truth   response
         16    setosa     setosa
         18    setosa     setosa
         21    setosa     setosa
---
        129 virginica  virginica
        134 virginica versicolor
        149 virginica  virginica
```

In this vignette, we showed a very simple use-case for stacking. In many real-world applications, stacking is done for multiple levels and on multiple representations of the dataset. On a lower level, different preprocessing methods can be defined in conjunction with several learners. On a higher level, we can then combine those predictions in order to form a very powerful model.

6.5.2.3. Multilevel Stacking

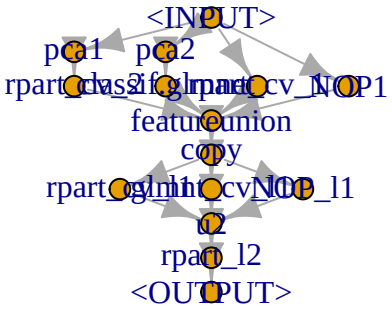
In order to showcase the power of `mlr3pipelines`, we will show a more complicated stacking example.

In this case, we train a `glmnet` and 2 different `rpart` models (some transform its inputs using `PipeOpPCA`) on our task in the "level 0" and concatenate them with the original features (via `gunion`). The result is then passed on to "level 1", where we copy the concatenated features 3 times and put this task into an `rpart` and a `glmnet` model. Additionally, we keep a version of the

"level 0" output (via PipeOpNOP) and pass this on to "level 2". In "level 2" we simply concatenate all "level 1" outputs and train a final decision tree.

In the following examples, use <lrn>$param_set$values$<param_name> = <param_value> to set hyperparameters for the different learner.

```
library("magrittr")
library("mlr3learners") # for classif.glmnet

rprt = lrn("classif.rpart", predict_type = "prob")
glmn = lrn("classif.glmnet", predict_type = "prob")

#  Create Learner CV Operators
lrn_0 = po("learner_cv", rprt, id = "rpart_cv_1")
lrn_0$param_set$values$maxdepth = 5L
lrn_1 = po("pca", id = "pca1") %>>% po("learner_cv", rprt, id = "rpart_cv_2")
lrn_1$param_set$values$rpart_cv_2.maxdepth = 1L
lrn_2 = po("pca", id = "pca2") %>>% po("learner_cv", glmn)

# Union them with a PipeOpNULL to keep original features
level_0 = gunion(list(lrn_0, lrn_1, lrn_2, po("nop", id = "NOP1")))

# Cbind the output 3 times, train 2 learners but also keep level
# 0 predictions
level_1 = level_0 %>>%
  po("featureunion", 4) %>>%
  po("copy", 3) %>>%
  gunion(list(
    po("learner_cv", rprt, id = "rpart_cv_l1"),
    po("learner_cv", glmn, id = "glmnt_cv_l1"),
    po("nop", id = "NOP_l1")
  ))

# Cbind predictions, train a final learner
level_2 = level_1 %>>%
  po("featureunion", 3, id = "u2") %>>%
  po("learner", rprt, id = "rpart_l2")

# Plot the resulting graph
level_2$plot(html = FALSE)
```




```
task = tsk("iris")
lrn = as_learner(level_2)
```

And we can again call `.$train` and `.$predict`:

```
lrn$
  train(task, train.idx)$
  predict(task, test.idx)$
  score()
```

```
classif.ce
       0.1
```

6.6. Adding new PipeOps

This section showcases how the `mlr3pipelines` package can be extended to include custom `PipeOp`s. To run the following examples, we will need a `Task`; we are using the well-known "Iris" task:

```
library("mlr3")
task = tsk("iris")
task$data()
```

```
     Species Petal.Length Petal.Width Sepal.Length Sepal.Width
1:    setosa          1.4         0.2          5.1         3.5
2:    setosa          1.4         0.2          4.9         3.0
```

```
  3:    setosa          1.3         0.2          4.7         3.2
  4:    setosa          1.5         0.2          4.6         3.1
  5:    setosa          1.4         0.2          5.0         3.6
 ---
146: virginica          5.2         2.3          6.7         3.0
147: virginica          5.0         1.9          6.3         2.5
148: virginica          5.2         2.0          6.5         3.0
149: virginica          5.4         2.3          6.2         3.4
150: virginica          5.1         1.8          5.9         3.0
```

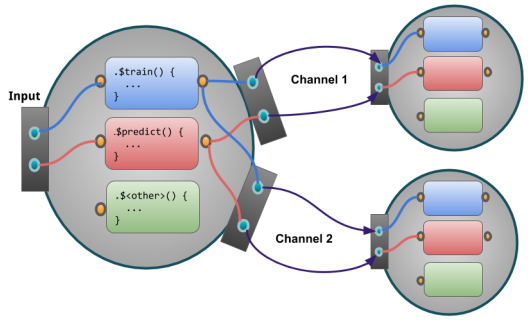
`mlr3pipelines` is fundamentally built around `R6`. When planning to create custom `PipeOp` objects, it can only help to familiarize yourself with it.

In principle, all a `PipeOp` must do is inherit from the `PipeOp` R6 class and implement the `.train()` and `.predict()` functions. There are, however, several auxiliary subclasses that can make the creation of *certain* operations much easier.

6.6.1. General Case Example: `PipeOpCopy`

A very simple yet useful `PipeOp` is `PipeOpCopy`, which takes a single input and creates a variable number of output channels, all of which receive a copy of the input data. It is a simple example that showcases the important steps in defining a custom `PipeOp`. We will show a simplified version here, **`PipeOpCopyTwo`**, that creates exactly two copies of its input data.

The following figure visualizes how our `PipeOp` is situated in the `Pipeline` and the significant in- and outputs.



6.6.1.1. First Steps: Inheriting from `PipeOp`

The first part of creating a custom `PipeOp` is inheriting from `PipeOp`. We make a mental note that we need to implement a `.train()` and a `.predict()` function, and that we probably want to have an `initialize()` as well:

```
PipeOpCopyTwo = R6::R6Class("PipeOpCopyTwo",
  inherit = mlr3pipelines::PipeOp,
  public = list(
    initialize = function(id = "copy.two") {
```

```
      ....
    },
  ),
  private == list(
    .train = function(inputs) {
      ....
    },

    .predict = function(inputs) {
      ....
    }
  )
)
```

Note, that **private** methods, e.g. `.train` and `.predict` etc are prefixed with a `.`.

6.6.1.2. Channel Definitions

We need to tell the `PipeOp` the layout of its channels: How many there are, what their names are going to be, and what types are acceptable. This is done on initialization of the `PipeOp` (using a `super$initialize` call) by giving the `input` and `output` `data.table` objects. These must have three columns: a `"name"` column giving the names of input and output channels, and a `"train"` and `"predict"` column naming the class of objects we expect during training and prediction as input / output. A special value for these classes is `"*"`, which indicates that any class will be accepted; our simple copy operator accepts any kind of input, so this will be useful. We have only one input, but two output channels.

By convention, we name a single channel `"input"` or `"output"`, and a group of channels [`"input1"`, `"input2"`, ...], unless there is a reason to give specific different names. Therefore, our `input` `data.table` will have a single row `<"input", "*", "*">`, and our `output` table will have two rows, `<"output1", "*", "*">` and `<"output2", "*", "*">`.

All of this is given to the `PipeOp` creator. Our `initialize()` will thus look as follows:

```
initialize = function(id = "copy.two") {
  input = data.table::data.table(name = "input", train = "*", predict = "*")
  # the following will create two rows and automatically fill the `train`
  # and `predict` cols with "*"
  output = data.table::data.table(
    name = c("output1", "output2"),
    train = "*", predict = "*"
  )
  super$initialize(id,
    input = input,
    output = output
  )
}
```

6.6.1.3. Train and Predict

Both `.train()` and `.predict()` will receive a `list` as input and must give a `list` in return. According to our `input` and `output` definitions, we will always get a list with a single element as input, and will need to return a list with two elements. Because all we want to do is create two copies, we will just create the copies using `c(inputs, inputs)`.

Two things to consider:

- The `.train()` function must always modify the `self$state` variable to something that is not `NULL` or `NO_OP`. This is because the `$state` slot is used as a signal that `PipeOp` has been trained on data, even if the state itself is not important to the `PipeOp` (as in our case). Therefore, our `.train()` will set `self$state = list()`.
- It is not necessary to "clone" our input or make deep copies, because we don't modify the data. However, if we were changing a reference-passed object, for example by changing data in a `Task`, we would have to make a deep copy first. This is because a `PipeOp` may never modify its input object by reference.

Our `.train()` and `.predict()` functions are now:

```
.train = function(inputs) {
  self$state = list()
  c(inputs, inputs)
}
```

```
.predict = function(inputs) {
  c(inputs, inputs)
}
```

6.6.1.4. Putting it Together

The whole definition thus becomes

```
PipeOpCopyTwo = R6::R6Class("PipeOpCopyTwo",
  inherit = mlr3pipelines::PipeOp,
  public = list(
    initialize = function(id = "copy.two") {
      super$initialize(id,
        input = data.table::data.table(name = "input", train = "*", predict = "*"),
        output = data.table::data.table(name = c("output1", "output2"),
                              train = "*", predict = "*")
      )
    }
  ),
  private = list(
    .train = function(inputs) {
```

```
      self$state = list()
      c(inputs, inputs)
    },

    .predict = function(inputs) {
      c(inputs, inputs)
    }
  )
)
```

We can create an instance of our PipeOp, put it in a graph, and see what happens when we train it on something:

```
library("mlr3pipelines")
poct = PipeOpCopyTwo$new()
gr = Graph$new()
gr$add_pipeop(poct)

print(gr)
```

```
Graph with 1 PipeOps:
       ID         State sccssors prdcssors
 copy.two <<UNTRAINED>>
```

```
result = gr$train(task)

str(result)
```

```
List of 2
 $ copy.two.output1:Classes 'TaskClassif', 'TaskSupervised', 'Task', 'R6' <TaskClassif:iris>
 $ copy.two.output2:Classes 'TaskClassif', 'TaskSupervised', 'Task', 'R6' <TaskClassif:iris>
```

6.6.2. Special Case: Preprocessing

Many PipeOps perform an operation on exactly one Task, and return exactly one Task. They may even not care about the "Target" / "Outcome" variable of that task, and only do some modification of some input data. However, it is usually important to them that the Task on which they perform prediction has the same data columns as the Task on which they train. For these cases, the auxiliary base class PipeOpTaskPreproc exists. It inherits from PipeOp itself, and other PipeOps should use it if they fall in the kind of use-case named above.

When inheriting from PipeOpTaskPreproc, one must either implement the private methods `.train_task()` and `.predict_task()`, or the methods `.train_dt()`, `.predict_dt()`, depending on whether wants to operate on a Task object or on its data as `data.tables`. In the second

case, one can optionally also overload the `.select_cols()` method, which chooses which of the incoming `Task`'s features are given to the `.train_dt()` / `.predict_dt()` functions.

The following will show two examples: `PipeOpDropNA`, which removes a `Task`'s rows with missing values during training (and implements `.train_task()` and `.predict_task()`), and `PipeOpScale`, which scales a `Task`'s numeric columns (and implements `.train_dt()`, `.predict_dt()`, and `.select_cols()`).

6.6.2.1. Example: `PipeOpDropNA`

Dropping rows with missing values may be important when training a model that can not handle them.

Because `mlr3` `"Task", text = "Tasks")` only contain a view to the underlying data, it is not necessary to modify data to remove rows with missing values. Instead, the rows can be removed using the `Task`'s `$filter` method, which modifies the `Task` in-place. This is done in the private method `.train_task()`. We take care that we also set the `$state` slot to signal that the `PipeOp` was trained.

The private method `.predict_task()` does not need to do anything; removing missing values during prediction is not as useful, since learners that cannot handle them will just ignore the respective rows. Furthermore, `mlr3` expects a `Learner` to always return just as many predictions as it was given input rows, so a `PipeOp` that removes `Task` rows during training can not be used inside a `GraphLearner`.

When we inherit from `PipeOpTaskPreproc`, it sets the `input` and `output` `data.table`s for us to only accept a single `Task`. The only thing we do during `initialize()` is therefore to set an `id` (which can optionally be changed by the user).

The complete `PipeOpDropNA` can therefore be written as follows. Note that it inherits from `PipeOpTaskPreproc`, unlike the `PipeOpCopyTwo` example from above:

```
PipeOpDropNA = R6::R6Class("PipeOpDropNA",
  inherit = mlr3pipelines::PipeOpTaskPreproc,
  public = list(
    initialize = function(id = "drop.na") {
      super$initialize(id)
    }
  ),

  private = list(
    .train_task = function(task) {
      self$state = list()
      featuredata = task$data(cols = task$feature_names)
      exclude = apply(is.na(featuredata), 1, any)
      task$filter(task$row_ids[!exclude])
    },

    .predict_task = function(task) {
```

```
        # nothing to be done
        task
      }
    )
  )
```

To test this PipeOp, we create a small task with missing values:

```
smalliris = iris[(1:5) * 30, ]
smalliris[1, 1] = NA
smalliris[2, 2] = NA
sitask = as_task_classif(smalliris, target = "Species")
print(sitask$data())
```

```
      Species Petal.Length Petal.Width Sepal.Length Sepal.Width
1:     setosa          1.6         0.2           NA         3.2
2: versicolor          3.9         1.4          5.2          NA
3: versicolor          4.0         1.3          5.5         2.5
4:  virginica          5.0         1.5          6.0         2.2
5:  virginica          5.1         1.8          5.9         3.0
```

We test this by feeding it to a new Graph that uses `PipeOpDropNA`.

```
gr = Graph$new()
gr$add_pipeop(PipeOpDropNA$new())

filtered_task = gr$train(sitask)[[1]]
print(filtered_task$data())
```

```
      Species Petal.Length Petal.Width Sepal.Length Sepal.Width
1: versicolor          4.0         1.3          5.5         2.5
2:  virginica          5.0         1.5          6.0         2.2
3:  virginica          5.1         1.8          5.9         3.0
```

6.6.2.2. Example: `PipeOpScaleAlways`

An often-applied preprocessing step is to simply **center** and/or **scale** the data to mean 0 and standard deviation 1. This fits the PipeOpTaskPreproc pattern quite well. Because it always replaces all columns that it operates on, and does not require any information about the task's target, it only needs to overload the `.train_dt()` and `.predict_dt()` functions. This saves some boilerplate-code from getting the correct feature columns out of the task, and replacing them after modification.

Because scaling only makes sense on numeric features, we want to instruct PipeOpTaskPreproc to give us only these numeric columns. We do this by overloading the `.select_cols()` function:

It is called by the class to determine which columns to pass to `.train_dt()` and `.predict_dt()`. Its input is the `Task` that is being transformed, and it should return a `character` vector of all features to work with. When it is not overloaded, it uses all columns; instead, we will set it to only give us numeric columns. Because the `levels()` of the data table given to `.train_dt()` and `.predict_dt()` may be different from the `Task`'s levels, these functions must also take a `levels` argument that is a named list of column names indicating their levels. When working with numeric data, this argument can be ignored, but it should be used instead of `levels(dt[[column]])` for factorial or character columns.

This is the first `PipeOp` where we will be using the `$state` slot for something useful: We save the centering offset and scaling coefficient and use it in `$.predict()`!

For simplicity, we are not using hyperparameters and will always scale and center all data. Compare this `PipeOpScaleAlways` operator to the one defined inside the `mlr3pipelines` package, `PipeOpScale`.

```
PipeOpScaleAlways = R6::R6Class("PipeOpScaleAlways",
  inherit = mlr3pipelines::PipeOpTaskPreproc,
  public = list(
    initialize = function(id = "scale.always") {
      super$initialize(id = id)
    }
  ),

  private = list(
    .select_cols = function(task) {
      task$feature_types[type == "numeric", id]
    },

    .train_dt = function(dt, levels, target) {
      sc = scale(as.matrix(dt))
      self$state = list(
        center = attr(sc, "scaled:center"),
        scale = attr(sc, "scaled:scale")
      )
      sc
    },

    .predict_dt = function(dt, levels) {
      t((t(dt) - self$state$center) / self$state$scale)
    }
  )
)
```

(Note for the observant: If you check `PipeOpScale.R` from the `mlr3pipelines` package, you will notice that is uses "`get("type")`" and "`get("id")`" instead of "`type`" and "`id`", because the static code checker on CRAN would otherwise complain about references to undefined variables. This is a "problem" with `data.table` and not exclusive to `mlr3pipelines`.)

We can, again, create a new Graph that uses this PipeOp to test it. Compare the resulting data to the original "iris" Task data printed at the beginning:

```
gr = Graph$new()
gr$add_pipeop(PipeOpScaleAlways$new())

result = gr$train(task)

result[[1]]$data()
```

```
       Species Petal.Length Petal.Width Sepal.Length Sepal.Width
  1:    setosa   -1.3357516  -1.3110521  -0.89767388  1.01560199
  2:    setosa   -1.3357516  -1.3110521  -1.13920048 -0.13153881
  3:    setosa   -1.3923993  -1.3110521  -1.38072709  0.32731751
  4:    setosa   -1.2791040  -1.3110521  -1.50149039  0.09788935
  5:    setosa   -1.3357516  -1.3110521  -1.01843718  1.24503015
 ---
146: virginica    0.8168591   1.4439941   1.03453895 -0.13153881
147: virginica    0.7035638   0.9192234   0.55148575 -1.27867961
148: virginica    0.8168591   1.0504160   0.79301235 -0.13153881
149: virginica    0.9301544   1.4439941   0.43072244  0.78617383
150: virginica    0.7602115   0.7880307   0.06843254 -0.13153881
```

6.6.3. Special Case: Preprocessing with Simple Train

It is possible to make even further simplifications for many PipeOps that perform mostly the same operation during training and prediction. The point of Task preprocessing is often to modify the training data in mostly the same way as prediction data (but in a way that *may* depend on training data).

Consider constant feature removal, for example: The goal is to remove features that have no variance, or only a single factor level. However, what features get removed must be decided during *training*, and may only depend on training data. Furthermore, the actual process of removing features is the same during training and prediction.

A simplification to make is therefore to have a private method `.get_state(task)` which sets the `$state` slot during training, and a private method `.transform(task)`, which gets called both during training *and* prediction. This is done in the PipeOpTaskPreprocSimple class. Just like PipeOpTaskPreproc, one can inherit from this and overload these functions to get a PipeOp that performs preprocessing with very little boilerplate code.

Just like PipeOpTaskPreproc, PipeOpTaskPreprocSimple offers the possibility to instead overload the `.get_state_dt(dt, levels)` and `.transform_dt(dt, levels)` methods (and optionally, again, the `.select_cols(task)` function) to operate on `data.table` feature data instead of the whole Task.

Even some methods that do not use PipeOpTaskPreprocSimple *could* work in a similar way: The `PipeOpScaleAlways` example from above will be shown to also work with this paradigm.

6.6.3.1. Example: `PipeOpDropConst`

A typical example of a preprocessing operation that does almost the same operation during training and prediction is an operation that drops features depending on a criterion that is evaluated during training. One simple example of this is dropping constant features. Because the `mlr3` `Task` class offers a flexible view on underlying data, it is most efficient to drop columns from the task directly using its `$select()` function, so the `.get_state_dt(dt, levels)` / `.transform_dt(dt, levels)` functions will *not* get used; instead we overload the `.get_state(task)` and `.transform(task)` methods.

The `.get_state()` function's result is saved to the `$state` slot, so we want to return something that is useful for dropping features. We choose to save the names of all the columns that have nonzero variance. For brevity, we use `length(unique(column)) > 1` to check whether more than one distinct value is present; a more sophisticated version could have a tolerance parameter for numeric values that are very close to each other.

The `.transform()` method is evaluated both during training *and* prediction, and can rely on the `$state` slot being present. All it does here is call the `Task$select` function with the columns we chose to keep.

The full `PipeOp` could be written as follows:

```
PipeOpDropConst = R6::R6Class("PipeOpDropConst",
  inherit = mlr3pipelines::PipeOpTaskPreprocSimple,
  public = list(
    initialize = function(id = "drop.const") {
      super$initialize(id = id)
    }
  ),

  private = list(
    .get_state = function(task) {
      data = task$data(cols = task$feature_names)
      nonconst = sapply(data, function(column) length(unique(column)) > 1)
      list(cnames = colnames(data)[nonconst])
    },

    .transform = function(task) {
      task$select(self$state$cnames)
    }
  )
)
```

This can be tested using the first five rows of the "Iris" `Task`, for which one feature (`"Petal.Width"`) is constant:

```
irishead = task$clone()$filter(1:5)
irishead$data()
```

```
   Species Petal.Length Petal.Width Sepal.Length Sepal.Width
1:  setosa          1.4         0.2          5.1         3.5
2:  setosa          1.4         0.2          4.9         3.0
3:  setosa          1.3         0.2          4.7         3.2
4:  setosa          1.5         0.2          4.6         3.1
5:  setosa          1.4         0.2          5.0         3.6
```

```
gr = Graph$new()$add_pipeop(PipeOpDropConst$new())
dropped_task = gr$train(irishead)[[1]]

dropped_task$data()
```

```
   Species Petal.Length Sepal.Length Sepal.Width
1:  setosa          1.4          5.1         3.5
2:  setosa          1.4          4.9         3.0
3:  setosa          1.3          4.7         3.2
4:  setosa          1.5          4.6         3.1
5:  setosa          1.4          5.0         3.6
```

We can also see that the `$state` was correctly set. Calling `$.predict()` with this graph, even with different data (the whole Iris `Task`!) will still drop the `"Petal.Width"` column, as it should.

```
gr$pipeops$drop.const$state
```

```
$cnames
[1] "Petal.Length" "Sepal.Length" "Sepal.Width"

$affected_cols
[1] "Petal.Length" "Petal.Width"  "Sepal.Length" "Sepal.Width"

$intasklayout
             id    type
1: Petal.Length numeric
2:  Petal.Width numeric
3: Sepal.Length numeric
4:  Sepal.Width numeric

$outtasklayout
             id    type
1: Petal.Length numeric
2: Sepal.Length numeric
3:  Sepal.Width numeric

$outtaskshell
Empty data.table (0 rows and 4 cols): Species,Petal.Length,Sepal.Length,Sepal.Width
```

```
dropped_predict = gr$predict(task)[[1]]

dropped_predict$data()
```

```
        Species Petal.Length Sepal.Length Sepal.Width
  1:     setosa          1.4          5.1         3.5
  2:     setosa          1.4          4.9         3.0
  3:     setosa          1.3          4.7         3.2
  4:     setosa          1.5          4.6         3.1
  5:     setosa          1.4          5.0         3.6
 ---
146: virginica          5.2          6.7         3.0
147: virginica          5.0          6.3         2.5
148: virginica          5.2          6.5         3.0
149: virginica          5.4          6.2         3.4
150: virginica          5.1          5.9         3.0
```

6.6.3.2. Example: `PipeOpScaleAlwaysSimple`

This example will show how a `PipeOpTaskPreprocSimple` can be used when only working on feature data in form of a `data.table`. Instead of calling the `scale()` function, the `center` and `scale` values are calculated directly and saved to the `$state` slot. The `.transform_dt()` function will then perform the same operation during both training and prediction: subtract the `center` and divide by the `scale` value. As in the `PipeOpScaleAlways` example above, we use `.select_cols()` so that we only work on numeric columns.

```
PipeOpScaleAlwaysSimple = R6::R6Class("PipeOpScaleAlwaysSimple",
  inherit = mlr3pipelines::PipeOpTaskPreprocSimple,
  public = list(
    initialize = function(id = "scale.always.simple") {
      super$initialize(id = id)
    }
  ),

  private = list(
    .select_cols = function(task) {
      task$feature_types[type == "numeric", id]
    },

    .get_state_dt = function(dt, levels, target) {
      list(
        center = sapply(dt, mean),
        scale = sapply(dt, sd)
      )
    },
```

```
20
21      .transform_dt = function(dt, levels) {
22        t((t(dt) - self$state$center) / self$state$scale)
23      }
24    )
25  )
```

We can compare this PipeOp to the one above to show that it behaves the same.

```
gr = Graph$new()$add_pipeop(PipeOpScaleAlways$new())
result_posa = gr$train(task)[[1]]

gr = Graph$new()$add_pipeop(PipeOpScaleAlwaysSimple$new())
result_posa_simple = gr$train(task)[[1]]
```

```
result_posa$data()
```

```
       Species Petal.Length Petal.Width Sepal.Length Sepal.Width
  1:    setosa   -1.3357516  -1.3110521  -0.89767388  1.01560199
  2:    setosa   -1.3357516  -1.3110521  -1.13920048 -0.13153881
  3:    setosa   -1.3923993  -1.3110521  -1.38072709  0.32731751
  4:    setosa   -1.2791040  -1.3110521  -1.50149039  0.09788935
  5:    setosa   -1.3357516  -1.3110521  -1.01843718  1.24503015
 ---
146: virginica    0.8168591   1.4439941   1.03453895 -0.13153881
147: virginica    0.7035638   0.9192234   0.55148575 -1.27867961
148: virginica    0.8168591   1.0504160   0.79301235 -0.13153881
149: virginica    0.9301544   1.4439941   0.43072244  0.78617383
150: virginica    0.7602115   0.7880307   0.06843254 -0.13153881
```

```
result_posa_simple$data()
```

```
       Species Petal.Length Petal.Width Sepal.Length Sepal.Width
  1:    setosa   -1.3357516  -1.3110521  -0.89767388  1.01560199
  2:    setosa   -1.3357516  -1.3110521  -1.13920048 -0.13153881
  3:    setosa   -1.3923993  -1.3110521  -1.38072709  0.32731751
  4:    setosa   -1.2791040  -1.3110521  -1.50149039  0.09788935
  5:    setosa   -1.3357516  -1.3110521  -1.01843718  1.24503015
 ---
146: virginica    0.8168591   1.4439941   1.03453895 -0.13153881
147: virginica    0.7035638   0.9192234   0.55148575 -1.27867961
148: virginica    0.8168591   1.0504160   0.79301235 -0.13153881
149: virginica    0.9301544   1.4439941   0.43072244  0.78617383
150: virginica    0.7602115   0.7880307   0.06843254 -0.13153881
```

6.6.4. Hyperparameters

mlr3pipelines uses the [paradox](https://paradox.mlr-org.com) package to define parameter spaces for PipeOps. Parameters for PipeOps can modify their behavior in certain ways, e.g. switch centering or scaling off in the PipeOpScale operator. The unified interface makes it possible to have parameters for whole Graphs that modify the individual PipeOp's behavior. The Graphs, when encapsulated in GraphLearners, can even be tuned using the tuning functionality in mlr3tuning.

Hyperparameters are declared during initialization, when calling the PipeOp's `$initialize()` function, by giving a `param_set` argument. The `param_set` must be a ParamSet from the paradox package; see the tuning chapter or Section 9.4 for more information on how to define parameter spaces. After construction, the ParamSet can be accessed through the `$param_set` slot. While it is *possible* to modify this ParamSet, using e.g. the `$add()` and `$add_dep()` functions, *after* adding it to the PipeOp, it is strongly advised against.

Hyperparameters can be set and queried through the `$values` slot. When setting hyperparameters, they are automatically checked to satisfy all conditions set by the `$param_set`, so it is not necessary to type check them. Be aware that it is always possible to *remove* hyperparameter values.

When a PipeOp is initialized, it usually does not have any parameter values—`$values` takes the value `list()`. It is possible to set initial parameter values in the `$initialize()` constructor; this must be done *after* the `super$initialize()` call where the corresponding ParamSet must be supplied. This is because setting `$values` checks against the current `$param_set`, which would fail if the `$param_set` was not set yet.

When using an underlying library function (the `scale` function in PipeOpScale, say), then there is usually a "default" behaviour of that function when a parameter is not given. It is good practice to use this default behaviour whenever a parameter is not set (or when it was removed). This can easily be done when using the mlr3misc library's `mlr3misc::invoke()` function, which has functionality similar to `"do.call()"`.

6.6.4.1. Hyperparameter Example: PipeOpScale

How to use hyperparameters can best be shown through the example of PipeOpScale, which is very similar to the example above, `PipeOpScaleAlways`. The difference is made by the presence of hyperparameters. PipeOpScale constructs a ParamSet in its `$initialize` function and passes this on to the `super$initialize` function:

```
1  PipeOpScale$public_methods$initialize
```

```
function (id = "scale", param_vals = list())
.__PipeOpScale__initialize(self = self, private = private, super = super,
    id = id, param_vals = param_vals)
<environment: namespace:mlr3pipelines>
```

The user has access to this and can set and get parameters. Types are automatically checked:

```
pss = po("scale")
print(pss$param_set)
```

```
<ParamSet:scale>
               id    class lower upper nlevels        default value
1:         center ParamLgl    NA    NA       2           TRUE
2:          scale ParamLgl    NA    NA       2           TRUE
3:         robust ParamLgl    NA    NA       2 <NoDefault[3]> FALSE
4: affect_columns ParamUty    NA    NA     Inf  <Selector[1]>
```

```
pss$param_set$values$center = FALSE
print(pss$param_set$values)
```

```
$robust
[1] FALSE

$center
[1] FALSE
```

```
pss$param_set$values$scale = "TRUE" # bad input is checked!
```

```
Error in self$assert(xs): Assertion on 'xs' failed: scale: Must be of type 'logical flag', not
```

How PipeOpScale handles its parameters can be seen in its `$.train_dt` method: It gets the relevant parameters from its `$values` slot and uses them in the `mlr3misc::invoke()` call. This has the advantage over calling `scale()` directly that if a parameter is not given, its default value from the `"scale()"` function will be used.

```
PipeOpScale$private_methods$.train_dt
```

```
function (dt, levels, target)
.__PipeOpScale__.train_dt(self = self, private = private, super = super,
    dt = dt, levels = levels, target = target)
<environment: namespace:mlr3pipelines>
```

Another change that is necessary compared to `PipeOpScaleAlways` is that the attributes `"scaled:scale"` and `"scaled:center"` are not always present, depending on parameters, and possibly need to be set to default values 1 or 0, respectively.

It is now even possible (if a bit pointless) to call PipeOpScale with both `scale` and `center` set to `FALSE`, which returns the original dataset, unchanged.

```
pss$param_set$values$scale = FALSE
pss$param_set$values$center = FALSE

gr = Graph$new()
gr$add_pipeop(pss)

result = gr$train(task)

result[[1]]$data()
```

```
        Species Petal.Length Petal.Width Sepal.Length Sepal.Width
  1:     setosa          1.4         0.2          5.1         3.5
  2:     setosa          1.4         0.2          4.9         3.0
  3:     setosa          1.3         0.2          4.7         3.2
  4:     setosa          1.5         0.2          4.6         3.1
  5:     setosa          1.4         0.2          5.0         3.6
 ---
146: virginica          5.2         2.3          6.7         3.0
147: virginica          5.0         1.9          6.3         2.5
148: virginica          5.2         2.0          6.5         3.0
149: virginica          5.4         2.3          6.2         3.4
150: virginica          5.1         1.8          5.9         3.0
```

6.7. Special Operators

This section introduces some special operators, that might be useful in numerous further applications.

6.7.1. Imputation: `PipeOpImpute`

Often you will be using data sets that have missing values. There are many methods of dealing with this issue, from relatively simple imputation using either mean, median or histograms to way more involved methods including using machine learning algorithms in order to predict missing values. These methods are called imputation.

The following `PipeOp`s, `PipeOpImpute`:

- Add an indicator column marking whether a value for a given feature was missing or not (numeric only)
- Impute numeric values from a histogram
- Impute categorical values using a learner
- We use `po("featureunion")` and `po("nop")` to cbind the missing indicator features. In other words to combine the indicator columns with the rest of the data.

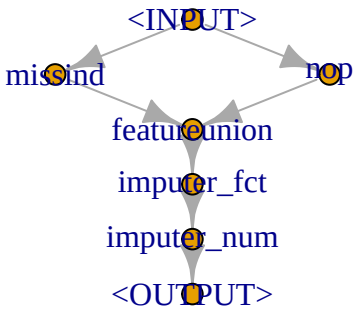
```
# Imputation example
task = tsk("penguins")
task$missings()
```

```
     species     bill_depth    bill_length      body_mass flipper_length
           0              2              2              2              2
      island            sex           year
           0             11              0
```

```
# Add missing indicator columns ("dummy columns") to the Task
pom = po("missind")
# Simply pushes the input forward
nop = po("nop")
# Imputes numerical features by histogram.
pon = po("imputehist", id = "imputer_num")
# combines features (used here to add indicator columns to original data)
pou = po("featureunion")
# Impute categorical features by fitting a Learner ("classif.rpart") for each feature.
pof = po("imputelearner", lrn("classif.rpart"), id = "imputer_fct", affect_columns = selecto
```

Now we construct the graph.

```
impgraph = list(
  pom,
  nop
) %>>% pou %>>% pof %>>% pon

impgraph$plot()
```



Now we get the new task and we can see that all of the missing values have been imputed.

```
new_task = impgraph$train(task)[[1]]

new_task$missings()
```

```
             species     missing_bill_depth    missing_bill_length
                   0                      0                      0
missing_body_mass    missing_flipper_length                 island
                   0                      0                      0
                year                    sex             bill_depth
                   0                      0                      0
         bill_length              body_mass         flipper_length
                   0                      0                      0
```

A learner can thus be equipped with automatic imputation of missing values by adding an imputation Pipeop.

```
polrn = po("learner", lrn("classif.rpart"))
lrn = as_learner(impgraph %>>% polrn)
```

6.7.2. Feature Engineering: `PipeOpMutate`

New features can be added or computed from a task using `PipeOpMutate` . The operator evaluates one or multiple expressions provided in an `alist`. In this example, we compute some new features on top of the `iris` task. Then we add them to the data as illustrated below:

`iris` dataset looks like this:

```
task = task = tsk("iris")
head(as.data.table(task))
```

```
   Species Petal.Length Petal.Width Sepal.Length Sepal.Width
1:  setosa          1.4         0.2          5.1         3.5
2:  setosa          1.4         0.2          4.9         3.0
3:  setosa          1.3         0.2          4.7         3.2
4:  setosa          1.5         0.2          4.6         3.1
5:  setosa          1.4         0.2          5.0         3.6
6:  setosa          1.7         0.4          5.4         3.9
```

Once we do the mutations, you can see the new columns:

```
pom = po("mutate")

# Define a set of mutations
mutations = list(
  Sepal.Sum = ~ Sepal.Length + Sepal.Width,
  Petal.Sum = ~ Petal.Length + Petal.Width,
  Sepal.Petal.Ratio = ~ (Sepal.Length / Petal.Length)
)
pom$param_set$values$mutation = mutations

new_task = pom$train(list(task))[[1]]
head(as.data.table(new_task))
```

```
   Species Petal.Length Petal.Width Sepal.Length Sepal.Width Sepal.Sum
1:  setosa          1.4         0.2          5.1         3.5       8.6
2:  setosa          1.4         0.2          4.9         3.0       7.9
3:  setosa          1.3         0.2          4.7         3.2       7.9
4:  setosa          1.5         0.2          4.6         3.1       7.7
5:  setosa          1.4         0.2          5.0         3.6       8.6
6:  setosa          1.7         0.4          5.4         3.9       9.3
2 variables not shown: [Petal.Sum, Sepal.Petal.Ratio]
```

If outside data is required, we can make use of the `env` parameter. Moreover, we provide an environment, where expressions are evaluated (`env` defaults to `.GlobalEnv`).

6.7.3. Training on data subsets: `PipeOpChunk`

In cases, where data is too big to fit into the machine's memory, an often-used technique is to split the data into several parts. Subsequently, the parts are trained on each part of the data.

After undertaking these steps, we aggregate the models. In this example, we split our data into 4 parts using `PipeOpChunk` . Additionally, we create 4 `PipeOpLearner` POS, which are then trained on each split of the data.

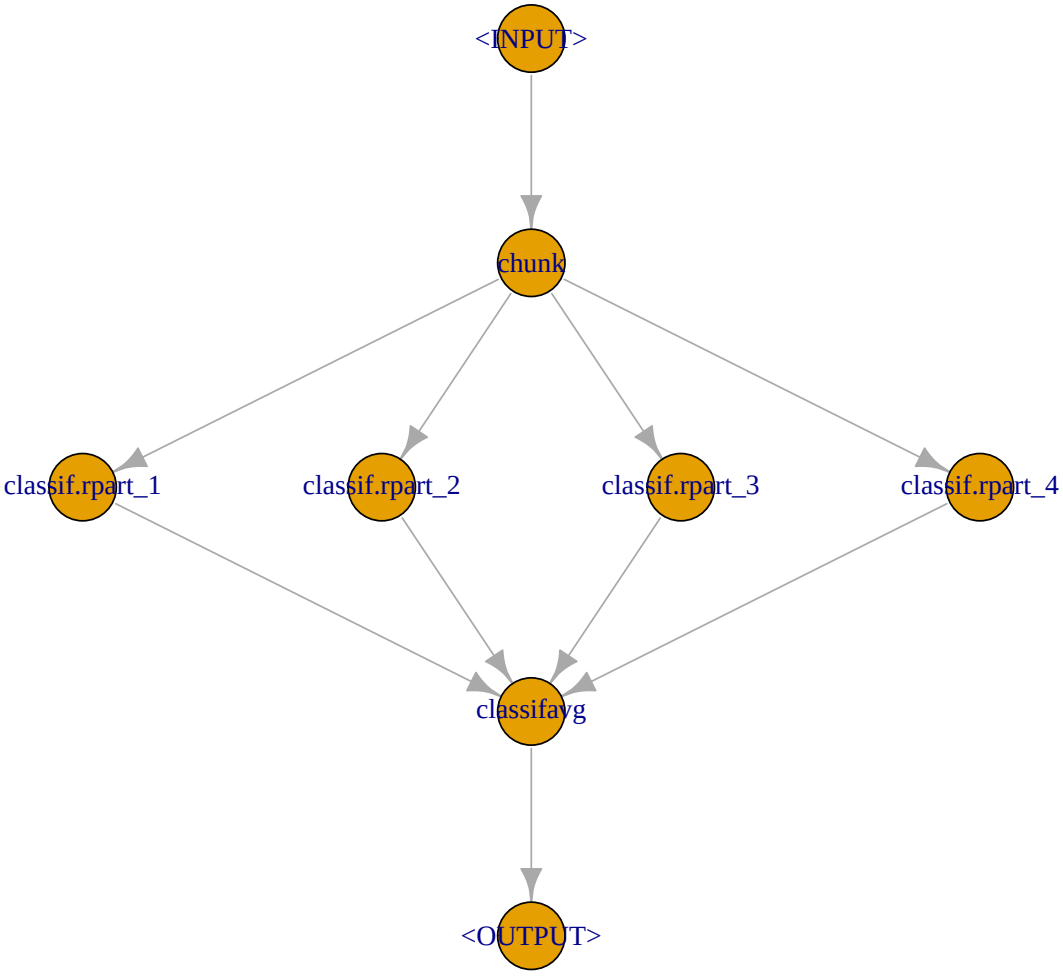
```
chks = po("chunk", 4)
lrns = ppl("greplicate", po("learner", lrn("classif.rpart")), 4)
```

Afterwards we can use `PipeOpClassifAvg` to aggregate the predictions from the 4 different models into a new one.

```
mjv = po("classifavg", 4)
```

We can now connect the different operators and visualize the full graph:

```
pipeline = chks %>>% lrns %>>% mjv
pipeline$plot(html = FALSE)
```




```
task = tsk("iris")
train.idx = sample(seq_len(task$nrow), 120)
test.idx = setdiff(seq_len(task$nrow), train.idx)

```

```
pipelrn = as_learner(pipeline)
pipelrn$train(task, train.idx)$
  predict(task, train.idx)$
  score()
```

```
classif.ce
 0.2083333
```

6.7.4. Feature Selection: `PipeOpFilter` and `PipeOpSelect`

The package `mlr3filters` contains many different `"mlr3filters::Filter"`)s that can be used to select features for subsequent learners. This is often required when the data has a large amount of features.

A `PipeOp` for filters is `PipeOpFilter`:

```
po("filter", mlr3filters::flt("information_gain"))
```

```
PipeOp: <information_gain> (not trained)
values: <list()>
Input channels <name [train type, predict type]>:
  input [Task,Task]
Output channels <name [train type, predict type]>:
  output [Task,Task]
```

How many features to keep can be set using `filter_nfeat`, `filter_frac` and `filter_cutoff`.

Filters can be selected / de-selected by name using `PipeOpSelect`.

6.8. In-depth look into mlr3pipelines

This vignette is an in-depth introduction to `mlr3pipelines`, the dataflow programming toolkit for machine learning in `R` using `mlr3`. It will go through basic concepts and then give a few examples that both show the simplicity as well as the power and versatility of using `mlr3pipelines`.

6.8.1. What's the Point

Machine learning toolkits often try to abstract away the processes happening inside machine learning algorithms. This makes it easy for the user to switch out one algorithm for another without having to worry about what is happening inside it, what kind of data it is able to operate on etc. The benefit of using `mlr3`, for example, is that one can create a `Learner`, a `Task`, a `Resampling` etc. and use them for typical machine learning operations. It is trivial to exchange individual components and therefore use, for example, a different `Learner` in the same experiment for comparison.

```
task = as_task_classif(iris, target = "Species")
lrn = lrn("classif.rpart")
rsmp = rsmp("holdout")
resample(task, lrn, rsmp)
```

```
<ResampleResult> of 1 iterations
* Task: iris
* Learner: classif.rpart
* Warnings: 0 in 0 iterations
* Errors: 0 in 0 iterations
```

However, this modularity breaks down as soon as the learning algorithm encompasses more than just model fitting, like data preprocessing, ensembles or other meta models. `mlr3pipelines` takes modularity one step further than `mlr3`: it makes it possible to build individual steps within a `Learner` out of building blocks called `PipeOp`s.

6.8.2. `PipeOp`: Pipeline Operators

The most basic unit of functionality within `mlr3pipelines` is the `PipeOp`, short for "pipeline operator", which represents a trans-formative operation on input (for example a training dataset) leading to output. It can therefore be seen as a generalized notion of a function, with a certain twist: `PipeOp`s behave differently during a "training phase" and a "prediction phase". The training phase will typically generate a certain model of the data that is saved as internal state. The prediction phase will then operate on the input data depending on the trained model.

An example of this behavior is the *principal component analysis* operation ("`PipeOpPCA`"): During training, it will transform incoming data by rotating it in a way that leads to uncorrelated features ordered by their contribution to total variance. It will *also* save the rotation matrix to be use for new data during the "prediction phase". This makes it possible to perform "prediction" with single rows of new data, where a row's scores on each of the principal components (the components of the training data!) is computed.

```
po = po("pca")
po$train(list(task))[[1]]$data()
```

```
       Species       PC1         PC2         PC3          PC4
  1:    setosa -2.684126 -0.31939725  0.02791483 -0.002262437
  2:    setosa -2.714142  0.17700123  0.21046427 -0.099026550
  3:    setosa -2.888991  0.14494943 -0.01790026 -0.019968390
  4:    setosa -2.745343  0.31829898 -0.03155937  0.075575817
  5:    setosa -2.728717 -0.32675451 -0.09007924  0.061258593
 ---
146: virginica  1.944110 -0.18753230 -0.17782509 -0.426195940
147: virginica  1.527167  0.37531698  0.12189817 -0.254367442
148: virginica  1.764346 -0.07885885 -0.13048163 -0.137001274
```

```
149: virginica  1.900942 -0.11662796 -0.72325156 -0.044595305
150: virginica  1.390189  0.28266094 -0.36290965  0.155038628
```

```
single_line_task = task$clone()$filter(1)
po$predict(list(single_line_task))[[1]]$data()
```

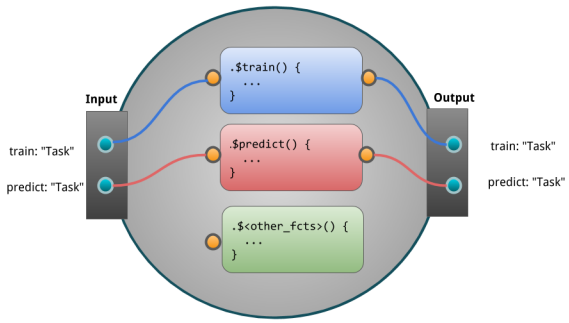
```
   Species       PC1        PC2        PC3          PC4
1:  setosa -2.684126 -0.3193972 0.02791483 -0.002262437
```

```
po$state
```

```
Standard deviations (1, .., p=4):
[1] 2.0562689 0.4926162 0.2796596 0.1543862

Rotation (n x k) = (4 x 4):
                     PC1         PC2         PC3        PC4
Petal.Length  0.85667061  0.17337266 -0.07623608  0.4798390
Petal.Width   0.35828920  0.07548102 -0.54583143 -0.7536574
Sepal.Length  0.36138659 -0.65658877  0.58202985 -0.3154872
Sepal.Width  -0.08452251 -0.73016143 -0.59791083  0.3197231
```

This shows the most important primitives incorporated in a `PipeOp`: * **`$train()`**, taking a list of input arguments, turning them into a list of outputs, meanwhile saving a state in `$state` * **`$predict()`**, taking a list of input arguments, turning them into a list of outputs, making use of the saved `$state` * **`$state`**, the "model" trained with `$train()` and utilized during `$predict()`.

Schematically we can represent the `PipeOp` like so:



6.8.2.1. Why the `$state`

It is important to take a moment and notice the importance of a `$state` variable and the `$train()` / `$predict()` dichotomy in a `PipeOp`. There are many preprocessing methods, for example scaling of parameters or imputation, that could in theory just be applied to training data and prediction / validation data separately, or they could be applied to a task before resampling is performed. This would, however, be fallacious:

- The preprocessing of each instance of prediction data should not depend on the remaining prediction dataset. A prediction on a single instance of new data should give the same result as prediction performed on a whole dataset.
- If preprocessing is performed on a task *before* resampling is done, information about the test set can leak into the training set. Resampling should evaluate the generalization performance of the *entire* machine learning method, therefore the behavior of this entire method must only depend only on the content of the *training* split during resampling.

6.8.2.2. Where to get PipeOps

Each PipeOp is an instance of an "R6" class, many of which are provided by the mlr3pipelines package itself. They can be constructed explicitly ("PipeOpPCA$new()") or retrieved from the mlr_pipeops dictionary: po("pca"). The entire list of available PipeOps, and some meta-information, can be retrieved using as.data.table():

```
as.data.table(mlr_pipeops)[, c("key", "input.num", "output.num")]
```

```
              key input.num output.num
 1:         boxcox         1          1
 2:         branch         1         NA
 3:          chunk         1         NA
 4: classbalancing         1          1
 5:     classifavg        NA          1
---
60:      threshold         1          1
61:  tunethreshold         1          1
62:       unbranch        NA          1
63:         vtreat         1          1
64:     yeojohnson         1          1
```

When retrieving PipeOps from the mlr_pipeops dictionary, it is also possible to give additional constructor arguments, such as an id or parameter values.

```
po("pca", rank. = 3)
```

```
PipeOp: <pca> (not trained)
values: <rank.=3>
Input channels <name [train type, predict type]>:
  input [Task,Task]
Output channels <name [train type, predict type]>:
  output [Task,Task]
```

6.8.3. PipeOp Channels

6.8.3.1. Input Channels

Just like functions, PipeOps can take multiple inputs. These multiple inputs are always given as elements in the input list. For example, there is a PipeOpFeatureUnion that combines multiple tasks with different features and "cbind()s" them together, creating one combined task. When two halves of the iris task are given, for example, it recreates the original task:

```
iris_first_half = task$clone()$select(c("Petal.Length", "Petal.Width"))
iris_second_half = task$clone()$select(c("Sepal.Length", "Sepal.Width"))

pofu = po("featureunion", innum = 2)

pofu$train(list(iris_first_half, iris_second_half))[[1]]$data()
```

```
        Species Petal.Length Petal.Width Sepal.Length Sepal.Width
  1:     setosa          1.4         0.2          5.1         3.5
  2:     setosa          1.4         0.2          4.9         3.0
  3:     setosa          1.3         0.2          4.7         3.2
  4:     setosa          1.5         0.2          4.6         3.1
  5:     setosa          1.4         0.2          5.0         3.6
 ---
146: virginica          5.2         2.3          6.7         3.0
147: virginica          5.0         1.9          6.3         2.5
148: virginica          5.2         2.0          6.5         3.0
149: virginica          5.4         2.3          6.2         3.4
150: virginica          5.1         1.8          5.9         3.0
```

Because PipeOpFeatureUnion effectively takes two input arguments here, we can say it has two **input channels**. An input channel also carries information about the *type* of input that is acceptable. The input channels of the pofu object constructed above, for example, each accept a Task during training and prediction. This information can be queried from the $input slot:

```
pofu$input
```

```
     name train predict
1: input1  Task    Task
2: input2  Task    Task
```

Other PipeOps may have channels that take different types during different phases. The backuplearner PipeOp, for example, takes a NULL and a Task during training, and a Prediction and a Task during prediction:

```
# TODO this is an important case to handle here, do not delete unless there is a better exam
# po("backuplearner")$input
```

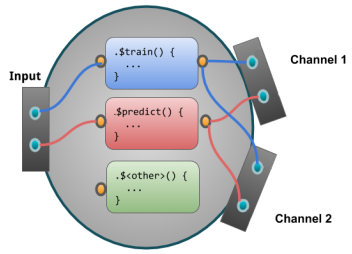
6.8.3.2. Output Channels

Unlike the typical notion of a function, PipeOps can also have multiple **output channels**. `$train()` and `$predict()` always return a list, so certain PipeOps may return lists with more than one element. Similar to input channels, the information about the number and type of outputs given by a PipeOp is available in the `$output` slot. The `chunk` PipeOp, for example, chunks a given Task into subsets and consequently returns multiple Task objects, both during training and prediction. The number of output channels must be given during construction through the `outnum` argument.

```
po("chunk", outnum = 3)$output
```

```
      name train predict
1: output1  Task    Task
2: output2  Task    Task
3: output3  Task    Task
```

Note that the number of output channels during training and prediction is the same. A schema of a PipeOp with two output channels:



6.8.3.3. Channel Configuration

Most PipeOps have only one input channel (so they take a list with a single element), but there are a few with more than one; In many cases, the number of input or output channels is determined during construction, e.g. through the `innum` / `outnum` arguments. The `input.num` and `output.num` columns of the `mlr_pipeops`-table above show the default number of channels, and `NA` if the number depends on a construction argument.

The default printer of a PipeOp gives information about channel names and types:

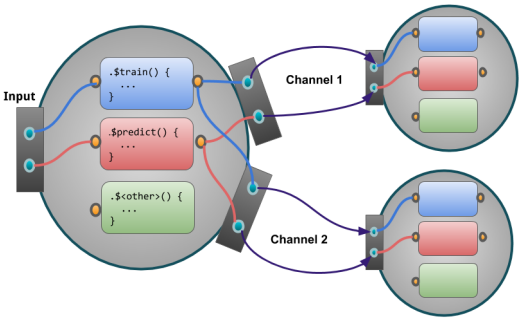
```
# po("backuplearner")
```

6.8.4. Graph: Networks of PipeOps

6.8.4.1. Basics

What is the advantage of this tedious way of declaring input and output channels and handling in/output through lists? Because each PipeOp has a known number of input and output channels that always produce or accept data of a known type, it is possible to network them together in Graphs. A Graph is a collection of PipeOps with "edges" that mandate that data should be flowing along them. Edges always pass between PipeOp *channels*, so it is not only possible to explicitly prescribe which position of an input or output list an edge refers to, it makes it possible to make different components of a PipeOp's output flow to multiple different other PipeOps, as well as to have a PipeOp gather its input from multiple other PipeOps.

A schema of a simple graph of PipeOps:



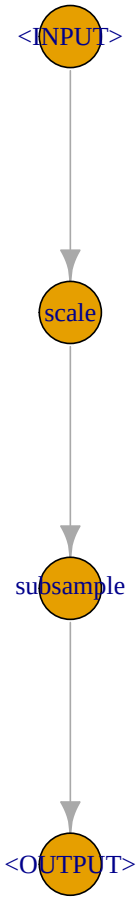
A Graph is empty when first created, and PipeOps can be added using the **$add_pipeop()** method. The **$add_edge()** method is used to create connections between them. While the printer of a Graph gives some information about its layout, the most intuitive way of visualizing it is using the $plot() function.

```
gr = Graph$new()
gr$add_pipeop(po("scale"))
gr$add_pipeop(po("subsample", frac = 0.1))
gr$add_edge("scale", "subsample")
```

```
print(gr)
```

```
Graph with 2 PipeOps:
        ID         State  sccssors prdcssors
     scale <<UNTRAINED>> subsample
 subsample <<UNTRAINED>>               scale
```

```
gr$plot(html = FALSE)
```



A `Graph` itself has a **`$train()`** and a **`$predict()`** method that accept some data and propagate this data through the network of `PipeOp`s. The return value corresponds to the output of the `PipeOp` output channels that are not connected to other `PipeOp`s.

```
gr$train(task)[[1]]$data()
```

```
      Species Petal.Length   Petal.Width Sepal.Length Sepal.Width
1:     setosa  -1.27910398 -1.3110521482  -1.01843718   0.7861738
2:     setosa  -1.22245633 -1.3110521482  -1.25996379   0.7861738
3:     setosa  -1.50569459 -1.4422448248  -1.86378030  -0.1315388
4:     setosa  -1.16580868 -1.3110521482  -0.53538397   0.7861738
```

```
 5:     setosa  -1.44904694 -1.3110521482  -1.01843718   0.3273175
 6:     setosa  -1.39239929 -1.3110521482  -1.74301699  -0.1315388
 7: versicolor   0.42032558  0.3944526477   0.67224905   0.3273175
 8: versicolor  -0.14615094 -0.2615107354  -1.01843718  -2.4258204
 9: versicolor  -0.08950329  0.1320672944  -0.29385737  -0.3609670
10: versicolor   0.42032558  0.3944526477   0.43072244  -1.9669641
11: versicolor   0.42032558  0.3944526477   0.18919584  -0.3609670
12: versicolor   0.36367793  0.0008746178  -0.41462067  -1.0492515
13: versicolor   0.47697323  0.2632599711   0.30995914  -0.1315388
14: versicolor   0.13708732  0.0008746178  -0.05233076  -1.0492515
15:  virginica   1.04344975  1.1816087073   0.67224905  -0.5903951
```

```
gr$predict(single_line_task)[[1]]$data()
```

```
   Species Petal.Length Petal.Width Sepal.Length Sepal.Width
1:  setosa    -1.335752   -1.311052   -0.8976739    1.015602
```

The collection of PipeOps inside a Graph can be accessed through the **$pipeops** slot. The set of edges in the Graph can be inspected through the **$edges** slot. It is possible to modify individual PipeOps and edges in a Graph through these slots, but this is not recommended because no error checking is performed and it may put the Graph in an unsupported state.

6.8.4.2. Networks

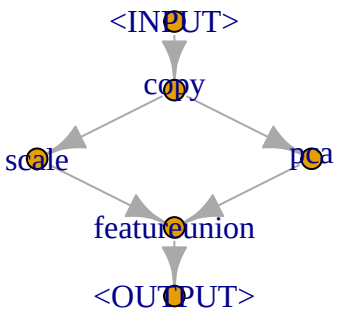
The example above showed a linear preprocessing pipeline, but it is in fact possible to build true "graphs" of operations, as long as no loops are introduced[1]. PipeOps with multiple output channels can feed their data to multiple different subsequent PipeOps, and PipeOps with multiple input channels can take results from different PipeOps. When a PipeOp has more than one input / output channel, then the Graph's `$add_edge()` method needs an additional argument that indicates which channel to connect to. This argument can be given in the form of an integer, or as the name of the channel.

The following constructs a Graph that copies the input and gives one copy each to a "scale" and a "pca" PipeOp. The resulting columns of each operation are put next to each other by "feature-union".

```
gr = Graph$new()$
  add_pipeop(po("copy", outnum = 2))$
  add_pipeop(po("scale"))$
  add_pipeop(po("pca"))$
  add_pipeop(po("featureunion", innum = 2))

gr$
```

[1] It is tempting to denote this as a "directed acyclic graph", but this would not be entirely correct because edges run between channels of PipeOps, not PipeOps themselves.

```
  add_edge("copy", "scale", src_channel = 1)$        # designating channel by index
  add_edge("copy", "pca", src_channel = "output2")$  # designating channel by name
  add_edge("scale", "featureunion", dst_channel = 1)$
  add_edge("pca", "featureunion", dst_channel = 2)

gr$plot(html = FALSE)
```



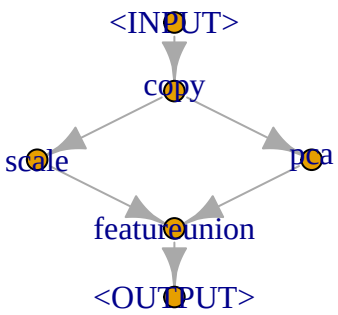

```
gr$train(iris_first_half)[[1]]$data()
```

```
      Species Petal.Length Petal.Width       PC1          PC2
  1:    setosa   -1.3357516  -1.3110521 -2.561012 -0.006922191
  2:    setosa   -1.3357516  -1.3110521 -2.561012 -0.006922191
  3:    setosa   -1.3923993  -1.3110521 -2.653190  0.031849692
  4:    setosa   -1.2791040  -1.3110521 -2.468834 -0.045694073
  5:    setosa   -1.3357516  -1.3110521 -2.561012 -0.006922191
 ---
146: virginica    0.8168591   1.4439941  1.755953  0.455479438
147: virginica    0.7035638   0.9192234  1.416510  0.164312126
148: virginica    0.8168591   1.0504160  1.639637  0.178946130
149: virginica    0.9301544   1.4439941  1.940308  0.377935674
150: virginica    0.7602115   0.7880307  1.469915  0.033362474
```

6.8.4.3. Syntactic Sugar

Although it is possible to create intricate `Graph`s with edges going all over the place (as long as no loops are introduced), there is usually a clear direction of flow between "layers" in the `Graph`. It is therefore convenient to build up a `Graph` from layers, which can be done using the **`%>>%`** ("double-arrow") operator. It takes either a `PipeOp` or a `Graph` on each of its sides and connects all of the outputs of its left-hand side to one of the inputs each of its right-hand side–the number of inputs therefore must match the number of outputs. Together with the `gunion()` operation, which takes `PipeOp`s or `Graph`s and arranges them next to each other akin to a (disjoint) graph union, the above network can more easily be constructed as follows:

```
gr = po("copy", outnum = 2) %>>%
  gunion(list(po("scale"), po("pca"))) %>>%
  po("featureunion", innum = 2)

gr$plot(html = FALSE)
```



6.8.4.4. `PipeOp` IDs and ID Name Clashes

`PipeOp`s within a graph are addressed by their **`$id`**-slot. It is therefore necessary for all `PipeOp`s within a `Graph` to have a unique `$id`. The `$id` can be set during or after construction, but it should not directly be changed after a `PipeOp` was inserted in a `Graph`. At that point, the **`$set_names()`**-method can be used to change `PipeOp` ids.

```
po1 = po("scale")
po2 = po("scale")
```

```
po1 %>>% po2 # name clash
```

```
Error in gunion(list(g1, g2), in_place = c(TRUE, TRUE)): Assertion on 'ids of pipe operators o
```

```
po2$id = "scale2"
gr = po1 %>>% po2
gr
```

```
Graph with 2 PipeOps:
     ID         State sccssors prdcssors
  scale <<UNTRAINED>>   scale2
 scale2 <<UNTRAINED>>              scale
```

```
# Alternative ways of getting new ids:
po("scale", id = "scale2")
```

```
PipeOp: <scale2> (not trained)
values: <robust=FALSE>
Input channels <name [train type, predict type]>:
  input [Task,Task]
Output channels <name [train type, predict type]>:
  output [Task,Task]
```

```
# sometimes names of PipeOps within a Graph need to be changed
gr2 = po("scale") %>>% po("pca")
gr %>>% gr2
```

```
Error in gunion(list(g1, g2), in_place = c(TRUE, TRUE)): Assertion on 'ids of pipe operators o
```

```
gr2$set_names("scale", "scale3")
gr %>>% gr2
```

```
Graph with 4 PipeOps:
     ID         State sccssors prdcssors
  scale <<UNTRAINED>>   scale2
 scale2 <<UNTRAINED>>   scale3     scale
 scale3 <<UNTRAINED>>      pca    scale2
    pca <<UNTRAINED>>             scale3
```

6.8.5. Learners in Graphs, Graphs in Learners

The true power of mlr3pipelines derives from the fact that it can be integrated seamlessly with mlr3. Two components are mainly responsible for this:

- PipeOpLearner, a PipeOp that encapsulates a mlr3 Learner and creates a PredictionData object in its $predict() phase
- GraphLearner, a mlr3 Learner that can be used in place of any other mlr3 Learner, but which does prediction using a Graph given to it

Note that these are dual to each other: One takes a Learner and produces a PipeOp (and by extension a Graph); the other takes a Graph and produces a Learner.

6.8.5.1. PipeOpLearner

The PipeOpLearner is constructed using a mlr3 Learner and will use it to create PredictionData in the $predict() phase. The output during $train() is NULL. It can be used after a preprocessing pipeline, and it is even possible to perform operations on the PredictionData, for example by averaging multiple predictions or by using the PipeOpBackupLearner" operator to impute predictions that a given model failed to create.

The following is a very simple Graph that performs training and prediction on data after performing principal component analysis.

```
gr = po("pca") %>>% po("learner",
  lrn("classif.rpart"))
```

```
gr$train(task)
```

```
$classif.rpart.output
NULL
```

```
gr$predict(task)
```

```
$classif.rpart.output
<PredictionClassif> for 150 observations:
    row_ids     truth  response
          1    setosa    setosa
          2    setosa    setosa
          3    setosa    setosa
---
        148 virginica virginica
        149 virginica virginica
        150 virginica virginica
```

6.8.5.2. GraphLearner

Although a Graph has `$train()` and `$predict()` functions, it can not be used directly in places where mlr3 `Learners` can be used like resampling or benchmarks. For this, it needs to be wrapped in a GraphLearner object, which is a thin wrapper that enables this functionality. The resulting Learner is extremely versatile, because every part of it can be modified, replaced, parameterized and optimized over. Resampling the graph above can be done the same way that resampling of the Learner was performed in the introductory example.

```
lrngrph = as_learner(gr)
resample(task, lrngrph, rsmp)
```

```
<ResampleResult> of 1 iterations
* Task: iris
* Learner: pca.classif.rpart
* Warnings: 0 in 0 iterations
* Errors: 0 in 0 iterations
```

6.8.6. Hyperparameters

mlr3pipelines relies on the paradox package to provide parameters that can modify each PipeOp's behavior. paradox parameters provide information about the parameters that can be changed, as well as their types and ranges. They provide a unified interface for benchmarks and parameter optimization ("tuning"). For a deep dive into paradox, see the tuning chapter or Section 9.4.

The ParamSet, representing the space of possible parameter configurations of a PipeOp, can be inspected by accessing the **`$param_set`** slot of a PipeOp or a Graph.

```
op_pca = po("pca")
op_pca$param_set
```

```
<ParamSet:pca>
               id    class lower upper nlevels       default value
1:         center ParamLgl    NA    NA       2          TRUE
2:         scale. ParamLgl    NA    NA       2         FALSE
3:          rank. ParamInt     1   Inf     Inf
4: affect_columns ParamUty    NA    NA     Inf <Selector[1]>
```

To set or retrieve a parameter, the **`$param_set$values`** slot can be accessed. Alternatively, the `param_vals` value can be given during construction.

```
op_pca$param_set$values$center = FALSE
op_pca$param_set$values
```

```
$center
[1] FALSE
```

```
op_pca = po("pca", center = TRUE)
op_pca$param_set$values
```

```
$center
[1] TRUE
```

Each PipeOp can bring its own individual parameters which are collected together in the Graph's $param_set. A PipeOp's parameter names are prefixed with its $id to prevent parameter name clashes.

```
gr = op_pca %>>% po("scale")
gr$param_set
```

```
<ParamSetCollection>
                     id    class lower upper nlevels        default value
1:           pca.center ParamLgl    NA    NA       2           TRUE  TRUE
2:           pca.scale. ParamLgl    NA    NA       2          FALSE
3:            pca.rank. ParamInt     1   Inf     Inf
4:   pca.affect_columns ParamUty    NA    NA     Inf  <Selector[1]>
5:         scale.center ParamLgl    NA    NA       2           TRUE
6:          scale.scale ParamLgl    NA    NA       2           TRUE
7:         scale.robust ParamLgl    NA    NA       2 <NoDefault[3]> FALSE
8: scale.affect_columns ParamUty    NA    NA     Inf  <Selector[1]>
```

```
gr$param_set$values
```

```
$pca.center
[1] TRUE

$scale.robust
[1] FALSE
```

Both PipeOpLearner and GraphLearner preserve parameters of the objects they encapsulate.

```
op_rpart = po("learner", lrn("classif.rpart"))
op_rpart$param_set
```

```
<ParamSet:classif.rpart>
                id    class lower upper nlevels        default value
 1:             cp ParamDbl     0     1     Inf           0.01
 2:     keep_model ParamLgl    NA    NA       2          FALSE
 3:     maxcompete ParamInt     0   Inf     Inf              4
 4:       maxdepth ParamInt     1    30      30             30
 5:   maxsurrogate ParamInt     0   Inf     Inf              5
 6:      minbucket ParamInt     1   Inf     Inf <NoDefault[3]>
 7:       minsplit ParamInt     1   Inf     Inf             20
 8: surrogatestyle ParamInt     0     1       2              0
 9:   usesurrogate ParamInt     0     2       3              2
10:           xval ParamInt     0   Inf     Inf             10     0
```

```
glrn = as_learner(gr %>>% op_rpart)
glrn$param_set
```

```
<ParamSetCollection>
                             id    class lower upper nlevels        default
 1:                  pca.center ParamLgl    NA    NA       2           TRUE
 2:                  pca.scale. ParamLgl    NA    NA       2          FALSE
 3:                   pca.rank. ParamInt     1   Inf     Inf
 4:           pca.affect_columns ParamUty    NA    NA     Inf  <Selector[1]>
 5:                scale.center ParamLgl    NA    NA       2           TRUE
 6:                 scale.scale ParamLgl    NA    NA       2           TRUE
 7:                scale.robust ParamLgl    NA    NA       2 <NoDefault[3]>
 8:         scale.affect_columns ParamUty    NA    NA     Inf  <Selector[1]>
 9:             classif.rpart.cp ParamDbl     0     1     Inf           0.01
10:     classif.rpart.keep_model ParamLgl    NA    NA       2          FALSE
11:     classif.rpart.maxcompete ParamInt     0   Inf     Inf              4
12:       classif.rpart.maxdepth ParamInt     1    30      30             30
13:   classif.rpart.maxsurrogate ParamInt     0   Inf     Inf              5
14:      classif.rpart.minbucket ParamInt     1   Inf     Inf <NoDefault[3]>
15:       classif.rpart.minsplit ParamInt     1   Inf     Inf             20
16: classif.rpart.surrogatestyle ParamInt     0     1       2              0
17:   classif.rpart.usesurrogate ParamInt     0     2       3              2
18:           classif.rpart.xval ParamInt     0   Inf     Inf             10
1 variable not shown: [value]
```

7. Preprocessing

TODO (150-200 WORDS)

8. Special Tasks

TODO (150-200 WORDS)

This chapter explores the different functions of `mlr3` when dealing with specific data sets that require further statistical modification to undertake sensible analysis. Following topics are discussed:

Survival Analysis

This sub-chapter explains how to conduct sound survival analysis in mlr3. Survival analysis is used to monitor the period of time until a specific event takes places. This specific event could be, e.g., death, the transmission of a disease, marriage, or divorce. Two considerations are important when conducting survival analysis:

- Whether the event occurred within the frame of the given data
- How much time it took until the event occurred

In summary, this sub-chapter explains how to account for these considerations and conduct survival analysis using the `mlr3proba` extension package.

Density Estimation

This sub-chapter explains how to conduct (unconditional) density estimation in mlr3. Density estimation is used to estimate the probability density function of a continuous variable. Unconditional density estimation is an unsupervised task, so there is no 'value' to predict. Instead, densities are *estimated*.

This sub-chapter explains how to estimate probability distributions for continuous variables using the `mlr3proba` extension package.

Spatiotemporal Analysis

Spatiotemporal analysis data observations entail reference information about spatial and temporal characteristics. One of the largest issues of spatiotemporal data analysis is the inevitable presence of auto-correlation in the data. Auto-correlation is especially severe in data with a marginal spatiotemporal variation. The sub-chapter on Spatiotemporal analysis provides instructions on how to account for spatiotemporal data.

Multilabel Classification

Multilabel classification deals with objects that can belong to more than one category at the same time. Numerous target labels are attributed to a single observation. Working with multilabel data requires one to use modified algorithms, to accommodate data specific characteristics. Two approaches to multilabel classification are prominently used:

- The problem transformation method
- The algorithm adaption method

Instructions on how to deal with multilabel classification in `mlr3` can be found in this sub-chapter.

Cost Sensitive Classification

This sub-chapter deals with the implementation of cost-sensitive classification. Regular classification aims to minimize the misclassification rate and thus all types of misclassification errors are deemed equally severe. Cost-sensitive classification is a setting where the costs caused by different kinds of errors are not assumed to be equal. The objective is to minimize the expected costs.

Analytical data for a big credit institution is used as a use case to illustrate the different features. Firstly, the sub-chapter provides guidance on how to implement a first model. Subsequently, the sub-chapter contains instructions on how to modify cost sensitivity measures, thresholding and threshold tuning.

Cluster Analysis

Cluster analysis aims to group data into clusters such that objects that are similar end up in the same cluster. Fundamentally, clustering and classification are similar. However, clustering is an unsupervised task because observations do not contain true labels while in classification, labels are needed in order to train a model.

This sub-chapter explains how to perform cluster analysis in `mlr3` with the help of `mlr3cluster` extension package.

Coming soon

In development we are also working on

- Multilabel classification - `mlr3multioutput`
- Functional data analysis - `mlr3fda`
- Ordinal analysis - `mlr3ordinal`
- Time-series analysis / forecasting - `mlr3temporal`

Send us a message if you want to help out on any of these!

8.1. Survival Analysis

> **Warning**
>
> Survival analysis with {mlr3proba} is currently in a fragile state after its removal from CRAN. Hence most code examples listed in this page will not work for the time being. We are actively working on a solution!

Survival analysis is a sub-field of supervised machine learning in which the aim is to predict the survival distribution of a given individual. Arguably the main feature of survival analysis is that, unlike classification and regression, learners are trained on two features:

1. the time until the event takes place

2. the event type: either censoring or death.

At a particular time-point, an individual is either: alive, dead, or censored. Censoring occurs if it is unknown if an individual is alive or dead. For example, say we are interested in patients in hospital and every day it is recorded if they are alive or dead, then after a patient leaves, it is unknown if they are alive or dead. Hence they are censored. If there was no censoring, then ordinary regression analysis could be used instead. Furthermore, survival data contains solely positive values and therefore needs to be transformed to avoid biases.

Note that survival analysis accounts for both censored and uncensored observations while adjusting respective model parameters.

The package `mlr3proba` (Sonabend et al. 2021) extends `mlr3` with the following objects for survival analysis:

- `TaskSurv` to define (censored) survival tasks
- `LearnerSurv` as base class for survival learners
- `PredictionSurv` as specialized class for `Prediction` objects
- `MeasureSurv` as specialized class for performance measures

For a good introduction to survival analysis see *Modelling Survival Data in Medical Research* (Collett 2014).

8.1.1. TaskSurv

Unlike `TaskClassif` and `TaskRegr` which have a single 'target' argument, `TaskSurv` mimics the `survival::Surv` object and has three to four target arguments (dependent on censoring type). A `TaskSurv` can be constructed with the function `as_task_surv()`:

```
library("mlr3")
library("mlr3proba")
library("survival")

as_task_surv(survival::bladder2[, -1L], id = "interval_censored",
  time = "start", event = "event", time2 = "stop", type = "interval")

# type = "right" is default
task = as_task_surv(survival::rats, id = "right_censored",
  time = "time", event = "status", type = "right")

print(task)

# the target column is a survival object:
head(task$truth())

# kaplan-meier plot
# library("mlr3viz")
autoplot(task)
```

8.1.2. Predict Types - crank, lp, and distr

Every PredictionSurv object can predict one or more of:

- `lp` - Linear predictor calculated as the fitted coefficients multiplied by the test data.
- `distr` - Predicted survival distribution, either discrete or continuous. Implemented in distr6.
- `crank` - Continuous risk ranking.
- `response` - Predicted survival time.

`lp` and `crank` can be used with measures of discrimination such as the concordance index. Whilst `lp` is a specific mathematical prediction, `crank` is any continuous ranking that identifies who is more or less likely to experience the event. So far the only implemented learner that only returns a continuous ranking is `surv.svm`. If a PredictionSurv returns an `lp` then the `crank` is identical to this. Otherwise `crank` is calculated as the expectation of the predicted survival distribution. Note that for linear proportional hazards models, the ranking (but not necessarily the `crank` score itself) given by `lp` and the expectation of `distr`, is identical.

The example below uses the `rats` task shipped with mlr3proba.

```
task = tsk("rats")
learn = lrn("surv.coxph")

train_set = sample(task$nrow, 0.8 * task$nrow)
test_set = setdiff(seq_len(task$nrow), train_set)

learn$train(task, row_ids = train_set)
prediction = learn$predict(task, row_ids = test_set)

print(prediction)
```

```
<PredictionSurv> for 60 observations:
    row_ids time status      crank         lp     distr
          2   49   TRUE -0.5038971 -0.5038971 <list[1]>
          3  104  FALSE -0.5038971 -0.5038971 <list[1]>
         12  102  FALSE -3.4446695 -3.4446695 <list[1]>
---
        281   89  FALSE -2.5217340 -2.5217340 <list[1]>
        295  104  FALSE  1.3955682  1.3955682 <list[1]>
        300  102  FALSE -2.4602050 -2.4602050 <list[1]>
```

8.1.3. Composition

Finally we take a look at the PipeOps implemented in mlr3proba, which are used for composition of predict types. For example, a predict linear predictor does not have a lot of meaning by itself, but it can be composed into a survival distribution. See mlr3pipelines for full tutorials and details on PipeOps.

```r
library("mlr3pipelines")
library("mlr3learners")
# PipeOpDistrCompositor - Train one model with a baseline distribution,
# (Kaplan-Meier or Nelson-Aalen), and another with a predicted linear predictor.
task = tsk("rats")
# remove the factor column for support with glmnet
task$select(c("litter", "rx"))
learner_lp = lrn("surv.glmnet")
learner_distr = lrn("surv.kaplan")
prediction_lp = learner_lp$train(task)$predict(task)
prediction_distr = learner_distr$train(task)$predict(task)
prediction_lp$distr

# Doesn't need training. Base = baseline distribution. ph = Proportional hazards.

pod = po("compose_distr", form = "ph", overwrite = FALSE)
prediction = pod$predict(list(base = prediction_distr, pred = prediction_lp))$output

# Now we have a predicted distr!

prediction$distr

# This can all be simplified by using the distrcompose pipeline

glm.distr = ppl("distrcompositor", learner = lrn("surv.glmnet"),
  estimator = "kaplan", form = "ph", overwrite = FALSE, graph_learner = TRUE)
glm.distr$train(task)$predict(task)
```

8.1.4. Benchmark Experiment

Finally, we conduct a small benchmark study on the `rats` task using some of the integrated survival learners:

```r
library("mlr3learners")

task = tsk("rats")

# some integrated learners
learners = lrns(c("surv.coxph", "surv.kaplan", "surv.ranger"))
print(learners)
```

```
$surv.coxph
<LearnerSurvCoxPH:surv.coxph>: Cox Proportional Hazards
* Model: -
* Parameters: list()
```

```
* Packages: mlr3, mlr3proba, survival, distr6
* Predict Types:  crank, [distr], lp
* Feature Types: logical, integer, numeric, factor
* Properties: weights

$surv.kaplan
<LearnerSurvKaplan:surv.kaplan>: Kaplan-Meier Estimator
* Model: -
* Parameters: list()
* Packages: mlr3, mlr3proba, survival, distr6
* Predict Types:  [crank], distr
* Feature Types: logical, integer, numeric, character, factor, ordered
* Properties: missings

$surv.ranger
<LearnerSurvRanger:surv.ranger>: Random Forest
* Model: -
* Parameters: num.threads=1
* Packages: mlr3, mlr3proba, mlr3extralearners, ranger
* Predict Types:  crank, [distr]
* Feature Types: logical, integer, numeric, character, factor, ordered
* Properties: importance, oob_error, weights
```

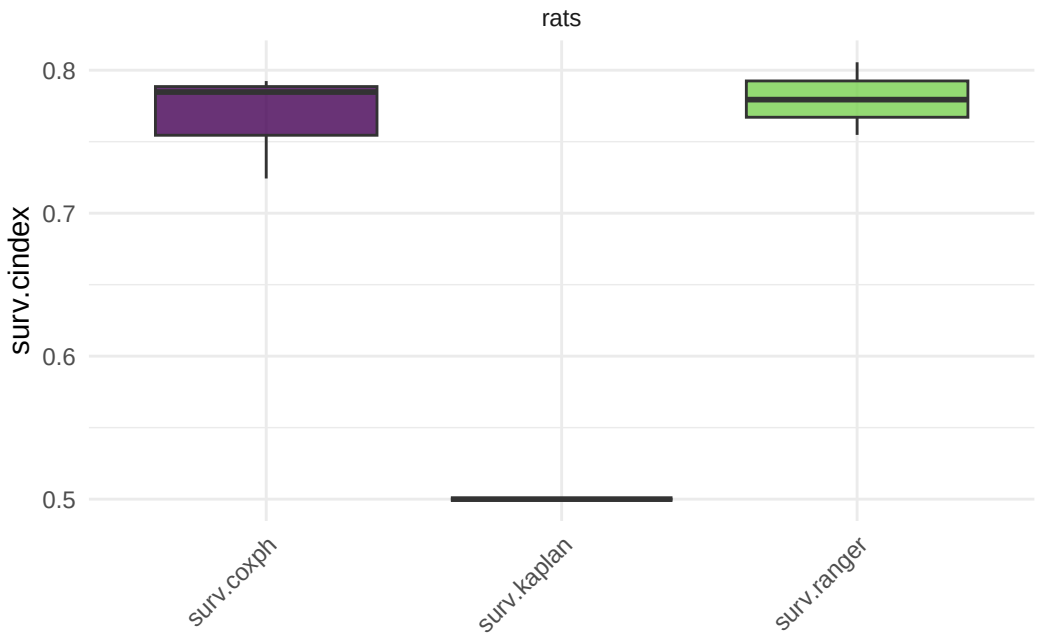
```
# Harrell's C-Index for survival
measure = msr("surv.cindex")
print(measure)
```

```
<MeasureSurvCindex:surv.cindex>
* Packages: mlr3, mlr3proba
* Range: [0, 1]
* Minimize: FALSE
* Average: macro
* Parameters: weight_meth=I, tiex=0.5, eps=0.001
* Properties: -
* Predict type: crank
* Return type: Score
```

```
set.seed(1)
bmr = benchmark(benchmark_grid(task, learners, rsmp("cv", folds = 3)))
bmr$aggregate(measure)
```

```
   nr      resample_result task_id  learner_id resampling_id iters surv.cindex
1:  1 <ResampleResult[21]>    rats  surv.coxph            cv     3   0.7671307
2:  2 <ResampleResult[21]>    rats surv.kaplan            cv     3   0.5000000
3:  3 <ResampleResult[21]>    rats surv.ranger            cv     3   0.7799153
```

```
autoplot(bmr, measure = measure)
```



The experiment indicates that both the Cox PH and the random forest have better discrimination than the Kaplan-Meier baseline estimator, but that the machine learning random forest is not consistently better than the interpretable Cox PH.

8.2. Density Estimation

> **Warning**
>
> Survival analysis with {mlr3proba} is currently in a fragile state after its removal from CRAN. Hence most code examples listed in this page will not work for the time being. We are actively working on a solution!

Density estimation is the learning task to find the unknown distribution from which an i.i.d. data set is generated. We interpret this broadly, with this distribution not necessarily being continuous (so may possess a mass not density). The conditional case, where a distribution is predicted conditional on covariates, is known as 'probabilistic supervised regression', and will be implemented in `mlr3proba` in the near-future. Unconditional density estimation is viewed as an unsupervised task. For a good overview to density estimation see *Density estimation for statistics and data analysis* (Silverman 1986).

The package `mlr3proba` extends `mlr3` with the following objects for density estimation:

- `TaskDens` to define density tasks
- `LearnerDens` as base class for density estimators

- PredictionDens as specialized class for Prediction objects
- MeasureDens as specialized class for performance measures

In this example we demonstrate the basic functionality of the package on the faithful data from the datasets package. This task ships as pre-defined TaskDens with mlr3proba.

```
library("mlr3")
library("mlr3proba")

task = tsk("precip")
print(task)
```

```
<TaskDens:precip> (70 x 1): Annual Precipitation
* Target: -
* Properties: -
* Features (1):
  - dbl (1): precip
```

```
# histogram and density plot
library("mlr3viz")
# FIXME
# autoplot(task, type = "overlay")
```

Unconditional density estimation is an unsupervised method. Hence, TaskDens is an unsupervised task which inherits directly from Task unlike TaskClassif and TaskRegr. However, TaskDens still has a `target` argument and a `$truth` field defined by:

- `target` - the name of the variable in the data for which to estimate density
- `$truth` - the values of the `target` column (which is *not* the true density, which is always unknown)

8.2.1. Train and Predict

Density learners have `train` and `predict` methods, though being unsupervised, 'prediction' is actually 'estimation'. In training, a distr6 object is created, see here for full tutorials on how to access the probability density function, `pdf`, cumulative distribution function, `cdf`, and other important fields and methods. The predict method is simply a wrapper around `self$model$pdf` and if available `self$model$cdf`, i.e. evaluates the pdf/cdf at given points. Note that in prediction the points to evaluate the pdf and cdf are determined by the `target` column in the TaskDens object used for testing.

```
# create task and learner

task_faithful = TaskDens$new(id = "eruptions", backend = datasets::faithful$eruptions)
learner = lrn("dens.hist")

```

```r
# train/test split
train_set = sample(task_faithful$nrow, 0.8 * task_faithful$nrow)
test_set = setdiff(seq_len(task_faithful$nrow), train_set)

# fitting KDE and model inspection
learner$train(task_faithful, row_ids = train_set)
learner$model
```

```
$distr
Histogram()

$hist
$breaks
[1] 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0 5.5

$counts
[1] 39 30  5  4 25 62 49  3

$density
[1] 0.35944700 0.27649770 0.04608295 0.03686636 0.23041475 0.57142857 0.45161290
[8] 0.02764977

$mids
[1] 1.75 2.25 2.75 3.25 3.75 4.25 4.75 5.25

$xname
[1] "dat"

$equidist
[1] TRUE

attr(,"class")
[1] "histogram"

attr(,"class")
[1] "dens.hist"
```

```r
class(learner$model)
```

```
[1] "dens.hist"
```

```r
# make predictions for new data
prediction = learner$predict(task_faithful, row_ids = test_set)
```

Every `PredictionDens` object can estimate:

- `pdf` - probability density function

Some learners can estimate:

- `cdf` - cumulative distribution function

8.2.2. Benchmark Experiment

Finally, we conduct a small benchmark study on the `precip` task using some of the integrated survival learners:

```
# some integrated learners
learners = lrns(c("dens.hist", "dens.kde"))
print(learners)
```

```
$dens.hist
<LearnerDensHistogram:dens.hist>: Histogram Density Estimator
* Model: -
* Parameters: list()
* Packages: mlr3, mlr3proba, distr6
* Predict Types:  [pdf], cdf, distr
* Feature Types: integer, numeric
* Properties: -

$dens.kde
<LearnerDensKDE:dens.kde>: Kernel Density Estimator
* Model: -
* Parameters: kernel=Epan, bandwidth=silver
* Packages: mlr3, mlr3proba, distr6
* Predict Types:  [pdf], distr
* Feature Types: integer, numeric
* Properties: missings
```

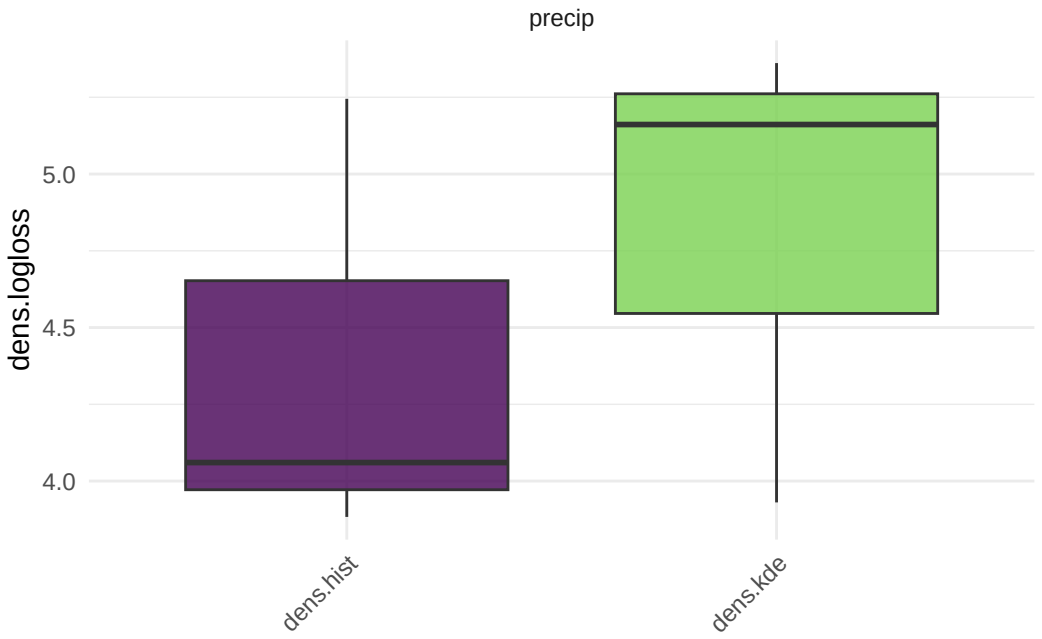
```
# Logloss for probabilistic predictions
measure = msr("dens.logloss")
print(measure)
```

```
<MeasureDensLogloss:dens.logloss>: Log Loss
* Packages: mlr3, mlr3proba
* Range: [0, Inf]
* Minimize: TRUE
* Average: macro
* Parameters: eps=1e-15
* Properties: -
* Predict type: pdf
```

```
set.seed(1)
bmr = benchmark(benchmark_grid(task, learners, rsmp("cv", folds = 3)))
bmr$aggregate(measure)
```

```
   nr      resample_result task_id learner_id resampling_id iters dens.logloss
1:  1 <ResampleResult[21]>  precip  dens.hist            cv     3     4.396138
2:  2 <ResampleResult[21]>  precip   dens.kde            cv     3     4.817715
```

```
autoplot(bmr, measure = measure)
```



The results of this experiment show that the sophisticated Penalized Density Estimator does not outperform the baseline histogram, but that the Kernel Density Estimator has at least consistently better (i.e. lower logloss) results.

8.3. Spatiotemporal Analysis

Data observations may entail reference information about spatial or temporal characteristics. Spatial information is stored as coordinates, usually named "x" and "y" or "lat"/"lon". Treating spatiotemporal data using non-spatial data methods can lead to over-optimistic performance estimates. Hence, methods specifically designed to account for the special nature of spatiotemporal data are needed.

In the `mlr3` framework, the following packages relate to this field:

- `mlr3spatiotempcv` (biased-reduced performance estimation)

- mlr3spatial (spatial prediction support)

The following (sub-)sections introduce the potential pitfalls of spatiotemporal data in machine learning and how to account for it. Note that not all functionality will be covered, and that some of the used packages are still in early lifecycles. If you want to contribute to one of the packages mentioned above, please contact Patrick Schratz.

8.3.1. Creating a spatial Task

To make use of spatial resampling methods, a {mlr3} task that is aware of its spatial characteristic needs to be created. Two `Task` child classes exist in {mlr3spatiotempcv} for this purpose:

- `TaskClassifST`
- `TaskRegrST`

To create one of these, you have multiple options:

1. Use the constructor of the `Task` directly via `$new()` - this only works for data.table backends (!)
2. Use the `as_task_*` converters (e.g. if your data is stored in an `sf` object)

We recommend the latter, as the `as_task_*` converters aim to make task construction easier, e.g., by creating the `DataBackend` (which is required to create a Task in {mlr3}) automatically and setting the `crs` and `coordinate_names` fields. Let's assume your (point) data is stored in with an `sf` object, which is a common scenario for spatial analysis in R.

```
# create 'sf' object
data_sf = sf::st_as_sf(ecuador, coords = c("x", "y"), crs = 32717)

# create `TaskClassifST` from `sf` object
task = as_task_classif_st(data_sf, id = "ecuador_task", target = "slides", positive = "TRUE"
```

You can also use a plain `data.frame`. In this case, `crs` and `coordinate_names` need to be passed along explicitly as they cannot be inferred directly from the `sf` object:

```
task = as_task_classif_st(ecuador, id = "ecuador_task", target = "slides",
  positive = "TRUE", coordinate_names = c("x", "y"), crs = 32717)
```

The `*ST` task family prints a subset of the coordinates by default:

```
print(task)
```

```
<TaskClassifST:ecuador_task> (751 x 11)
* Target: slides
* Properties: twoclass
* Features (10):
  - dbl (10): carea, cslope, dem, distdeforest, distroad,
    distslidespast, hcurv, log.carea, slope, vcurv
```

```
* Coordinates:
            x       y
  1: 712882.5 9560002
  2: 715232.5 9559582
  3: 715392.5 9560172
  4: 715042.5 9559312
  5: 715382.5 9560142
 ---
747: 714472.5 9558482
748: 713142.5 9560992
749: 713322.5 9560562
750: 715392.5 9557932
751: 713802.5 9560862
```

All `*ST` tasks can be treated as their super class equivalents `TaskClassif` or `TaskRegr` in subsequent {mlr3} modeling steps.

8.3.2. Autocorrelation

Data which includes spatial or temporal information requires special treatment in machine learning (similar to survival, ordinal and other task types listed in the special tasks chapter). In contrast to non-spatial/non-temporal data, observations inherit a natural grouping, either in space or time or in both space and time (Legendre 1993). This grouping causes observations to be autocorrelated, either in space (spatial autocorrelation (SAC)), time (temporal autocorrelation (TAC)) or both space and time (spatiotemporal autocorrelation (STAC)). For simplicity, the acronym STAC is used as a generic term in the following chapter for all the different characteristics introduced above.

What effects does STAC have in statistical/machine learning?

The overarching problem is that STAC violates the assumption that the observations in the train and test datasets are independent (Hastie, Friedman, and Tibshirani 2001). If this assumption is violated, the reliability of the resulting performance estimates, for example retrieved via cross-validation, is decreased. The magnitude of this decrease is linked to the magnitude of STAC in the dataset, which cannot be determined easily.

One approach to account for the existence of STAC is to use dedicated resampling methods. `mlr3spatiotempcv` provides access to the most frequently used spatiotemporal resampling methods. The following example showcases how a spatial dataset can be used to retrieve a bias-reduced performance estimate of a learner.

The following examples use the `ecuador` dataset created by Jannes Muenchow. It contains information on the occurrence of landslides (binary) in the Andes of Southern Ecuador. The landslides were mapped from aerial photos taken in 2000. The dataset is well suited to serve as an example because it it relatively small and of course due to the spatial nature of the observations. Please refer to Muenchow, Brenning, and Richter (2012) for a detailed description of the dataset.

To account for the spatial autocorrelation probably present in the landslide data, we will make use one of the most used spatial partitioning methods, a cluster-based k-means grouping (Brenning 2012), (`spcv_coords` in `mlr3spatiotempcv`). This method performs a clustering in 2D space which

contrasts with the commonly used random partitioning for non-spatial data. The grouping has the effect that train and test data are more separated in space as they would be by conducting a random partitioning, thereby reducing the effect of STAC.

By contrast, when using the classical random partitioning approach with spatial data, train and test observations would be located side-by-side across the full study area (a visual example is provided further below). This leads to a high similarity between train and test sets, resulting in "better" but biased performance estimates in every fold of a CV compared to the spatial CV approach. However, these low error rates are mainly caused due to the STAC in the observations and the lack of appropriate partitioning methods and not by the power of the fitted model.

8.3.3. Spatiotemporal Cross-Validation and Partitioning

One part of spatiotemporal machine learning is dealing with the spatiotemporal components of the data during performance estimation. Performance is commonly estimated via cross-validation and `mlr3spatiotempcv` provides specialized resamplings methods for spatiotemporal data. The following chapters showcases how these methods can be applied and how they differ compared to non-spatial resampling methods, e.g. random partitioning. In addition, examples which show how resamplings with spatial information can be visualized using `mlr3spatiotempcv`.

Besides performance estimation, prediction on spatiotemporal data is another challenging task. See Section 8.3.6 for more information about how this topic is handled within the mlr3 framework.

8.3.3.1. Spatial CV vs. Non-Spatial CV

In the following a spatial and non-spatial CV will be applied to showcase the mentioned performance differences.

The performance of a simple classification tree (`"classif.rpart"`) is evaluated on a random partitioning (`repeated_cv`) with four folds and two repetitions. The chosen evaluation measure is "classification error" (`"classif.ce"`).

For the spatial example, `repeated_spcv_coords` is chosen whereas `repeated_cv` represents the non-spatial example.

> **Note**
>
> The selection of `repeated_spcv_coords` in this example is arbitrary. For your use case, you might want to use a different spatial partitioning method (but not necessarily!). Have a look at the "Getting Started" vignette of `mlr3spatiotempcv` to see all available methods and choose one which **fits your data and its prediction purpose**.

8.3.3.1.1. Non-Spatial CV

In this example the `ecuador` example task is taken to estimate the performance of an `rpart` learner with fixed parameters on it.

> **Warning**
>
> In practice you usually might want to tune the hyperparameters of the learner in this case and apply a nested CV in which the inner loop is used for hyperparameter tuning.

```
library("mlr3")
library("mlr3spatiotempcv")
set.seed(42)

# be less verbose
lgr::get_logger("bbotk")$set_threshold("warn")
lgr::get_logger("mlr3")$set_threshold("warn")

task = tsk("ecuador")

learner = lrn("classif.rpart", maxdepth = 3, predict_type = "prob")
resampling_nsp = rsmp("repeated_cv", folds = 4, repeats = 2)
rr_nsp = resample(
  task = task, learner = learner,
  resampling = resampling_nsp)

rr_nsp$aggregate(measures = msr("classif.ce"))
```

```
classif.ce
 0.3388575
```

8.3.3.1.2. Spatial CV

```
task = tsk("ecuador")

learner = lrn("classif.rpart", maxdepth = 3, predict_type = "prob")
resampling_sp = rsmp("repeated_spcv_coords", folds = 4, repeats = 2)
rr_sp = resample(
  task = task, learner = learner,
  resampling = resampling_sp)

rr_sp$aggregate(measures = msr("classif.ce"))
```

```
classif.ce
  0.412529
```

Here, the performance of the classification tree learner is around 7 percentage points worse when using Spatial Cross-Validation (SpCV) compared to Non-Spatial Cross-Validation (NSpCV). The resulting difference in performance is variable as it depends on the dataset, the magnitude of STAC

and the learner itself. For algorithms with a higher tendency of overfitting to the training set, the difference between the two methods will be larger.

Now, what does it mean that the performance in the spatial case is worse? Should you ditch SpCV and keep using non-spatial partitioning? The answer is **NO**. The reason why the spatial partitioning scenario results in a lower predictive performance is because throughout the CV the model has been trained on data that is less similar than the test data compared against the non-spatial scenario. Or in other words: in the non-spatial scenario, train and test data are almost identical (due to spatial autocorrelation).

This means that the result from the SpCV setting is more close to the true predictive power of the model - whereas the result from non-spatial CV is overoptimistic and biased.

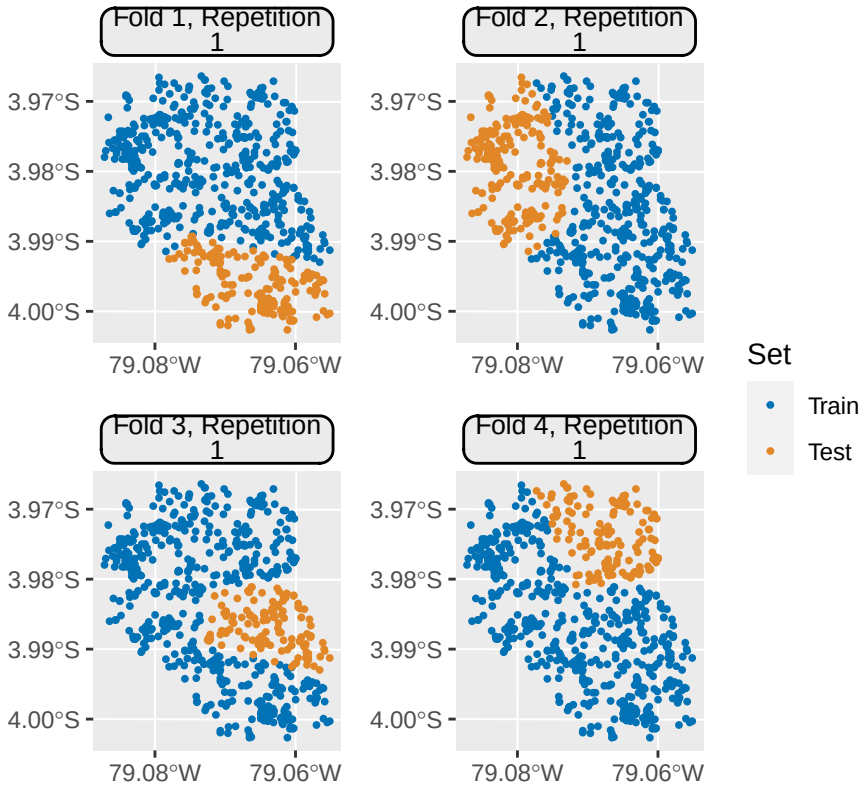
> **Note**
>
> The result of the SpCV setting is by no means the absolute truth - it is also biased, but (most often) less compared to the non-spatial setting.

8.3.4. Visualization of Spatiotemporal Partitions

Every partitioning method in `mlr3spatiotempcv` comes with S3 methods for `plot()` and `autoplot()` to visualize the created groups. In a 2D space `ggplot2` is used in the backgroudn while for spatiotemporal methods 3D visualizations via `plotly` are created.

The following examples shows how the `resampling_sp` object from the previous example can be visualized. In this case I want to look at the first four partitions of the first repetition. The point size is adjusted via argument `size`. After the plot creation, additional `scale_*` calls are used to adjust the coordinate labels on the x and y axes, respectively.

```
autoplot(resampling_sp, task, fold_id = c(1:4), size = 0.7) *
  ggplot2::scale_y_continuous(breaks = seq(-3.97, -4, -0.01)) *
  ggplot2::scale_x_continuous(breaks = seq(-79.06, -79.08, -0.02))
```

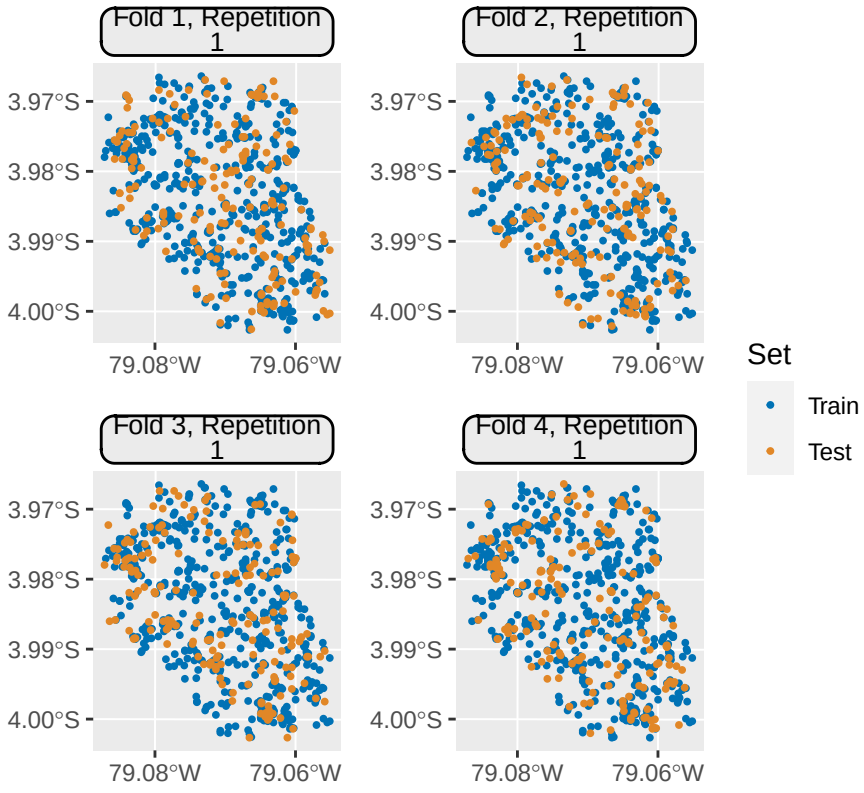


> **Warning**
>
> Note that setting the correct CRS for the given data is important which is done **during task creation**. Spatial offsets of up to multiple meters may occur if the wrong CRS is supplied initially.

This example used a built-in mlr3 task via `tsk()`. In practice however, one needs to create a spatiotemporal task via `TaskClassifST`/`TaskRegrST` and set the `crs` argument (unless a `sf` object is handed over).

`mlr3spatiotempcv` can also visualize non-spatial partitonings. This helps to visually compare differences. Let's use the objects from the previous example again, this time `resampling_nsp`.

```
autoplot(resampling_nsp, task, fold_id = c(1:4), size = 0.7) *
  ggplot2::scale_y_continuous(breaks = seq(-3.97, -4, -0.01)) *
  ggplot2::scale_x_continuous(breaks = seq(-79.06, -79.08, -0.02))
```



The visualization show very well how close train and test observations are located next to each other.

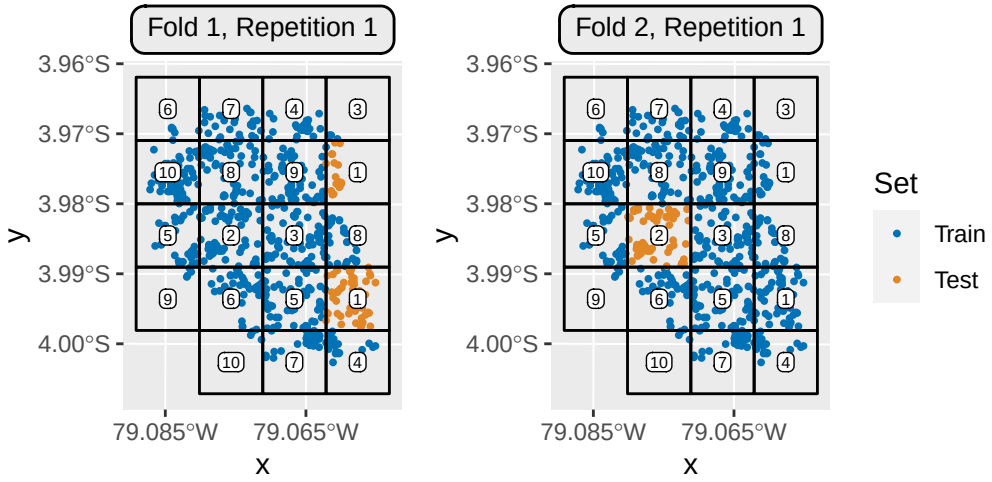
8.3.4.1. Spatial Block Visualization

This examples showcases another SpCV method: `spcv_block`. This method makes use of rectangular blocks to divide the study area into equally-sized parts. {mlr3spatiotempcv} has support for visualizing the created blocks and displaying their respective fold ID to get a better understanding how the final folds were composed out of the partitions. E.g. the "Fold 1 Repetition 1" plot shows that the test set is composed out of two "blocks" with the ID "1" in this case.

> **Note**
>
> The use of `range = 1000L` is arbitrary here and should not be copy-pasted into a real application.

```
task = tsk("ecuador")
resampling = rsmp("spcv_block", range = 1000L)

# Visualize train/test splits of multiple folds
autoplot(resampling, task, size = 0.7,
```

```
    fold_id = c(1, 2), show_blocks = TRUE, show_labels = TRUE) *
    ggplot2::scale_x_continuous(breaks = seq(-79.085, -79.055, 0.02))
```



8.3.4.2. Spatiotemporal Visualization

When going spatiotemporal, two dimensions are not enough anymore. To visualize space and time together, a 3D solution is needed. {mlr3spatiotempcv} makes use of `plotly` for this purpose.

The following examples uses a modified version of the `cookfarm_mlr3` task for showcasing reasons. By adjusting some levels, the individual partitions can be recognized very well.

> **Warning**
>
> In practice, you should not modify your data to achieve "good looking" visualizations as done in this example. This is only done for (visual) demonstration purposes.

In the following we use the `sptcv_cstf` method after Meyer et al. (2018). Only the temporal variable is used in this first example, denoted by setting the column role "time" to variable "Date". This column role is then picked up by the resampling method. Last, `autoplot()` is called with an explicit definition of `plot3D = TRUE`. This is because `sptcv_cstf` can also be visualized in 2D (which only makes sense if the "space" column role is used for partitioning).

Last, `sample_fold_n` is used to take a stratified random sample from all partitions. The call to `plotly::layout()` only adjusts the default viewing angle of the plot - in interactive visualizations, this is not needed and the viewing angle can be adjusted with the mouse.

> **Warning**
>
> This is done to reduce the final plot size and keep things small for demos like this one. We don't recommend doing this in actual studies - unless you prominently communicate this alongside the resulting plot.

```
data = cookfarm_mlr3
set.seed(42)
data$Date = sample(rep(c(
  "2020-01-01", "2020-02-01", "2020-03-01", "2020-04-01",
  "2020-05-01"), times = 1, each = 35768))
task_spt = as_task_regr_st(data,
  id = "cookfarm", target = "PHIHOX",
  coordinate_names = c("x", "y"), coords_as_features = FALSE,
  crs = 26911)
task_spt$set_col_roles("Date", roles = "time")

rsmp_cstf_time = rsmp("sptcv_cstf", folds = 5)

plot = autoplot(rsmp_cstf_time,
  fold_id = 5, task = task_spt, plot3D = TRUE,
  sample_fold_n = 3000L
)
plotly::layout(plot, scene = list(camera = list(eye = list(z = 0.58))))
```

If both space and time are used for partitioning in `sptcv_cstf`, the visualization becomes even more powerful as it allows to also show the observations which are omitted, i.e., not being used in either train and test sets for a specific fold.

```
task_spt$set_col_roles("SOURCEID", roles = "space")
task_spt$set_col_roles("Date", roles = "time")

rsmp_cstf_space_time = rsmp("sptcv_cstf", folds = 5)

plot = autoplot(rsmp_cstf_space_time,
  fold_id = 4, task = task_spt, plot3D = TRUE,
  show_omitted = TRUE, sample_fold_n = 3000L)

plotly::layout(plot, scene = list(camera =
list(eye = list(z = 0.58, x = -1.4, y = 1.6))))
```

Combining multiple spatiotemporal plots with `plotly::layout()` is possible but somewhat cumbersome. First, a list of plots containing the individuals plots must be created. These plots can then be passed to `plotly::subplot()`. This return is then passed to `plotly::layout()`.

```r
pl = autoplot(rsmp_cstf_space_time, task = task_spt,
  fold_id = c(1, 2, 3, 4), point_size = 3,
  axis_label_fontsize = 10, plot3D = TRUE,
  sample_fold_n = 3000L, show_omitted = TRUE
)

# Warnings can be ignored
pl_subplot = plotly::subplot(pl)

plotly::layout(pl_subplot,
  title = "Individual Folds",
  scene = list(
    domain = list(x = c(0, 0.5), y = c(0.5, 1)),
    aspectmode = "cube",
    camera = list(eye = list(z = 0.20, x = -1.4, y = 1.6))
  ),
  scene2 = list(
    domain = list(x = c(0.5, 1), y = c(0.5, 1)),
    aspectmode = "cube",
    camera = list(eye = list(z = 0.1, x = -1.4, y = 1.6))
  ),
  scene3 = list(
    domain = list(x = c(0, 0.5), y = c(0, 0.5)),
    aspectmode = "cube",
    camera = list(eye = list(z = 0.1, x = -1.4, y = 1.6))
  ),
  scene4 = list(
    domain = list(x = c(0.5, 1), y = c(0, 0.5)),
    aspectmode = "cube",
    camera = list(eye = list(z = 0.58, x = -1.4, y = 1.6))
  )
)
```

Unfortunately, titles in subplots cannot be created dynamically. However, there is a manual workaround via annotations show in this RPubs post.

8.3.5. Choosing a Resampling Method

While the example in this section made use of the `spcv_coords` method, this should by no means infer that this method is the best or only method suitable for this task. Even though this method is quite popular, it was mainly chosen because of the clear visual grouping differences when being applied on the `ecuador` task when compared to random partitioning.

In fact, most often multiple spatial partitioning methods can be used for a dataset. It is recommended (required) that users familiarize themselves with each implemented method and decide which method to choose based on the specific characteristics of the dataset. For almost all methods implemented in `mlr3spatiotempcv`, there is a scientific publication describing the strengths and

weaknesses of the respective approach (either linked in the help file of `mlr3spatiotempcv` or its respective dependency packages).

> **Tip**
>
> In the example above, a cross-validation without hyperparameter tuning was shown. If a nested CV is desired, it is recommended to use the same spatial partitioning method for the inner loop (= tuning level). See Schratz et al. (2019) for more details and chapter 11 of Geocomputation with R (Lovelace, Nowosad, and Muenchow 2019).

> **Tip**
>
> A list of all implemented methods in `mlr3spatiotempcv` can be found in the Getting Started vignette of the package.

If you want to learn even more about the field of spatial partitioning, STAC and the problems associated with it, the works of Prof. Hanna Meyer and Prof. Alexander Brenning are very much recommended for further reference.

8.3.6. Spatial Prediction

Support for (parallel) spatial prediction with `terra`, `raster`, `stars` and `sf` objects is available via `mlr3spatial`.

`mlr3spatial` has two main scopes:

- Provide DataBackends for spatial objects (vector and raster data)
- Simplify spatial prediction tasks

Overall it aims to reduce the roundtripping between spatial objects -> data.frame / data.table -> spatial object during modeling.

8.3.6.1. Spatial Data Backends

A common scenario is the existence of spatial information in (point) vector data. `mlr3spatial` provides `as_task_*` helpers to directly convert these into a spatiotemporal (ST) task:

```
library(mlr3verse)
library(mlr3spatial)
library(sf)

# load sample points
leipzig_vector = sf::read_sf(system.file("extdata",
  "leipzig_points.gpkg", package = "mlr3spatial"),
  stringsAsFactors = TRUE)

# create land cover task
```

```
tsk_leipzig = as_task_classif_st(leipzig_vector, target = "land_cover")
tsk_leipzig
```

```
<TaskClassifST:leipzig_vector> (97 x 9)
* Target: land_cover
* Properties: multiclass
* Features (8):
  - dbl (8): b02, b03, b04, b06, b07, b08, b11, ndvi
* Coordinates:
           X       Y
 1: 732480.1 5693957
 2: 732217.4 5692769
 3: 732737.2 5692469
 4: 733169.3 5692777
 5: 732202.2 5692644
---
93: 733018.7 5692342
94: 732551.4 5692887
95: 732520.4 5692589
96: 732542.2 5692204
97: 732437.8 5692300
```

This saves users from stripping the coordinates from the vector data or transforming the `sf` object to a `data.frame` or `data.table` in the first place.

`mlr3spatial` adds support for the following spatial data classes:

- `stars` (from package `stars`)
- `SpatRaster` (from package `terra`)
- `RasterLayer` (from package `raster`)
- `RasterStack` (from package `raster`)

8.3.6.2. Spatial prediction

The goal of spatial prediction is usually a raster image that covers a specific area. Most often this area is quite large and contains millions of pixels. The goal is to predict on each pixel and return a raster image containing these predictions.

To save users from having to go the extra mile of extracting the final model and using it with the respective `predict()` function of the spatial R package of their desired outcome class, `mlr3spatial` provides `predict_spatial()`. `predict_spatial()` let's users

- choose the output class of the resulting raster image
- optionally predict in parallel via the `future` package, using a parallel backend of their choice

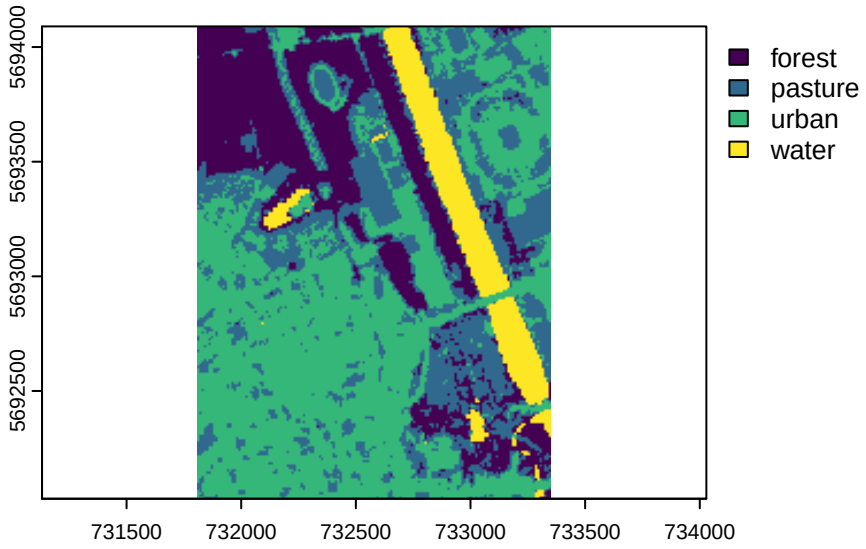
To use a raster image for prediction, it must be wrapped into a `TaskUnsupervised` for internal `mlr3` reasons. Next, the learner can be used to predict on the task.

```
leipzig_raster = terra::rast(system.file("extdata", "leipzig_raster.tif",
  package = "mlr3spatial"))
tsk_predict = as_task_unsupervised(leipzig_raster)

lrn = lrn("classif.ranger")
lrn$train(tsk_leipzig)

# plan("multisession") # optional parallelization
pred = predict_spatial(tsk_predict, lrn, format = "terra")
class(pred)
```

```
[1] "SpatRaster"
attr(,"package")
[1] "terra"
```

The resulting object can be visualized and treated as any other `terra` object. Thanks to the improved handling of factor variables in `terra`, the raster image contains the correct labeled classes from the prediction right away.

```
library(terra, exclude = "resample")
plot(pred, col = c("#440154FF", "#443A83FF", "#31688EFF",
  "#21908CFF", "#35B779FF", "#8FD744FF", "#FDE725FF"))
```



If you are interested in the performance of parallel spatial prediction, have a look at the Spatial Prediction Benchmark vignette - the resulting plot is shown below.

⚠ The results of the shown benchmark results should be taken with care as something seems to go wrong when using all-core parallelization with `terra::predict()`. Also both relative and absolute numbers will vary on your local machine and results might change depending on eventual package updates in the future.

8.4. 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. Cost-sensitive classification does not assume that the costs caused by different kinds of errors are equal. The objective of cost-sensitive classification is to minimize the expected costs.

Imagine you are an analyst for a big credit institution. Let's also assume that a correct bank decision would result in 35% of the profit at the end of a specific period. A correct decision means that the bank predicts that a customer will pay their bills (hence would obtain a loan), and the customer indeed has good credit. On the other hand, a wrong decision means that the bank predicts that the customer's credit is in good standing, but the opposite is true. This would result in a loss of 100% of the given loan.

	Good Customer (truth)	Bad Customer (truth)
Good Customer (predicted)	+ 0.35	- 1.0
Bad Customer (predicted)	0	0

Expressed as costs (instead of profit), we can write down the cost-matrix as follows:

```
costs = matrix(c(-0.35, 0, 1, 0), nrow = 2)
dimnames(costs) = list(response = c("good", "bad"), truth = c("good", "bad"))
print(costs)
```

```
        truth
response  good bad
    good -0.35   1
    bad   0.00   0
```

An exemplary data set for such a problem is the German Credit task:

```
library("mlr3verse")
task = tsk("german_credit")
table(task$truth())
```

```
good  bad
 700  300
```

The data has 70% of customers who can pay back their credit and 30% of bad customers who default on their debt. A manager, who doesn't have any model, could decide to give either everybody credit or to give nobody credit. The resulting costs for the German credit data are:

```
# nobody:
(700 * costs[2, 1] + 300 * costs[2, 2]) / 1000
```

```
[1] 0
```

```
# everybody
(700 * costs[1, 1] + 300 * costs[1, 2]) / 1000
```

```
[1] 0.055
```

If the average loan is $20,000, the credit institute will lose more than one million dollars if it would grant everybody a credit:

```
# average profit * average loan * number of customers
0.055 * 20000 * 1000
```

```
[1] 1100000
```

Our goal is to find a model that minimizes the costs (and maximizes the expected profit).

8.4.1. A First Model

For our first model, we choose an ordinary logistic regression (implemented in add-on package `mlr3learners`). We first create a classification task, then resample the model using 10-fold cross-validation and extract the resulting confusion matrix:

```
learner = lrn("classif.log_reg")
rr = resample(task, learner, rsmp("cv"))

confusion = rr$prediction()$confusion
print(confusion)
```

```
        truth
response good bad
    good  606 154
    bad    94 146
```

To calculate the average costs like above, we can simply multiply the elements of the confusion matrix with the elements of the previously introduced cost matrix and sum the values of the resulting matrix:

```
avg_costs = sum(confusion * costs) / 1000
print(avg_costs)
```

```
[1] -0.0581
```

With an average loan of $20,000, the logistic regression yields the following costs:

```
avg_costs * 20000 * 1000
```

```
[1] -1162000
```

Instead of losing over $1,000,000, the credit institute now can expect a profit of more than $1,000,000.

8.4.2. Cost-sensitive Measure

Our natural next step would be to further improve the modeling step in order to maximize the profit. For this purpose, we first create a cost-sensitive classification measure that calculates the costs based on our cost matrix. This allows us to conveniently quantify and compare modeling decisions. Fortunately, there already is a predefined measure `Measure` for this purpose: `MeasureClassifCosts`. The costs have to be provided as a numeric matrix whose columns and rows are named with class labels (just like the previously constructed `costs` matrix):

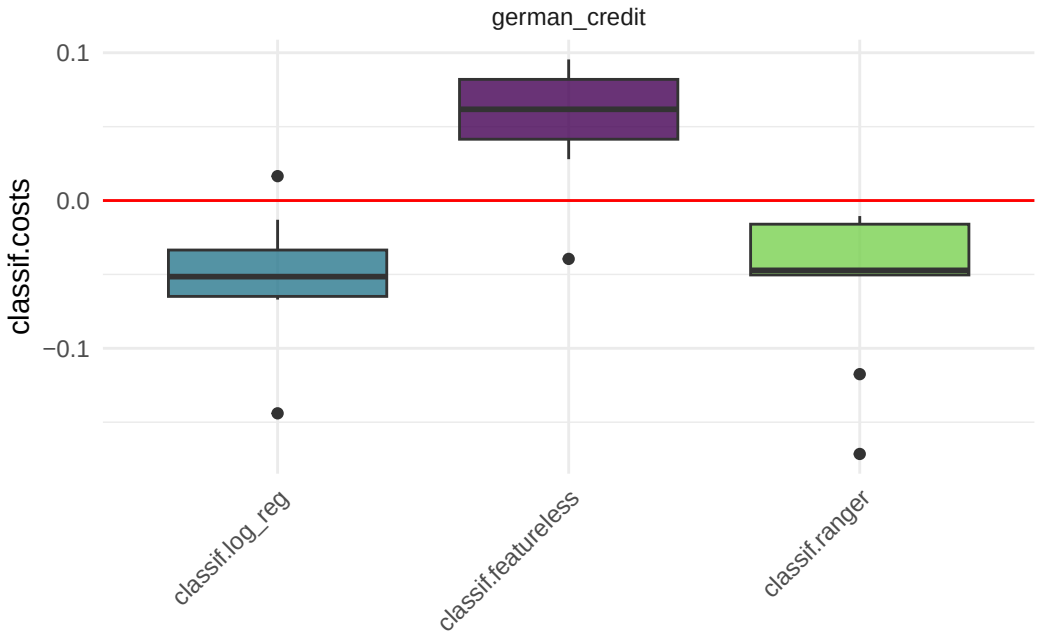
```
cost_measure = msr("classif.costs", costs = costs)
print(cost_measure)
```

```
<MeasureClassifCosts:classif.costs>: Cost-sensitive Classification
* Packages: mlr3
* Range: [-Inf, Inf]
* Minimize: TRUE
* Average: macro
* Parameters: normalize=TRUE
* Properties: -
* Predict type: response
```

If we now call `resample()` or `benchmark()`, the cost-sensitive measures will be evaluated. We compare the logistic regression to a simple featureless learner and to a random forest from package `ranger` :

```
learners = list(
  lrn("classif.log_reg"),
  lrn("classif.featureless"),
  lrn("classif.ranger")
```

```
)
cv10 = rsmp("cv", folds = 10)
bmr = benchmark(benchmark_grid(task, learners, cv10))
autoplot(bmr, measure = cost_measure) + ggplot2::geom_hline(yintercept = 0, colour = "red")
```



As expected, the featureless learner is performing comparably badly. The logistic regression and the random forest both yield a profit on average.

8.4.3. Thresholding

Although we now correctly evaluate the models in a cost-sensitive fashion, the models themselves are unaware of the classification costs. They assume the same costs for both wrong classification decisions (false positives and false negatives). Some learners natively support cost-sensitive classification (e.g., XXX). However, we will concentrate on a more generic approach that works for all models which can predict probabilities for class labels: thresholding.

Most learners can calculate the probability p for the positive class. If p exceeds the threshold 0.5, they predict the positive class and the negative class otherwise.

For our binary classification case of the credit data, we primarily want to minimize the errors where the model predicts "good", but truth is "bad" (i.e., the number of false positives) as this is the more expensive error. If we now increase the threshold to values > 0.5, we reduce the number of false negatives. Note that we increase the number of false positives simultaneously, or, in other words, we are trading false positives for false negatives.

```
# fit models with probability prediction
learner = lrn("classif.log_reg", predict_type = "prob")
rr = resample(task, learner, rsmp("cv"))
p = rr$prediction()
print(p)
```

```
<PredictionClassif> for 1000 observations:
    row_ids truth response  prob.good  prob.bad
          2   bad      bad 0.40126720 0.5987328
         17  good     good 0.97406360 0.0259364
         46  good     good 0.74870171 0.2512983
---
        973   bad      bad 0.09917846 0.9008215
        976  good     good 0.78358973 0.2164103
        997  good     good 0.51492948 0.4850705
```

```
# helper function to try different threshold values interactively
with_threshold = function(p, th) {
  p$set_threshold(th)
  list(confusion = p$confusion, costs = p$score(measures = cost_measure))
}

with_threshold(p, 0.5)
```

```
$confusion
        truth
response good bad
    good  598 152
    bad   102 148

$costs
classif.costs
      -0.0573
```

```
with_threshold(p, 0.75)
```

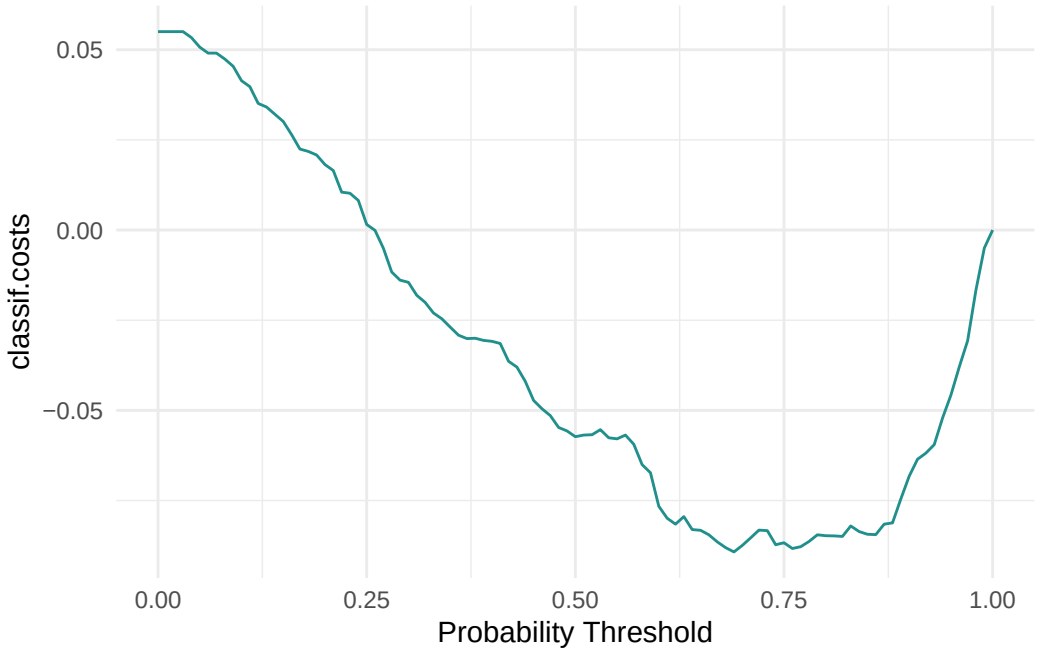
```
$confusion
        truth
response good bad
    good  462  75
    bad   238 225

$costs
classif.costs
      -0.0867
```

```
with_threshold(p, 1.0)
```

```
$confusion
        truth
response good bad
    good    0   0
    bad   700 300

$costs
classif.costs
            0
```

There is also an `autoplot()` method which systematically varies the threshold between 0 and 1 and calculates the corresponding scores:

```
autoplot(p, type = "threshold", measure = cost_measure)
```



Instead of manually or visually searching for good values, the base R function `optimize()` can do the job for us:

```
# simple wrapper function that takes a threshold and returns the resulting model performance
# this wrapper is passed to optimize() to find its minimum for thresholds in [0.5, 1]
f = function(th) {
  with_threshold(p, th)$costs
}
```

```
best = optimize(f, c(0.5, 1))
print(best)
```

```
$minimum
[1] 0.6905289

$objective
classif.costs
     -0.08925
```

```
# optimized confusion matrix:
with_threshold(p, best$minimum)$confusion
```

```
        truth
response good bad
    good  515  91
    bad   185 209
```

Note that the function `"optimize()"` is intended for unimodal functions and, therefore, may converge to a local optimum here. See the next section for better alternatives to tune the threshold.

8.4.4. Threshold Tuning

Currently `mlr3pipelines` offers two main strategies towards adjusting `classification thresholds`. We can either expose the thresholds as a `hyperparameter` of the Learner by using `PipeOpThreshold`. This allows us to tune the `thresholds` via an outside optimizer from `mlr3tuning`. Alternatively, we can also use `PipeOpTuneThreshold` which automatically tunes the threshold after each learner is fit. Both methods are described in the following subsections.

8.4.5. PipeOpThreshold

`PipeOpThreshold` can be put directly after a `Learner`.

A simple example would be:

```
gr = lrn("classif.rpart", predict_type = "prob") %>>% po("threshold")
l = as_learner(gr)
```

Note, that `predict_type = "prob"` is required for `po("threshold")` to have any effect.

The `thresholds` are now exposed as a `hyperparameter` of the `GraphLearner` we created:

```
l$param_set
```

```
<ParamSetCollection>
                              id    class lower upper nlevels        default
 1:             classif.rpart.cp ParamDbl     0     1     Inf           0.01
 2:     classif.rpart.keep_model ParamLgl    NA    NA       2          FALSE
 3:     classif.rpart.maxcompete ParamInt     0   Inf     Inf              4
 4:       classif.rpart.maxdepth ParamInt     1    30      30             30
 5:   classif.rpart.maxsurrogate ParamInt     0   Inf     Inf              5
 6:      classif.rpart.minbucket ParamInt     1   Inf     Inf <NoDefault[3]>
 7:       classif.rpart.minsplit ParamInt     1   Inf     Inf             20
 8: classif.rpart.surrogatestyle ParamInt     0     1       2              0
 9:   classif.rpart.usesurrogate ParamInt     0     2       3              2
10:           classif.rpart.xval ParamInt     0   Inf     Inf             10
11:         threshold.thresholds ParamUty    NA    NA     Inf <NoDefault[3]>
1 variable not shown: [value]
```

We can now tune those thresholds from the outside as follows:

Before tuning, we have to define which hyperparameters we want to tune over. In this example, we only tune over the `thresholds` parameter of the `threshold` pipe operator. You can easily imagine that we can also jointly tune over additional hyperparameters, i.e., rpart's `cp` parameter.

As the `Task` we aim to optimize for is a binary task, we can simply specify the threshold param:

```
library("paradox")
ps = ps(threshold.thresholds = p_dbl(lower = 0, upper = 1))
```

We now create a `AutoTuner` which automatically tunes the supplied learner over the `ParamSet` we supplied above.

```
at = AutoTuner$new(
  learner = l,
  resampling = rsmp("cv", folds = 3L),
  measure = msr("classif.ce"),
  search_space = ps,
  terminator = trm("evals", n_evals = 5L),
  tuner = tnr("random_search")
)

at$train(tsk("german_credit"))
```

Inside the `trafo`, we simply collect all set params into a named vector via `map_dbl` and store it in the `threshold.thresholds` slot expected by the learner.

Again, we create a `AutoTuner`, which automatically tunes the supplied learner over the `ParamSet` we supplied above.

One drawback of this strategy is that this requires us to fit a new model for each new threshold setting. While setting a threshold and computing performance is relatively cheap, fitting the learner is often more computationally demanding. An often better strategy is, therefore, to optimize the thresholds separately after each model fit.

8.4.6. PipeOpTunethreshold

PipeOpTuneThreshold on the other hand works together with PipeOpLearnerCV. It directly optimizes the `cross-validated` predictions made by this PipeOp. This is necessary to avoid over-fitting the threshold tuning.

A simple example would be:

```
gr = po("learner_cv", lrn("classif.rpart", predict_type = "prob")) %>>% po("tunethreshold")
l2 = as_learner(gr)
```

Note, that `predict_type` = "prob" is required for `po("tunethreshold")` to work. Additionally, note that this time no `threshold` parameter is exposed, and it is automatically tuned internally.

```
l2$param_set
```

```
<ParamSetCollection>
                                       id    class lower upper nlevels
 1:        classif.rpart.resampling.method ParamFct    NA    NA       2
 2:         classif.rpart.resampling.folds ParamInt     2   Inf     Inf
 3: classif.rpart.resampling.keep_response ParamLgl    NA    NA       2
 4:                     classif.rpart.cp ParamDbl     0     1     Inf
 5:               classif.rpart.keep_model ParamLgl    NA    NA       2
 6:               classif.rpart.maxcompete ParamInt     0   Inf     Inf
 7:                 classif.rpart.maxdepth ParamInt     1    30      30
 8:             classif.rpart.maxsurrogate ParamInt     0   Inf     Inf
 9:                classif.rpart.minbucket ParamInt     1   Inf     Inf
10:                 classif.rpart.minsplit ParamInt     1   Inf     Inf
11:           classif.rpart.surrogatestyle ParamInt     0     1       2
12:             classif.rpart.usesurrogate ParamInt     0     2       3
13:                     classif.rpart.xval ParamInt     0   Inf     Inf
14:           classif.rpart.affect_columns ParamUty    NA    NA     Inf
15:                 tunethreshold.measure ParamUty    NA    NA     Inf
16:               tunethreshold.optimizer ParamUty    NA    NA     Inf
17:               tunethreshold.log_level ParamUty    NA    NA     Inf
2 variables not shown: [default, value]
```

Note that we can set `rsmp("intask")` as a resampling strategy for "learner_cv" in order to evaluate predictions on the "training" data. This is generally not advised, as it might lead to over-fitting on the thresholds but can significantly reduce runtime.

For more information, see the post on Threshold Tuning on the mlr3 gallery.

8.5. Cluster Analysis

Cluster analysis is a type of unsupervised machine learning where the goal is to group data into clusters, where each cluster contains similar observations. The similarity is based on specified

metrics that are task and application-dependent. Cluster analysis is closely related to classification in the sense that each observation needs to be assigned to a cluster or a class. However, unlike classification problems where each observation is labeled, clustering works on data sets without true labels or class assignments.

The package `mlr3cluster` extends `mlr3` with the following objects for cluster analysis:

- `TaskClust` to define clustering tasks
- `LearnerClust` as base class for clustering learners
- `PredictionClust` as specialized class for `Prediction` objects
- `MeasureClust` as specialized class for performance measures

Since clustering is a type of unsupervised learning, `TaskClust` is slightly different from `TaskRegr` and `TaskClassif` objects. More specifically:

- `truth()` function is missing because observations are not labeled.
- `target` field is empty and will return `character(0)` if accessed anyway.

Additionally, `LearnerClust` provides two extra fields that are absent from supervised learners:

- `assignments` returns cluster assignments for training data. It returns `NULL` if accessed before training.
- `save_assignments` is a boolean field that controls whether or not to store training set assignments in a learner.

Finally, `PredictionClust` contains two additional fields:

- `partition` stores cluster partitions.
- `prob` stores cluster probabilities for each observation.

8.5.1. Train and Predict

Clustering learners provide both `train` and `predict` methods. The analysis typically consists of building clusters using all available data. To be consistent with the rest of the library, we refer to this process as training.

Some learners can assign new observations to existing groups with `predict`. However, prediction does not always make sense, as is the case for hierarchical clustering. In hierarchical clustering, the goal is to build a hierarchy of nested clusters by either splitting large clusters into smaller ones or merging smaller clusters into bigger ones. The final result is a tree or dendrogram which can change if a new data point is added. For consistency with the rest of the ecosystem, `mlr3cluster` offers `predict` method for hierarchical clusterers but it simply assigns all points to a specified number of clusters by cutting the resulting tree at a corresponding level. Moreover, some learners estimate the probability of each observation belonging to a given cluster. `predict_types` field gives a list of prediction types for each learner.

After training, the `model` field stores a learner's model that looks different for each learner depending on the underlying library. `predict` returns a `PredictionClust` object that gives a simplified view of the learned model. If the data given to the `predict` method is the same as the one on which the learner was trained, `predict` simply returns cluster assignments for the "training" observations.

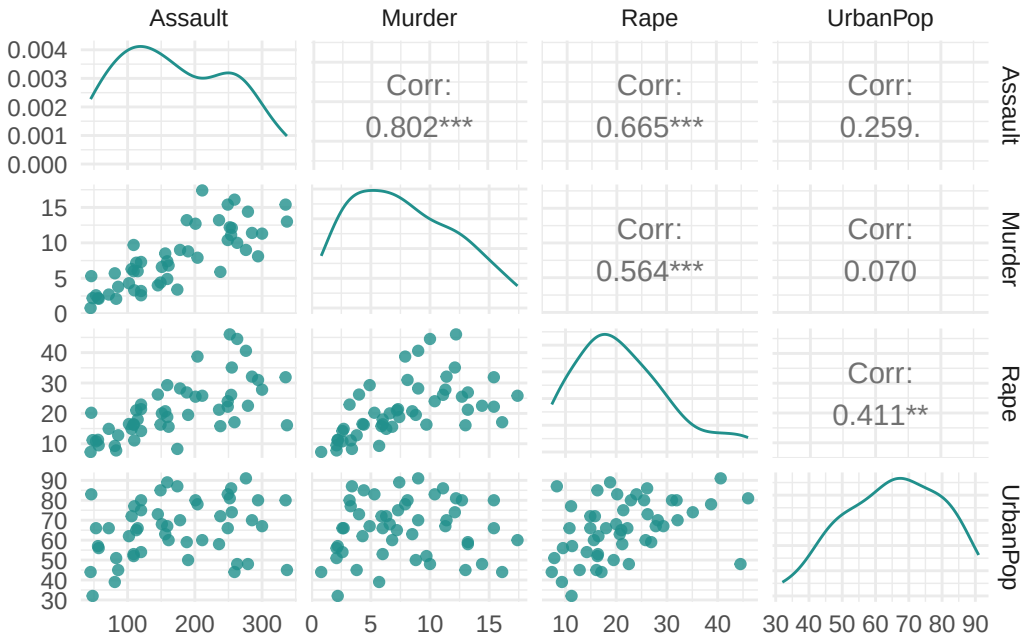
On the other hand, if the test set contains new data, `predict` will estimate cluster assignments for that data set. Some learners do not support estimating cluster partitions on new data and will instead return assignments for training data and print a warning message.

In the following example, a `$k$-means learner` is applied on the `US arrest data set`. The class labels are predicted and the contribution of the task features to assignment of the respective class are visualized.

```
library("mlr3")
library("mlr3cluster")
library("mlr3viz")
set.seed(1L)

# create an example task
task = tsk("usarrests")
print(task)
```

```
<TaskClust:usarrests> (50 x 4): US Arrests
* Target: -
* Properties: -
* Features (4):
  - int (2): Assault, UrbanPop
  - dbl (2): Murder, Rape
```

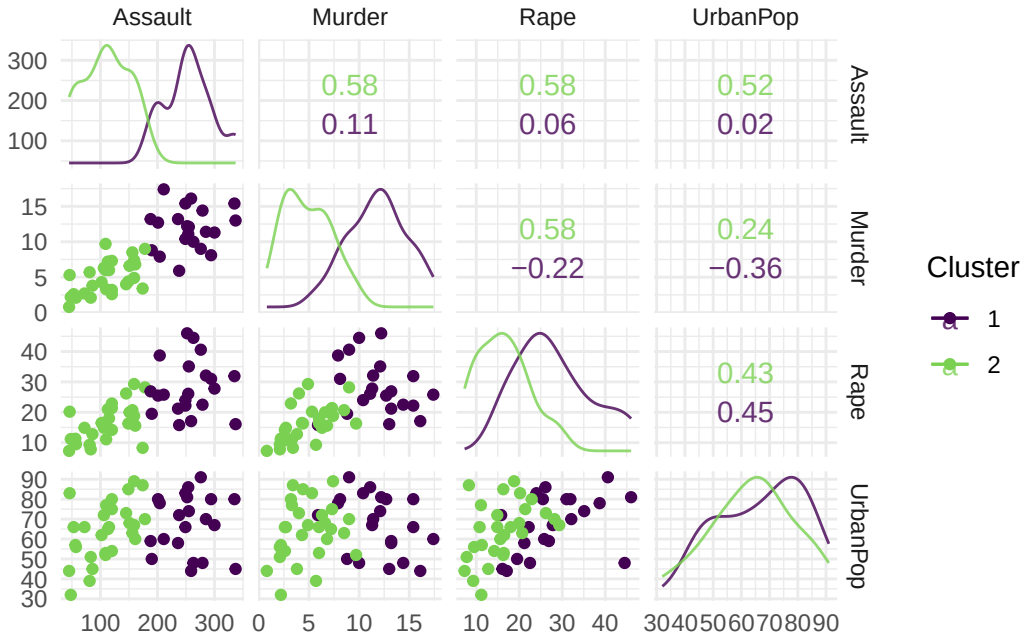
```
autoplot(task)
```



```
# create a k-means learner
learner = lrn("clust.kmeans")

# assigning each observation to one of the two clusters (default in clust.kmeans)
learner$train(task)
learner$model
```

```
K-means clustering with 2 clusters of sizes 21, 29

Cluster means:
   Assault    Murder     Rape UrbanPop
1 255.0000 11.857143 28.11429 67.61905
2 109.7586  4.841379 16.24828 64.03448

Clustering vector:
 [1] 1 1 1 1 1 1 2 1 1 1 2 2 1 2 2 2 2 1 2 1 2 1 2 1 2 2 2 1 2 2 1 1 1 2 2 2 2 2
[39] 2 1 2 1 1 2 2 2 2 2 2 2

Within cluster sum of squares by cluster:
[1] 41636.73 54762.30
 (between_SS / total_SS =  72.9 %)

Available components:

[1] "cluster"      "centers"      "totss"        "withinss"     "tot.withinss"
[6] "betweenss"    "size"         "iter"         "ifault"
```

```
# make "predictions" for the same data
prediction = learner$predict(task)
autoplot(prediction, task)
```



8.5.2. Measures

The difference between supervised and unsupervised learning is that there is no ground truth data in unsupervised learning. In a supervised setting, such as classification, we would need to compare our predictions to true labels. Since clustering is an example of unsupervised learning, there are no true labels to which we can compare. However, we can still measure the quality of cluster assignments by quantifying how closely objects within the same cluster are related (cluster cohesion) as well as how distinct different clusters are from each other (cluster separation).

There are a few built-in evaluation metrics available to assess the quality of clustering. One of them is `within sum of squares (WSS)` which calculates the sum of squared differences between observations and centroids. WSS is useful because it quantifies cluster cohesion. The range of this measure is $[0, \infty)$ where a smaller value means that clusters are more compact.

Another measure is `silhouette quality index` that quantifies how well each point belongs to its assigned cluster versus neighboring cluster. Silhouette values are in $[-1, 1]$ range.

Points with silhouette closer to:

- 1 are well clustered
- 0 lie between two clusters
- -1 likely placed in the wrong cluster

The following is an example of conducting a benchmark experiment with various learners on `iris data set` without target variable and assessing the quality of each learner with both within sum of squares and silhouette measures.

```
design = benchmark_grid(
  tasks = TaskClust$new("iris", iris[-5]),
  learners = list(
    lrn("clust.kmeans", centers = 3L),
    lrn("clust.pam", k = 2L),
    lrn("clust.cmeans", centers = 3L)),
  resamplings = rsmp("insample"))
print(design)
```

```
             task                  learner               resampling
1: <TaskClust[46]> <LearnerClustKMeans[38]> <ResamplingInsample[20]>
2: <TaskClust[46]>    <LearnerClustPAM[38]> <ResamplingInsample[20]>
3: <TaskClust[46]> <LearnerClustCMeans[38]> <ResamplingInsample[20]>
```

```
# execute benchmark
bmr = benchmark(design)

# define measure
measures = list(msr("clust.wss"), msr("clust.silhouette"))
bmr$aggregate(measures)
```

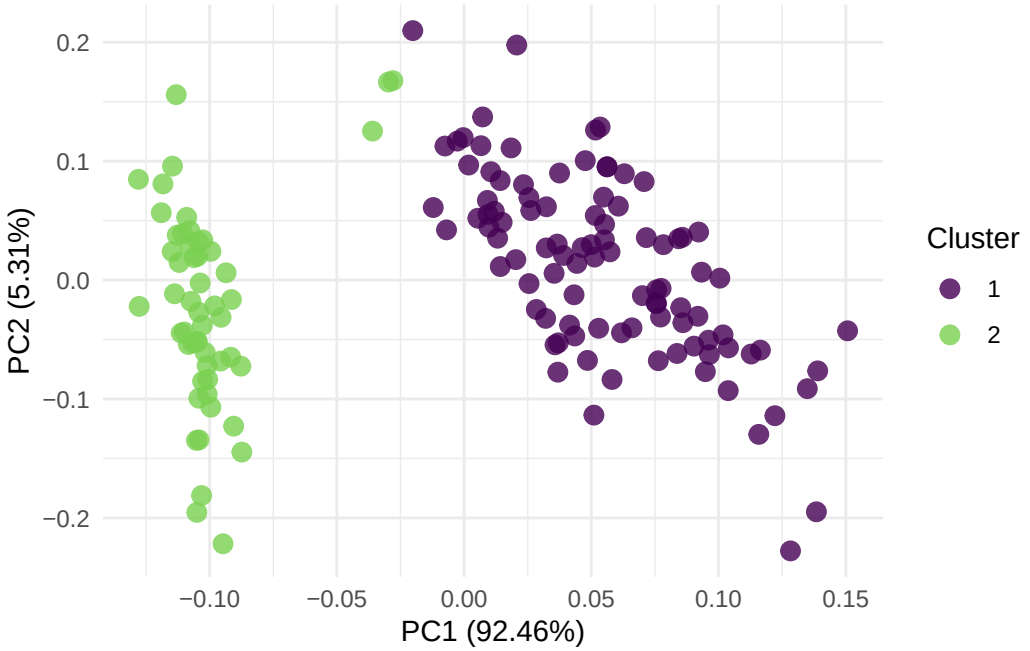
```
   nr      resample_result task_id   learner_id resampling_id iters clust.wss
1:  1 <ResampleResult[21]>    iris clust.kmeans      insample     1  78.85144
2:  2 <ResampleResult[21]>    iris    clust.pam      insample     1 153.32572
3:  3 <ResampleResult[21]>    iris clust.cmeans      insample     1  79.02617
1 variable not shown: [clust.silhouette]
```

The experiment shows that using k-means algorithm with three centers produces a better within sum of squares score than any other learner considered. However, pam (partitioning around medoids) learner with two clusters performs the best when considering silhouette measure which takes into the account both cluster cohesion and separation.

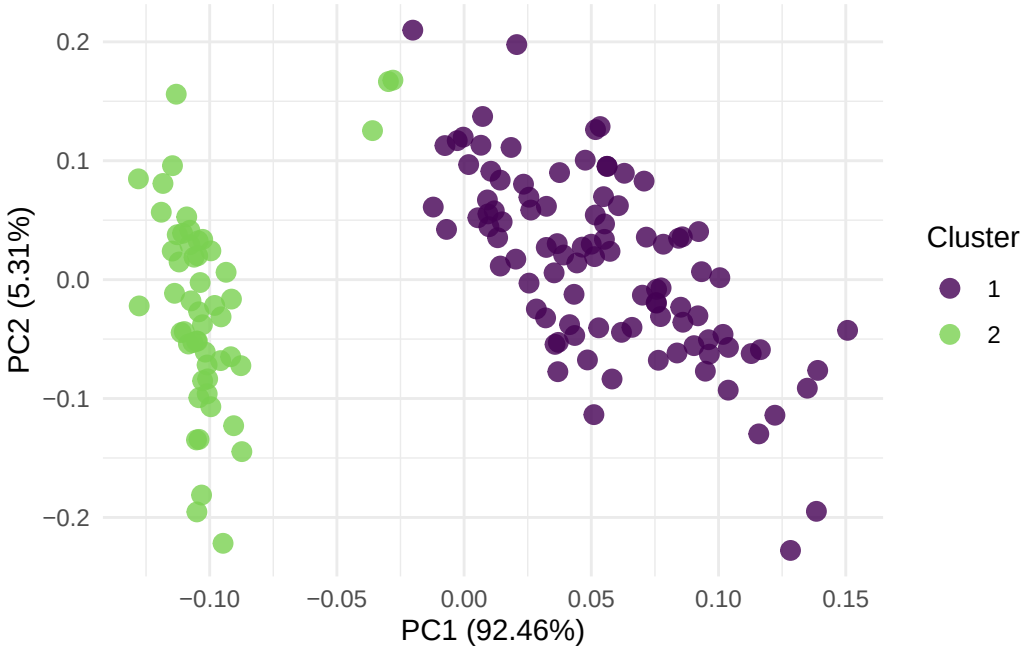
8.5.3. Visualization

Cluster analysis in `mlr3` is integrated with `mlr3viz` which provides a number of useful plots. Some of those plots are shown below.

```
task = TaskClust$new("iris", iris[-5])
learner = lrn("clust.kmeans")
learner$train(task)
prediction = learner$predict(task)

# performing PCA on task and showing assignments
autoplot(prediction, task, type = "pca")
```

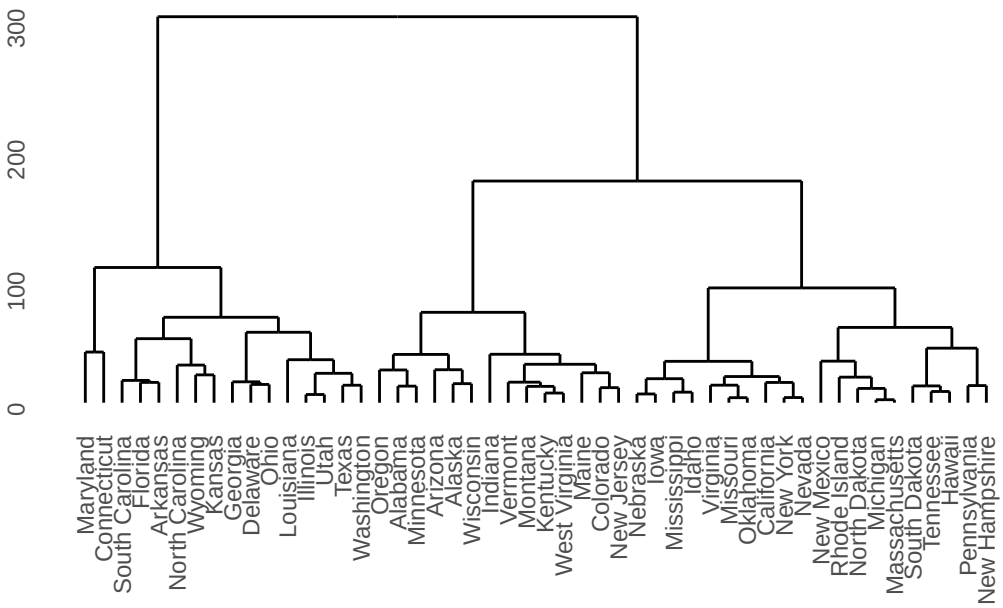



```
# same as above but with probability ellipse that assumes normal distribution
autoplot(prediction, task, type = "pca", frame = TRUE, frame.type = "norm")
```



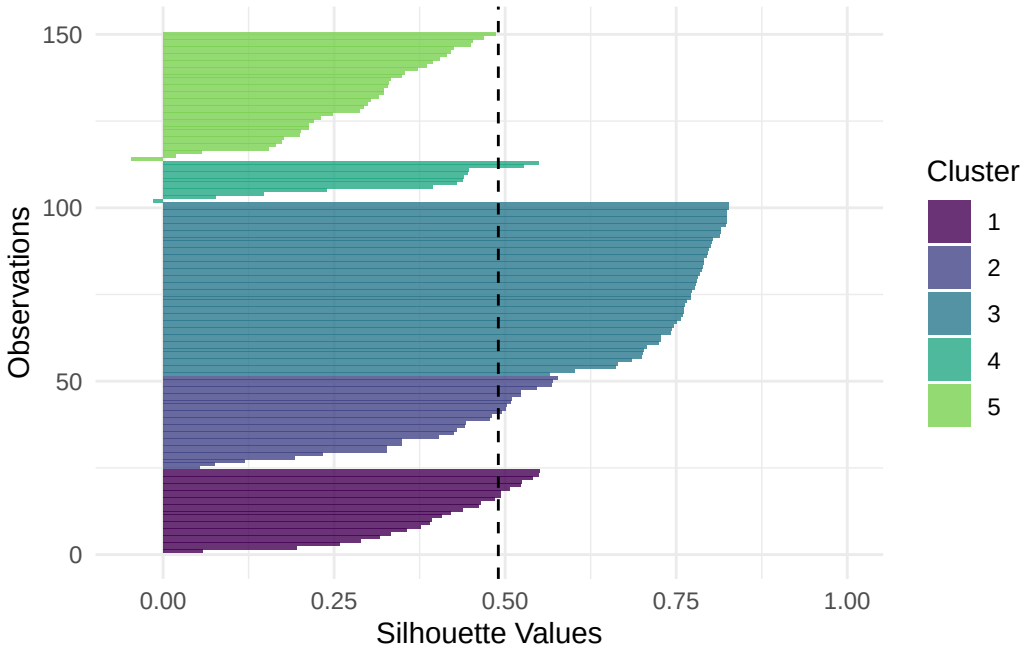

```
task = tsk("usarrests")
learner = lrn("clust.hclust")
learner$train(task)
```

```
# de
autc
```



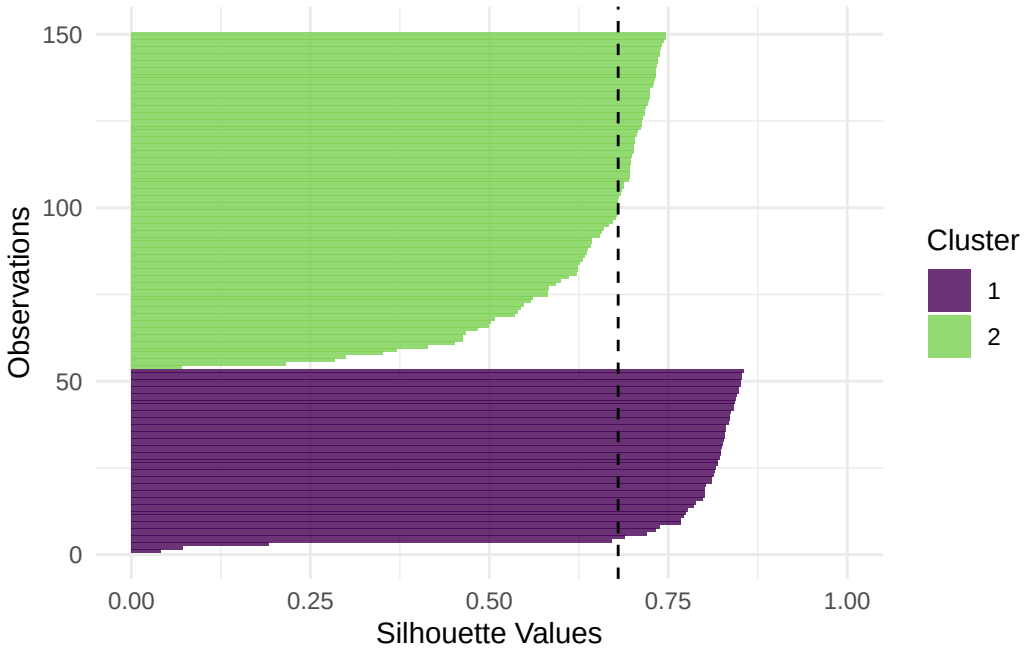
Silhouette plots can help to visually assess the quality of the analysis and help choose a number of clusters for a given data set. The red dotted line shows the mean silhouette value and each bar represents a data point. If most points in each cluster have an index around or higher than mean silhouette, the number of clusters is chosen well.

```
# silhouette plot allows to visually inspect the quality of clustering
task = TaskClust$new("iris", iris[-5])
learner = lrn("clust.kmeans")
learner$param_set$values = list(centers = 5L)
learner$train(task)
prediction = learner$predict(task)
autoplot(prediction, task, type = "sil")
```



The plot shows that all points in cluster 5 and almost all points in clusters 4, 2 and 1 are below average silhouette index. This means that a lot of observations lie either on the border of clusters or are likely assigned to the wrong cluster.

```
learner = lrn("clust.kmeans")
learner$param_set$values = list(centers = 2L)
learner$train(task)
prediction = learner$predict(task)
autoplot(prediction, task, type = "sil")
```



Setting the number of centers to two improves both the average silhouette score as well as the overall quality of clustering because almost all points in cluster 1 are higher than, and a lot of points in cluster 2 are close to the mean silhouette. Hence, having two centers might be a better choice for the number of clusters.

9. Technical

TODO (150-200 WORDS)

This chapter provides an overview of the technical details of the `mlr3` framework. This includes the following topics:

- Parallelization with the `future` framework (Section 9.1),
- how to handle errors and troubleshoot (Section 9.2),
- working with out-of-memory data, e.g., data stored in databases (Section 9.3),
- working with hyperparameters (Section 9.4), and
- adjust the logger to your needs (Section 9.5).

9.1. Parallelization

Parallelization refers to running multiple jobs in parallel, i.e., executing them simultaneously on multiple CPU cores, CPUs, or computational nodes. This process allows for significant savings in computing power.

In general, there are many possibilities to parallelize, depending on the hardware to run the computations: If you only have a single CPU with multiple cores, threads or forks are ways to utilize all cores. If you have multiple machines, they need a way to communicate and exchange information, e.g. via protocols like network sockets or the Message Passing Interface (MPI). We don't want to delve too deep into such details here, but want to introduce some terminology:

- We call the parallelization platform together with its implementation for R the **parallelization backend**. As many parallelization backends have a different API, we are using the `future` package as an additional abstraction layer. `mlr3` just interfaces `future` while the user can control how the code is executed.
- The R session or process which orchestrates the computational work is called **main**, and it starts computational **jobs**.
- The R sessions, processes, forks or machines which receive the jobs, do the calculation and then send back the result are called **workers**.

We distinguish between *implicit parallelism* and *explicit parallelism*. For the former, no special directives are required to enable the parallelization, everything works fully automatically. For the latter, parallelization has to be manually configured. On the one hand, this gives you full control over the execution, but on the other hand, this poses a greater obstacle for non-experts.

> **Note**
>
> We don't cover parallelization on GPUs here. `mlr3` only distributes the fitting of multiple learners, e.g., during resampling, benchmarking, or tuning. On this rather abstract level, GPU parallelization doesn't work efficiently. Some learning procedures can be compiled against CUDA/OpenCL to utilize the GPU while fitting a single model. We refer to the respective documentation of the learner's implementation, e.g., here for `xgboost`.

9.1.1. Implicit Parallelization

We talk about implicit parallelization in the context of `mlr3`, if `mlr3` calls external code (i.e., code from foreign CRAN packages which implements a `Learner`) that itself runs in parallel. Note that this definition includes GPU acceleration.

Many machine learning algorithms can parallelize their model fit using threading, e.g., the random forest implementation in `ranger` or the boosting implemented in `xgboost`. During threading, the implementation instructs some sequential parts of the code to be executed independently of the other parts in the same process.

For example, while fitting a decision tree, each split that divides the data into two disjoint partitions requires a search for the best cut point on all p features. So instead of iterating over all features sequentially, the search can be broken down into p threads, each searching for the best cut point on a single feature. These threads can easily be parallelized by the scheduler of the operating system, as there is no need for communication between the threads. After all threads have finished, the results are collected and merged before terminating the threads. I.e., for our example of the decision tree, (1) the p best cut points per feature are collected and then (2) aggregated to the single best cut point across all features by just iterating over the p results sequentially.

> **Warning**
>
> It does not make practical sense to actually execute in parallel every operation that can be parallelized. Starting and terminating workers (here: threads) as well as possible communication between workers comes at a price in the form of additionally required runtime which is called (parallelization) overhead. The overhead must be related to the runtime of the sequential execution. If the sequential execution is comparably fast, enabling parallelization often just introduces additional complexity and slows down the execution.

Unfortunately, threading conflicts with certain parallel backends used during explicit parallelization, causing the system to be overutilized in the best case and causing hangs or segfaults in the worst case. For this reason, we introduced the convention that implicit parallelization is turned off per default. Hyperparameters that control the number of threads are tagged with the label `"threads"`. Currently, controlling the number of threads is possible for some learners and filters from the `mlr3filters` package:

```
library("mlr3learners") # for the ranger learner

learner = lrn("classif.ranger")
```

```
learner$param_set$ids(tags = "threads")
```

```
[1] "num.threads"
```

To enable the parallelization for this learner, we provide the helper function `set_threads()` which

```
# use 4 CPUs
set_threads(learner, n = 4)
```

```
<LearnerClassifRanger:classif.ranger>
* Model: -
* Parameters: num.threads=4
* Packages: mlr3, mlr3learners, ranger
* Predict Types:  [response], prob
* Feature Types: logical, integer, numeric, character, factor, ordered
* Properties: hotstart_backward, importance, multiclass, oob_error,
  twoclass, weights
```

```
# auto-detect cores on the local machine
set_threads(learner)
```

```
<LearnerClassifRanger:classif.ranger>
* Model: -
* Parameters: num.threads=2
* Packages: mlr3, mlr3learners, ranger
* Predict Types:  [response], prob
* Feature Types: logical, integer, numeric, character, factor, ordered
* Properties: hotstart_backward, importance, multiclass, oob_error,
  twoclass, weights
```

Danger

Automatic detection of the number of CPUs is sometimes flaky, and utilizing all available cores is occasionally counterproductive as overburdening the system often has negative effects on the overall runtime. The function which determines the number of CPUs for `mlr3` is implemented in `parallelly::availableCores()` and comes with reasonable heuristics for many setups. See this blog post for some background information about the heuristic. However, there are still some scenarios where it is better to reduce the number of utilized CPUs manually:

- You want to simultaneously work on the same system, e.g., browse the web or watch a video.
- You are on a multi-user system and want to spare some resources for other users.
- You have energy-efficient CPU cores, for example, the "Icestorm" cores on a Mac M1 chip. These are comparably slower than the high-performance "Firestorm" cores and

not well suited for heavy computations.
- You have linked R to a threaded BLAS implementation like OpenBLAS, and your learners make heavy use of linear algebra.

You can manually set the number of CPUs to overrule the heuristic via option `"mc.cores"`:

```
options(mc.cores = 4)
```

We recommend setting this in your system's `.Rprofile` file, c.f. `Startup`.

9.1.2. Explicit Parallelization

Here, we talk about explicit parallelization if `mlr3` starts and controls the parallelization itself. For this purpose, an additional abstraction layer is used to be able to operate on a unified interface for a broad range of parallel backends: the `future` package. There are two operations where `mlr3` calls the `future` package: while performing resampling via `resample()` and while benchmarking via `benchmark()`. During resampling, because all resampling iterations are independent of each other, all iterations can be executed in parallel. The same holds for benchmarking, where additionally to the independent model fits of a single resampling, all combinations in the provided design are also independent. These iterations are performed by `future` using the parallel backend configured with `future::plan()`. Extension packages like `mlr3tuning` internally call `benchmark()` during tuning and thus work in parallel, too.

Tip

When computational problems are so easy to parallelize, they are often referred to as "embarrassingly parallel".
Whenever you loop over elements with a map-like function (e.g., `lapply()`, `sapply()`, `mapply()`, `vapply()` or a function from package `purrr`), you are facing an embarrassingly parallel problem. Such problems are straightforward to parallelize with R, e.g., with the `furrr` package providing map-like functions executed in parallel via the `future` framework. The same holds for `for`-loops with independent iterations, i.e., loops where the current iteration does not rely on the results of previous iterations.

In this section, we will use the `spam task` and a simple `classification tree` to showcase the explicit parallelization. We use the `future::multisession` parallel backend that should work on all systems.

```
# select the multisession backend to use
future::plan("multisession")

# define objects to perform a resampling
task = tsk("spam")
learner = lrn("classif.rpart")
resampling = rsmp("cv", folds = 3)

```

```
time = proc.time()[3]
resample(task, learner, resampling)
diff = proc.time()[3] - time
```

By default, all CPUs of your machine are used unless you specify the argument `workers` in `future::plan()` (possible problems with this default have already been discussed for implicit parallelization). You should see a decrease in the reported elapsed time, but in practice, you cannot expect the runtime to fall linearly as the number of cores increases (Amdahl's law). In contrast to threads, the technical overhead for starting workers, communicating objects, sending back results, and shutting down the workers is quite large for the multisession backend. Therefore, it is advised to only consider parallelization for resamplings where each iteration runs at least several seconds.

Figure 9.1 illustrates the parallelization from the above example. From left to right:

1. The main process calls the `resample()` function.
2. The task is split into 3 folds.
3. The folds are passed to three workers, each fitting a model on the respective subset of the task and predicting on the left-out observations.
4. The predictions (and trained models) are communicated back to main process which combines them into a `ResampleResult`.

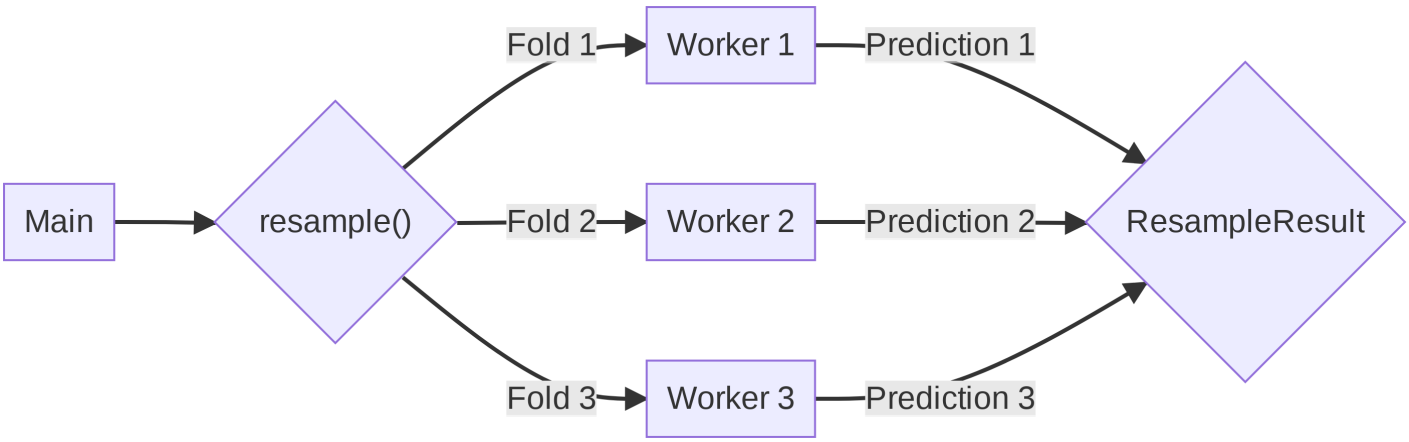


Figure 9.1.: Parallelization of a resampling using a 3-fold cross-validation

> **Note**
>
> If you are transitioning from `mlr`, you might be used to selecting different parallelization levels, e.g., for resampling, benchmarking, or tuning. In `mlr3`, this is no longer required (except for nested resampling, briefly described in the following section). All kind of experiments are rolled out on the same level. Therefore, there is no need to decide whether you want to parallelize the tuning OR the resampling.
> Just lean back and let the machine do the work :-)

9.1.3. Reproducibility

Usually reproducibility is a major concern during parallelization as special pseudorandom number generators (PRNGs) are required. Luckily, this problem is already solved for us by the excellent `future` package `mlr3` calls under the hood. `future` ensures that all workers will receive the exactly same PRNG streams. Although this alone does not guarantee full reproducibility, it is one problem less to worry about.

You can find more details about the used pseudo RNG in this blog post.

9.1.4. Nested Resampling Parallelization

Nested resampling results in two nested resampling loops, and the user can choose which of them should be parallelized. Let's consider the following example: You want to tune the `minsplit` argument of a classification tree using the `AutoTuner` of `mlr3tuning` (simplified version taken from the nested resampling section):

```
library("mlr3tuning")
```

```
Loading required package: paradox
```

```
learner = lrn("classif.rpart",
  minsplit  = to_tune(2, 128, logscale = TRUE)
)

at = auto_tuner(
  method = tnr("random_search"),
  learner = learner,
  resampling = rsmp("cv", folds = 2), # inner CV
  measure = msr("classif.ce"),
  term_evals = 20,
)
```

To evaluate the performance on an independent test set, resampling is used:

```
resample(
  task = tsk("penguins"),
  learner = at,
  resampling = rsmp("cv", folds = 5) # outer CV
)
```

```
<ResampleResult> of 5 iterations
* Task: penguins
* Learner: classif.rpart.tuned
* Warnings: 0 in 0 iterations
* Errors: 0 in 0 iterations
```

Here, we have two opportunities to tune: the inner cross-validation of the auto tuner with 2 folds, or the outer cross-validation of the resampling with 5 folds. Let's say that we have a single CPU with four cores available.

If we opt to parallelize the outer CV, all four cores would be utilized first with the computation of the first 4 resampling iterations. The computation of the fifth iteration has to wait, i.e., depending on the parallelization backend and its scheduling strategy,

(a) until all four iterations have been finished, and the results have been collectively reported back to the main process, or
(b) either one of the four cores has terminated – the first core reporting back will get a new task as soon as possible.

> **Note**
>
> The former method usually comes with less synchronization overhead and is best suited for short jobs with homogeneous runtimes. The latter yields better runtimes if the runtimes are heterogeneous, especially if the parallelization overhead is neglectable in comparison with the runtime for the computation. E.g., for `parallel::mclapply()`, the behavior of the scheduler can be controlled with the `mc.preschedule` option. For many backends, you cannot control the scheduling. However, `future` allows you to first chunk jobs together which combines multiple tasks into blocks that run sequentially on a worker, avoiding the intermediate synchronization steps.

The resulting CPU utilization of the nested resampling example on 4 CPUs is visualized in two Figures:

- Figure 9.2 as an example for parallelizing the outer 5-fold cross-validation.

  ```
  # Runs the outer loop in parallel and the inner loop sequentially
  future::plan(list("multisession", "sequential"))
  ```

  We assume that each fit during the inner resampling takes 4 seconds to compute and that there is no other significant overhead. First, each of the four workers starts with the computation of an inner 2-fold cross-validation. As there are more jobs than workers, the remaining fifth iteration of the outer resampling is queued on CPU1 **after** the first 4 iterations are finished after 8 secs. During the computation of the 5th outer resampling iteration, only CPU1 is utilized, the other 3 CPUs are idling.

- Figure 9.3 as an example for parallelizing the inner 2-fold cross-validation.

  ```
  # Runs the outer loop sequentially and the inner loop in parallel
  future::plan(list("sequential", "multisession"))
  ```

  Here, the outer loop runs sequentially and distributes the 2 computations for the inner resampling on 2 CPUs. Meanwhile, CPU3 and CPU4 are idling.

Both possibilities for parallelization are not exploiting the full potential of the 4 CPUs. With parallelization of the outer loop, all results are computed after 16s, in contrast to parallelization of the inner loop where the results are only available after 20s.

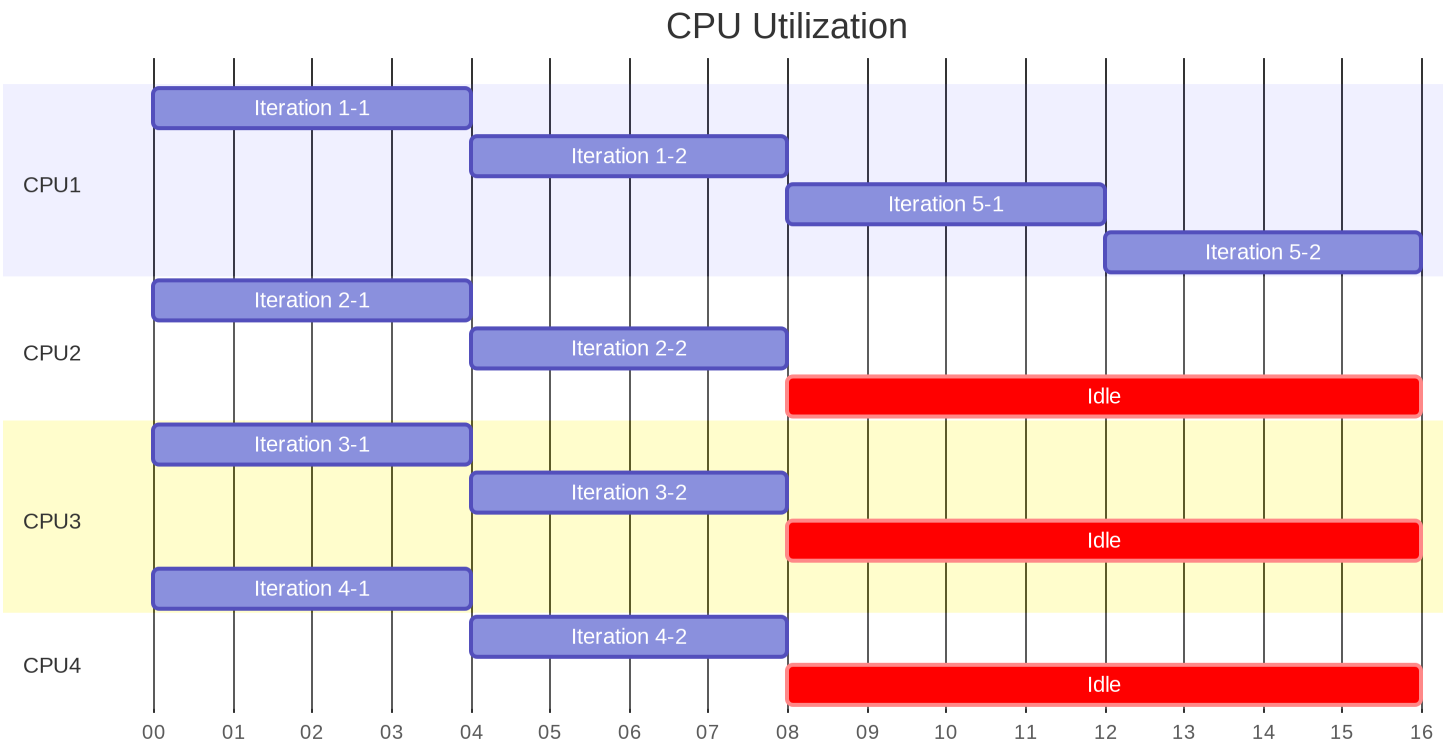


Figure 9.2.: CPU utilization while parallelizing the outer resampling of a 2-fold cross-validation nested inside a 5-fold cross-validation on 4 CPUs.

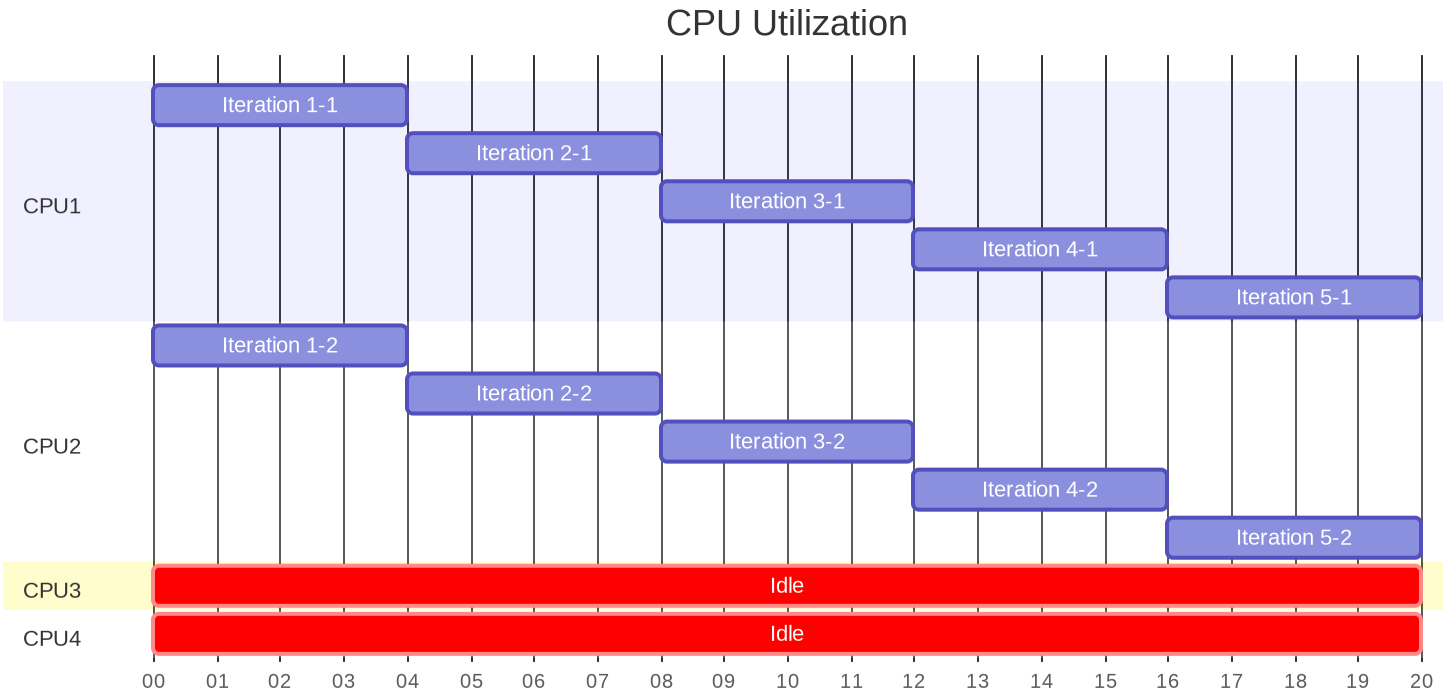


Figure 9.3.: CPU utilization while parallelizing the inner resampling of a 2-fold cross-validation nested inside a 5-fold cross-validation on 4 CPUs.

If possible, the number of iterations can be adapted to the available hardware. There is no law set in stone that you have to do, e.g., 10 folds in cross-validation. If you have 4 CPUs and a reasonable variance, 8 iterations are often sufficient, or you do 12 iterations because you get the last two iterations basically for free.

Alternatively, you can also enable parallelization for both loops for nested parallelization, even on different parallelization backends. While nesting real parallelization backends is often unintended and causes unnecessary overhead, it is useful in some distributed computing setups. In this case, the number of workers must be manually tweaked so that the system does not get overburdened:

```
# Runs both loops in parallel
future::plan(list(
  future::tweak("multisession", workers = 2),
  future::tweak("multisession", workers = 4)
))
```

This example would run on 8 cores (`= 2 * 4`) on the local machine. The vignette of the `future` package gives more insight into nested parallelization. For more background information about parallelization during tuning, see Section 6.7 of Bischl et al. (2021).

Danger

During tuning with `mlr3tuning`, you can often adjust the **batch size** of the `Tuner`, i.e., control how many hyperparameter configurations are evaluated in parallel. If you want full parallelization, make sure that the batch size multiplied by the number of (inner) resampling iterations is at least equal to the number of available workers. If you expect homogeneous runtimes, i.e., you are tuning over a single learner or linear pipeline and you have no hyperparameter which is likely to influence the performance, aim for a multiple of the number of workers.
In general, larger batches mean more parallelization, while smaller batches imply a more frequent evaluation of termination criteria. We default to a `batch_size` of 1 that ensures that all `Terminators` work as intended, i.e., you cannot exceed the computational budget.

9.2. Error Handling

In ML, it is not uncommon for something to break. This is because the algorithms have to process arbitrary data, and not all eventualities can always be handled. While we try to identify obvious problems before execution, such as when missing values occur, but a learner can't handle them, other problems are far more complex to detect. Examples include correlations or collinearity that make model fitting impossible, outliers that lead to numerical problems, or new levels of categorical variables emerging in the predict step. The learners behave quite differently when encountering such problems: some models signal a warning during the train step that they failed to fit but return a baseline model while other models stop the execution. During prediction, some learners just refuse to predict the response for observations they cannot handle while others predict a missing value. How to deal with these problems even in more complex setups like benchmarking or tuning is the topic of this section.

For illustration (and internal testing) of error handling, `mlr3` ships with the learners `classif.debug` and `regr.debug`. Here, we will concentrate on the debug learner for classification:

```
task = tsk("penguins")
learner = lrn("classif.debug")
print(learner)
```

```
<LearnerClassifDebug:classif.debug>: Debug Learner for Classification
* Model: -
* Parameters: list()
* Packages: mlr3
* Predict Types:  [response], prob
* Feature Types: logical, integer, numeric, character, factor, ordered
* Properties: hotstart_forward, missings, multiclass, twoclass
```

This learner comes with special hyperparameters that let us simulate problems frequently encountered in ML. E.g., the debug learner comes with hyperparameters to control

1. what conditions should be signaled (message, warning, error, segfault) with what probability,
2. during which stage the conditions should be signaled (train or predict), and
3. the ratio of predictions being `NA` (`predict_missing`).

```
learner$param_set
```

```
<ParamSet>
                     id    class lower upper nlevels        default value
 1:        error_predict ParamDbl     0     1     Inf              0
 2:          error_train ParamDbl     0     1     Inf              0
 3:      message_predict ParamDbl     0     1     Inf              0
 4:        message_train ParamDbl     0     1     Inf              0
 5:      predict_missing ParamDbl     0     1     Inf              0
 6: predict_missing_type ParamFct    NA    NA       2             na
 7:           save_tasks ParamLgl    NA    NA       2          FALSE
 8:     segfault_predict ParamDbl     0     1     Inf              0
 9:       segfault_train ParamDbl     0     1     Inf              0
10:          sleep_train ParamUty    NA    NA     Inf <NoDefault[3]>
11:        sleep_predict ParamUty    NA    NA     Inf <NoDefault[3]>
12:              threads ParamInt     1   Inf     Inf <NoDefault[3]>
13:      warning_predict ParamDbl     0     1     Inf              0
14:        warning_train ParamDbl     0     1     Inf              0
15:                    x ParamDbl     0     1     Inf <NoDefault[3]>
16:                 iter ParamInt     1   Inf     Inf              1
```

With the learner's default settings, the learner will do nothing special: The learner remembers a random label and constantly predicts this label:

```
task = tsk("penguins")
learner$train(task)$predict(task)$confusion
```

```
           truth
response    Adelie Chinstrap Gentoo
  Adelie         0         0      0
  Chinstrap      0         0      0
  Gentoo       152        68    124
```

We now set a hyperparameter to let the debug learner signal an error during the train step. By default, mlr3 does not catch conditions such as warnings or errors raised while calling learners:

```
# set probability to signal an error to 1
learner$param_set$values = list(error_train = 1)

learner$train(tsk("penguins"))
```

```
Error in .__LearnerClassifDebug__.train(self = self, private = private, : Error from classif.de
```

If this has been a regular learner, we could now start debugging with `traceback()` (or create a Minimal Reproducible Example (MRE) to file a bug report upstream).

> **Note**
>
> If you start debugging, make sure you have disabled parallelization to avoid various pitfalls related to parallelization. It may also be helpful to set the option `mlr3.debug` to `TRUE`. If this flag is set, mlr3 does not call into the `future` package, resulting in an easier-to-interpret program flow and `traceback()`.

9.2.1. Encapsulation

Since ML algorithms are confronted with arbitrary, often messy data, errors are not uncommon here, and we often just need to move on during benchmarking or tuning. Thus, we need a mechanism to

1. capture all signaled conditions such as messages, warnings and errors so that we can analyze them post-hoc (called "encapsulation", covered in this section), and
2. a statistically sound way to proceed while being able to aggregate over partial results (next Section 9.2.2).

Encapsulation ensures that signaled conditions (such as messages, warnings and errors) are intercepted: all conditions raised during the training or predict step are logged into the learner, and errors do not interrupt the program flow. I.e., the execution of the calling function or package (here: mlr3) continues as if there had been no error, though the result (fitted model during `train()`, predictions during `predict()`) are missing. Each `Learner` has a field `encapsulate` to control how

the train or predict steps are wrapped. The easiest way to encapsulate the execution is provided by the package `evaluate` which evaluates R expressions while tracking conditions such as outputs, messages, warnings or errors (see the documentation of the `encapsulate()` helper function for more details):

```
task = tsk("penguins")
learner = lrn("classif.debug")

# this learner throws a warning and then stops with an error during train()
learner$param_set$values = list(warning_train = 1, error_train = 1)

# enable encapsulation for train() and predict()
learner$encapsulate = c(train = "evaluate", predict = "evaluate")

learner$train(task)
```

After training the learner, one can access the recorded log via the fields `log`, `warnings` and `errors`:

```
learner$log
```

```
   stage   class                                 msg
1: train warning Warning from classif.debug->train()
2: train   error   Error from classif.debug->train()
```

```
learner$warnings
```

```
[1] "Warning from classif.debug->train()"
```

```
learner$errors
```

```
[1] "Error from classif.debug->train()"
```

Another method for encapsulation is implemented in the `callr` package. In contrast to `evaluate`, the computation is taken out in a separate R process. This guards the calling session against segfaults which otherwise would tear down the complete R session. On the downside, starting new processes comes with comparably more computational overhead.

```
learner$encapsulate = c(train = "callr", predict = "callr")
learner$param_set$values = list(segfault_train = 1)
learner$train(task = task)
learner$errors
```

```
[1] "callr process exited with status -11"
```

With either of these encapsulation methods, we can now catch errors and post-hoc analyze the messages, warnings and error messages. Unfortunately, this is only half the battle. Without a model, it is not possible to get predictions:

```
learner$predict(task)
```

```
Error: Cannot predict, Learner 'classif.debug' has not been trained yet
```

To handle the missing predictions gracefully during `resample()`, `benchmark()` or tuning, fallback learners are introduced next.

9.2.2. Fallback learners

Fallback learners have the purpose of allowing scoring results in cases where a `Learner` failed to fit a model, refuses to provide predictions for all observations or predicts missing values.

We will first handle the case that a learner fails to fit a model during training, e.g., if some convergence criterion is not met or the learner ran out of memory. There are in general three possibilities to proceed:

1. Ignore missing scores. Although this is arguably the most frequent approach in practice, it is **not** statistically sound. For example, consider the case where a researcher wants a specific learner to look better in a benchmark study. To do this, the researcher takes an existing learner but introduces a small adaptation: If an internal goodness-of-fit measure is not achieved, an error is thrown. In other words, the learner only fits a model if the model can be reasonably well learned on the given training data. In comparison with the learning procedure without this adaptation and a good threshold, however, we now compare the mean over only the "easy" splits with the mean over all splits - an unfair advantage.
2. Penalize failing learners. If a score is missing, we can simply impute the worst possible score (as defined by the `Measure`) and thereby heavily penalize the learner for failing. However, this often seems too harsh for many problems, and for some measures there is no reasonable value to impute.
3. Impute a value that corresponds to a (weak) baseline. Instead of imputing with the worst possible score, impute with a reasonable baseline, e.g., by just predicting the majority class or the mean of the response in the training data. Such simple baselines are implemented as featureless learners (`mlr_learners_classif.featureless` or `mlr_learners_regr.featureless`). Note that a reasonable baseline value is different in different training splits. Retrieving these values after a larger benchmark study has been conducted is possible, but tedious.

We strongly recommend option (3): it is statistically sound and very flexible. To make this procedure very convenient during resampling and benchmarking, we support fitting a proper baseline with a fallback learner. In the next example, in addition to the debug learner, we attach a simple featureless learner to the debug learner. So whenever the debug learner fails (which is every single time with the given parametrization) and encapsulation is enabled, `mlr3` falls back to the predictions of the featureless learner internally:

```
task = tsk("penguins")

learner = lrn("classif.debug")
learner$param_set$values = list(error_train = 1)
learner$fallback = lrn("classif.featureless")

learner$train(task)
learner
```

```
<LearnerClassifDebug:classif.debug>: Debug Learner for Classification
* Model: -
* Parameters: error_train=1
* Packages: mlr3
* Predict Types:  [response], prob
* Feature Types: logical, integer, numeric, character, factor, ordered
* Properties: hotstart_forward, missings, multiclass, twoclass
* Errors: Error from classif.debug->train()
```

Note that we don't have to enable encapsulation explicitly; it is automatically set to `"evaluate"` for the training and the predict step while setting a fallback learner for a learner without encapsulation enabled. Furthermore, the log contains the captured error (which is also included in the print output), and although we don't have a model, we can still get predictions:

```
learner$model
```

```
NULL
```

```
prediction = learner$predict(task)
prediction$score()
```

```
classif.ce
 0.5581395
```

In this stepwise train-predict procedure, the fallback learner is of limited use. However, it is invaluable for larger benchmark studies.

In the following snippet, we compare the previously created debug learner with a simple classification tree. We re-parametrize the debug learner to fail in roughly 30% of the resampling iterations during the training step:

```
learner$param_set$values = list(error_train = 0.3)

bmr = benchmark(benchmark_grid(tsk("penguins"), list(learner, lrn("classif.rpart")), rsmp("c
aggr = bmr$aggregate(conditions = TRUE)
```

```
aggr[, .(learner_id, warnings, errors, classif.ce)]
```

```
      learner_id warnings errors classif.ce
1: classif.debug        0      8 0.56915966
2: classif.rpart        0      0 0.06403361
```

Even though the debug learner occasionally failed to provide predictions, we still got a statistically sound aggregated performance value which we can compare to the aggregated performance of the classification tree. It is also possible to split the benchmark up into separate `ResampleResult` objects which sometimes helps to get more context. E.g., if we only want to have a closer look into the debug learner, we can extract the errors from the corresponding resample results:

```
rr = aggr[learner_id == "classif.debug"]$resample_result[[1L]]
rr$errors
```

```
   iteration                                msg
1:         1 Error from classif.debug->train()
2:         4 Error from classif.debug->train()
3:         5 Error from classif.debug->train()
4:         6 Error from classif.debug->train()
5:         7 Error from classif.debug->train()
6:         8 Error from classif.debug->train()
7:         9 Error from classif.debug->train()
8:        10 Error from classif.debug->train()
```

A similar problem to failed model fits emerges when a learner predicts only a subset of the observations in the test set (and predicts `NA` or no value for others). A typical case is, e.g., when new and unseen factor levels are encountered in the test data. Imagine again that our goal is to benchmark two algorithms using cross-validation on some binary classification task:

- Algorithm A is an ordinary logistic regression.
- Algorithm B is also an ordinary logistic regression, but with a twist: If the logistic regression is rather certain about the predicted label ($> 90\%$ probability), it returns the label and returns a missing value otherwise.

Clearly, at its core, this is the same problem as outlined before. Algorithm B would easily outperform algorithm A, but you have not factored in that you can not generate predictions for all observations. Long story short, if a fallback learner is involved, missing predictions of the base learner will be automatically replaced with predictions from the fallback learner. This is illustrated in the following example:

```
task = tsk("penguins")
learner = lrn("classif.debug")

# this hyperparameter sets the ratio of missing predictions
```

```
learner$param_set$values = list(predict_missing = 0.5)

# without fallback
p = learner$train(task)$predict(task)
table(p$response, useNA = "always")
```

```
Adelie Chinstrap    Gentoo      <NA>
   172         0         0       172
```

```
# with fallback
learner$fallback = lrn("classif.featureless")
p = learner$train(task)$predict(task)
table(p$response, useNA = "always")
```

```
Adelie Chinstrap    Gentoo      <NA>
   172         0       172         0
```

Summed up, by combining encapsulation and fallback learners, it is possible to benchmark even quite unreliable or unstable learning algorithms in a convenient and statistically sound fashion.

9.2.3. Actionable Errors

All problems demonstrated so far are artificial and non-actionable. The usefulness of encapsulation and error logging usually only really becomes apparent in large benchmarks, especially in combination with parallelization. For a fair comparison, you need to distinguish between the following cases:

(a) You have made a mistake, e.g., forgot a required preprocessing step in your pipeline. Action: Fix problems, restart computation.
(b) Temporary problems related to the executing system, e.g., network hiccups. Action: Restart computation.
(c) Intrinsic, deterministic and reproducible problem with the model fitting. Action: Impute with fallback learner.

The package mlr3batchmark provides functionality to map jobs of a benchmark to computational jobs for the package `batchtools`. This provides a convenient way get fine-grained control over the execution of each single resampling iteration and then combine the results afterwards to a `BenchmarkResult` again to proceed with the analysis.

9.3. Data Backends

In mlr3, `Tasks` store their data in an abstract data object, the `DataBackend`. A backend provides a unified API to retrieve subsets of the data or query information about it, regardless of how the data is actually stored. The default backend uses `data.table` via the `DataBackendDataTable` as a very fast and efficient in-memory database. For example, we can query some information of the `mlr_tasks_penguins` task:

```
task = tsk("penguins")
backend = task$backend
backend$nrow
```

```
[1] 344
```

```
backend$ncol
```

```
[1] 9
```

For bigger data, or when working with many tasks simultaneously in the same R session, it can be necessary to interface out-of-memory data to reduce the memory requirements. This way, only the part of the data which is currently required by the learners will be placed in the main memory to operate on. There are multiple options to archive this:

1. `DataBackendDplyr` which interfaces the R package `dbplyr`, extending `dplyr` to work on many popular databases like MariaDB, PostgreSQL or SQLite.
2. `DataBackendDuckDB` for the impressive DuckDB database connected via `duckdb`: a fast, zero-configuration alternative to SQLite.
3. `DataBackendDuckDB`, again, but for Parquet files. The data does not need to be converted to DuckDB's native storage format, you can work directly on directories containing one or multiple files stored in the popular Parquet format.

9.3.1. Databases with DataBackendDplyr

To demonstrate the `DataBackendDplyr` we use the NYC flights data set from the `nycflights13` package and move it into a SQLite database. Although `as_sqlite_backend()` provides a convenient function to perform this step, we construct the database manually here.

```
# load data
requireNamespace("DBI")
requireNamespace("RSQLite")
requireNamespace("nycflights13")
data("flights", package = "nycflights13")
str(flights)
```

```
tibble [336,776 x 19] (S3: tbl_df/tbl/data.frame)
 $ year          : int [1:336776] 2013 2013 2013 2013 2013 2013 2013 2013 2013 2013 ...
 $ month         : int [1:336776] 1 1 1 1 1 1 1 1 1 1 ...
 $ day           : int [1:336776] 1 1 1 1 1 1 1 1 1 1 ...
 $ dep_time      : int [1:336776] 517 533 542 544 554 554 555 557 557 558 ...
 $ sched_dep_time: int [1:336776] 515 529 540 545 600 558 600 600 600 600 ...
 $ dep_delay     : num [1:336776] 2 4 2 -1 -6 -4 -5 -3 -3 -2 ...
 $ arr_time      : int [1:336776] 830 850 923 1004 812 740 913 709 838 753 ...
 $ sched_arr_time: int [1:336776] 819 830 850 1022 837 728 854 723 846 745 ...
 $ arr_delay     : num [1:336776] 11 20 33 -18 -25 12 19 -14 -8 8 ...
 $ carrier       : chr [1:336776] "UA" "UA" "AA" "B6" ...
 $ flight        : int [1:336776] 1545 1714 1141 725 461 1696 507 5708 79 301 ...
 $ tailnum       : chr [1:336776] "N14228" "N24211" "N619AA" "N804JB" ...
 $ origin        : chr [1:336776] "EWR" "LGA" "JFK" "JFK" ...
 $ dest          : chr [1:336776] "IAH" "IAH" "MIA" "BQN" ...
 $ air_time      : num [1:336776] 227 227 160 183 116 150 158 53 140 138 ...
 $ distance      : num [1:336776] 1400 1416 1089 1576 762 ...
 $ hour          : num [1:336776] 5 5 5 5 6 5 6 6 6 6 ...
 $ minute        : num [1:336776] 15 29 40 45 0 58 0 0 0 0 ...
 $ time_hour     : POSIXct[1:336776], format: "2013-01-01 05:00:00" "2013-01-01 05:00:00" ...
```

```
# add column of unique row ids
flights$row_id = 1:nrow(flights)

# create sqlite database in temporary file
path = tempfile("flights", fileext = ".sqlite")
con = DBI::dbConnect(RSQLite::SQLite(), path)
tbl = DBI::dbWriteTable(con, "flights", as.data.frame(flights))
DBI::dbDisconnect(con)

# remove in-memory data
rm(flights)
```

With the SQLite database stored in file `path`, we now re-establish a connection and switch to dplyr/dbplyr for some essential preprocessing.

```
# establish connection
con = DBI::dbConnect(RSQLite::SQLite(), path)

# select the "flights" table, enter dplyr
library("dplyr")
```

```
Attaching package: 'dplyr'

The following objects are masked from 'package:data.table':
```

```
    between, first, last

The following objects are masked from 'package:stats':

    filter, lag

The following objects are masked from 'package:base':

    intersect, setdiff, setequal, union
```

```
library("dbplyr")
```

```
Attaching package: 'dbplyr'

The following objects are masked from 'package:dplyr':

    ident, sql
```

```
tbl = tbl(con, "flights")
```

First, we select a subset of columns to work on:

```
keep = c("row_id", "year", "month", "day", "hour", "minute", "dep_time",
  "arr_time", "carrier", "flight", "air_time", "distance", "arr_delay")
tbl = select(tbl, all_of(keep))
```

Additionally, we remove those observations where the arrival delay (`arr_delay`) has a missing value:

```
tbl = filter(tbl, !is.na(arr_delay))
```

To keep runtime reasonable for this toy example, we filter the data to only use every second row:

```
tbl = filter(tbl, row_id %% 2 == 0)
```

The factor levels of the feature `carrier` are merged so that infrequent carriers are replaced by level "other":

```
tbl = mutate(tbl, carrier = case_when(
  carrier %in% c("OO", "HA", "YV", "F9", "AS", "FL", "VX", "WN") ~ "other",
  TRUE ~ carrier))
```

Next, the processed table is used to create a `mlr3db::DataBackendDplyr` from `mlr3db`:

```
library("mlr3db")
b = as_data_backend(tbl, primary_key = "row_id")
```

We can now use the interface of DataBackend to query some basic information about the data:

```
b$nrow
```

```
[1] 163707
```

```
b$ncol
```

```
[1] 13
```

```
b$head()
```

```
   row_id year month day hour minute dep_time arr_time carrier flight air_time
1:      2 2013     1   1    5     29      533      850      UA   1714      227
2:      4 2013     1   1    5     45      544     1004      B6    725      183
3:      6 2013     1   1    5     58      554      740      UA   1696      150
4:      8 2013     1   1    6      0      557      709      EV   5708       53
5:     10 2013     1   1    6      0      558      753      AA    301      138
6:     12 2013     1   1    6      0      558      853      B6     71      158
2 variables not shown: [distance, arr_delay]
```

Note that the DataBackendDplyr does not know about any rows or columns we have filtered out with dplyr before, it just operates on the view we provided.

As we now have constructed a backend, we can switch over to mlr3 for model fitting and create the following mlr3 objects:

- A regression task, based on the previously created mlr3db::DataBackendDplyr.
- A regression learner (regr.rpart).
- A resampling strategy: 3 times repeated subsampling using 2% of the observations for training ("subsampling")
- Measures "mse", "time_train" and "time_predict"

```
task = as_task_regr(b, id = "flights_sqlite", target = "arr_delay")
learner = lrn("regr.rpart")
measures = mlr_measures$mget(c("regr.mse", "time_train", "time_predict"))
resampling = rsmp("subsampling", repeats = 3, ratio = 0.02)
```

We pass all these objects to resample() to perform a simple resampling with three iterations. In each iteration, only the required subset of the data is queried from the SQLite database and passed to rpart::rpart():

```
rr = resample(task, learner, resampling)
print(rr)
```

```
<ResampleResult> of 3 iterations
* Task: flights_sqlite
* Learner: regr.rpart
* Warnings: 0 in 0 iterations
* Errors: 0 in 0 iterations
```

```
rr$aggregate(measures)
```

```
    regr.mse   time_train time_predict
1246.0767508    0.3503333    2.2830000
```

Note that we still have an active connection to the database. To properly close it, we remove the `tbl` object referencing the connection and then close the connection.

```
rm(tbl)
DBI::dbDisconnect(con)
```

9.3.2. Parquet Files with DataBackendDuckDB

While storing the Task's data in memory is most efficient w.r.t. accessing it for model fitting, this has two major disadvantages:

1. Although you might only need a small proportion of the data, the complete data frame sits in memory and consumes memory. This is especially a problem if you work with many tasks simultaneously.
2. During parallelization, the complete data needs to be transferred to the workers which can cause significant overhead.

A very simple way to avoid this is given by just converting the `DataBackendDataTable` to a `DataBackendDuckDB`. As we have already demonstrated how to operate on a SQLite database, and DuckDB is not different in that regard. To convert a `data.frame` to DuckDB, we provide the helper function `as_duckdb_backend()`. Only two arguments are required: the `data.frame` to convert, and a `path` to store the data.

While this is useful while working with many tasks simultaneously in order to keep the memory requirements reasonable, the more frequent use case for DuckDB are nowadays Parquet files. Parquet is a popular column-oriented data storage format supporting efficient compression, making it far superior to other popular data exchange formats such as CSV.

To demonstrate working with Parquet files, we first query the location of an example data set shipped with `mlr3db`:

```
path = system.file(file.path("extdata", "spam.parquet"), package = "mlr3db")
```

We can then create a DataBackendDuckDB based on this file and convert the backend to a classification task, all without loading the dataset into memory:

```
backend = as_duckdb_backend(path)
task = as_task_classif(backend, target = "type")
print(task)
```

```
<TaskClassif:backend> (4601 x 58)
* Target: type
* Properties: twoclass
* Features (57):
  - dbl (57): address, addresses, all, business, capitalAve,
    capitalLong, capitalTotal, charDollar, charExclamation, charHash,
    charRoundbracket, charSemicolon, charSquarebracket, conference,
    credit, cs, data, direct, edu, email, font, free, george, hp, hpl,
    internet, lab, labs, mail, make, meeting, money, num000, num1999,
    num3d, num415, num650, num85, num857, order, original, our, over,
    parts, people, pm, project, re, receive, remove, report, table,
    technology, telnet, will, you, your
```

Accessing the data internally triggers a query and data is fetched to be stored in an in-memory `data.frame`, but only the required subsets.

9.4. Parameters (using paradox)

> **Note**
>
> We are currently revising the book. This section contains a lot of legacy code. You can find the new paradox syntax in the Defining a Tuning Spaces section.

The paradox package offers a language for the description of *parameter spaces*, as well as tools for useful operations on these parameter spaces. A parameter space is often useful when describing:

- A set of sensible input values for an R function
- The set of possible values that slots of a configuration object can take
- The search space of an optimization process

The tools provided by paradox therefore relate to:

- **Parameter checking**: Verifying that a set of parameters satisfies the conditions of a parameter space
- **Parameter sampling**: Generating parameter values that lie in the parameter space for systematic exploration of program behavior depending on these parameters

paradox is, by nature, an auxiliary package that derives its usefulness from other packages that make use of it. It is heavily utilized in other mlr-org packages such as mlr3, mlr3pipelines, and mlr3tuning.

9.4.1. Reference Based Objects

paradox is the spiritual successor to the ParamHelpers package and was written from scratch using the R6 class system. The most important consequence of this is that all objects created in paradox are "reference-based", unlike most other objects in R. When a change is made to a ParamSet object, for example by adding a parameter using the `$add()` function, all variables that point to this ParamSet will contain the changed object. To create an independent copy of a ParamSet, the `$clone()` method needs to be used:

```
library("paradox")

ps = ParamSet$new()
ps2 = ps
ps3 = ps$clone(deep = TRUE)
print(ps) # the same for ps2 and ps3
```

```
<ParamSet>
Empty.
```

```
ps$add(ParamLgl$new("a"))
```

```
print(ps)  # ps was changed
```

```
<ParamSet>
   id    class lower upper nlevels        default value
1:  a ParamLgl    NA    NA       2 <NoDefault[3]>
```

```
print(ps2) # contains the same reference as ps
```

```
<ParamSet>
   id    class lower upper nlevels        default value
1:  a ParamLgl    NA    NA       2 <NoDefault[3]>
```

```
print(ps3) # is a "clone" of the old (empty) ps
```

```
<ParamSet>
Empty.
```

9.4.2. Defining a Parameter Space

9.4.2.1. Single Parameters

The basic building block for describing parameter spaces is the `Param` class. It represents a single parameter, which usually can take a single atomic value. Consider, for example, trying to configure the `rpart` package's `rpart.control` object. It has various components (`minsplit`, `cp`, ...) that all take a single value, and that would all be represented by a different instance of a `Param` object.

The `Param` class has various subclasses that represent different value types:

- `ParamInt`: Integer numbers
- `ParamDbl`: Real numbers
- `ParamFct`: String values from a set of possible values, similar to R `factor`s
- `ParamLgl`: Truth values (`TRUE` / `FALSE`), as `logical`s in R
- `ParamUty`: Parameter that can take any value

A particular instance of a parameter is created by calling the attached `$new()` function:

```
library("paradox")
parA = ParamLgl$new(id = "A")
parB = ParamInt$new(id = "B", lower = 0, upper = 10, tags = c("tag1", "tag2"))
parC = ParamDbl$new(id = "C", lower = 0, upper = 4, special_vals = list(NULL))
parD = ParamFct$new(id = "D", levels = c("x", "y", "z"), default = "y")
parE = ParamUty$new(id = "E", custom_check = function(x) checkmate::checkFunction(x))
```

Every parameter must have:

- **id** - A name for the parameter within the parameter set
- **default** - A default value
- **special_vals** - A list of values that are accepted even if they do not conform to the type
- **tags** - Tags that can be used to organize parameters

The numeric (`Int` and `Dbl`) parameters furthermore allow for specification of a **lower** and **upper** bound. Meanwhile, the `Fct` parameter must be given a vector of **levels** that define the possible states its parameter can take. The `Uty` parameter can also have a **`custom_check`** function that must return `TRUE` when a value is acceptable and may return a `character(1)` error description otherwise. The example above defines `parE` as a parameter that only accepts functions.

All values which are given to the constructor are then accessible from the object for inspection using `$`. Although all these values can be changed for a parameter after construction, this can be a bad idea and should be avoided when possible.

Instead, a new parameter should be constructed. Besides the possible values that can be given to a constructor, there are also the `$class`, `$nlevels`, `$is_bounded`, `$has_default`, `$storage_type`, `$is_number` and `$is_categ` slots that give information about a parameter.

A list of all slots can be found in `?Param`.

```
parB$lower
```

```
[1] 0
```

```
parA$levels
```

```
[1]  TRUE FALSE
```

```
parE$class
```

```
[1] "ParamUty"
```

It is also possible to get all information of a Param as data.table by calling as.data.table().

```
as.data.table(parA)
```

```
   id    class lower upper      levels nlevels is_bounded special_vals
1:  A ParamLgl    NA    NA  TRUE,FALSE       2       TRUE    <list[0]>
3 variables not shown: [default, storage_type, tags]
```

9.4.2.1.1. Type / Range Checking

A Param object offers the possibility to check whether a value satisfies its condition, i.e. is of the right type, and also falls within the range of allowed values, using the $test(), $check(), and $assert() functions. test() should be used within conditional checks and returns TRUE or FALSE, while check() returns an error description when a value does not conform to the parameter (and thus plays well with the "checkmate::assert()" function). assert() will throw an error whenever a value does not fit.

```
parA$test(FALSE)
```

```
[1] TRUE
```

```
parA$test("FALSE")
```

```
[1] FALSE
```

```
parA$check("FALSE")
```

```
[1] "Must be of type 'logical flag', not 'character'"
```

Instead of testing single parameters, it is often more convenient to check a whole set of parameters using a ParamSet.

9.4.2.2. Parameter Sets

The ordered collection of parameters is handled in a ParamSet[1]. It is initialized using the `$new()` function and optionally takes a list of Params as argument. Parameters can also be added to the constructed ParamSet using the `$add()` function. It is even possible to add whole ParamSets to other ParamSets.

```
ps = ParamSet$new(list(parA, parB))
ps$add(parC)
ps$add(ParamSet$new(list(parD, parE)))
print(ps)
```

```
<ParamSet>
   id    class lower upper nlevels        default value
1:  A ParamLgl    NA    NA       2 <NoDefault[3]>
2:  B ParamInt     0    10      11 <NoDefault[3]>
3:  C ParamDbl     0     4     Inf <NoDefault[3]>
4:  D ParamFct    NA    NA       3               y
5:  E ParamUty    NA    NA     Inf <NoDefault[3]>
```

The individual parameters can be accessed through the `$params` slot. It is also possible to get information about all parameters in a vectorized fashion using mostly the same slots as for individual Params (i.e. `$class`, `$levels` etc.), see `?ParamSet` for details.

It is possible to reduce ParamSets using the **`$subset`** method. Be aware that it modifies a ParamSet in-place, so a "clone" must be created first if the original ParamSet should not be modified.

```
psSmall = ps$clone()
psSmall$subset(c("A", "B", "C"))
print(psSmall)
```

```
<ParamSet>
   id    class lower upper nlevels        default value
1:  A ParamLgl    NA    NA       2 <NoDefault[3]>
2:  B ParamInt     0    10      11 <NoDefault[3]>
3:  C ParamDbl     0     4     Inf <NoDefault[3]>
```

Just as for Params, and much more useful, it is possible to get the ParamSet as a `data.table` using `as.data.table()`. This makes it easy to subset parameters on certain conditions and aggregate information about them, using the variety of methods provided by `data.table`.

```
as.data.table(ps)
```

[1] Although the name is suggestive of a "Set"-valued Param, this is unrelated to the other objects that follow the `ParamXxx` naming scheme.

```
   id    class lower upper      levels nlevels is_bounded special_vals
1:  A ParamLgl    NA    NA TRUE,FALSE       2       TRUE    <list[0]>
2:  B ParamInt     0    10                 11       TRUE    <list[0]>
3:  C ParamDbl     0     4                Inf       TRUE    <list[1]>
4:  D ParamFct    NA    NA       x,y,z       3       TRUE    <list[0]>
5:  E ParamUty    NA    NA                 Inf      FALSE    <list[0]>
3 variables not shown: [default, storage_type, tags]
```

9.4.2.2.1. Type / Range Checking

Similar to individual Params, the ParamSet provides `$test()`, `$check()` and `$assert()` functions that allow for type and range checking of parameters. Their argument must be a named list with values that are checked against the respective parameters. It is possible to check only a subset of parameters.

```
ps$check(list(A = TRUE, B = 0, E = identity))
```

```
[1] TRUE
```

```
ps$check(list(A = 1))
```

```
[1] "A: Must be of type 'logical flag', not 'double'"
```

```
ps$check(list(Z = 1))
```

```
[1] "Parameter 'Z' not available. Did you mean 'A' / 'B' / 'C'?"
```

9.4.2.2.2. Values in a ParamSet

Although a ParamSet fundamentally represents a value space, it also has a slot `$values` that can contain a point within that space. This is useful because many things that define a parameter space need similar operations (like parameter checking) that can be simplified. The `$values` slot contains a named list that is always checked against parameter constraints. When trying to set parameter values, e.g. for mlr3 Learners, it is the `$values` slot of its `$param_set` that needs to be used.

```
ps$values = list(A = TRUE, B = 0)
ps$values$B = 1
print(ps$values)
```

```
$A
[1] TRUE

$B
[1] 1
```

The parameter constraints are automatically checked:

```
ps$values$B = 100
```

```
Error in self$assert(xs): Assertion on 'xs' failed: B: Element 1 is not <= 10.
```

9.4.2.2.3. Dependencies

It is often the case that certain parameters are irrelevant or should not be given depending on values of other parameters. An example would be a parameter that switches a certain algorithm feature (for example regularization) on or off, combined with another parameter that controls the behavior of that feature (e.g. a regularization parameter). The second parameter would be said to *depend* on the first parameter having the value `TRUE`.

A dependency can be added using the `$add_dep` method, which takes both the ids of the "depender" and "dependee" parameters as well as a `Condition` object. The `Condition` object represents the check to be performed on the "dependee". Currently it can be created using `CondEqual$new()` and `CondAnyOf$new()`. Multiple dependencies can be added, and parameters that depend on others can again be depended on, as long as no cyclic dependencies are introduced.

The consequence of dependencies are twofold: For one, the `$check()`, `$test()` and `$assert()` tests will not accept the presence of a parameter if its dependency is not met. Furthermore, when sampling or creating grid designs from a `ParamSet`, the dependencies will be respected (see Parameter Sampling, in particular Hierarchical Sampler).

The following example makes parameter `D` depend on parameter `A` being `FALSE`, and parameter `B` depend on parameter `D` being one of `"x"` or `"y"`. This introduces an implicit dependency of `B` on `A` being `FALSE` as well, because `D` does not take any value if `A` is `TRUE`.

```
ps$add_dep("D", "A", CondEqual$new(FALSE))
ps$add_dep("B", "D", CondAnyOf$new(c("x", "y")))
```

```
ps$check(list(A = FALSE, D = "x", B = 1))          # OK: all dependencies met
```

```
[1] TRUE
```

```
ps$check(list(A = FALSE, D = "z", B = 1))          # B's dependency is not met
```

```
[1] "The parameter 'B' can only be set if the following condition is met 'D  {x, y}'. Instead
```

```
ps$check(list(A = FALSE, B = 1))                    # B's dependency is not met
```

```
[1] "The parameter 'B' can only be set if the following condition is met 'D   {x, y}'. Instead
```

```
ps$check(list(A = FALSE, D = "z"))                  # OK: B is absent
```

```
[1] TRUE
```

```
ps$check(list(A = TRUE))                            # OK: neither B nor D present
```

```
[1] TRUE
```

```
ps$check(list(A = TRUE, D = "x", B = 1))            # D's dependency is not met
```

```
[1] "The parameter 'D' can only be set if the following condition is met 'A = FALSE'. Instead t
```

```
ps$check(list(A = TRUE, B = 1))                     # B's dependency is not met
```

```
[1] "The parameter 'B' can only be set if the following condition is met 'D   {x, y}'. Instead
```

Internally, the dependencies are represented as a `data.table`, which can be accessed listed in the `$deps` slot. This `data.table` can even be mutated, to e.g. remove dependencies. There are no sanity checks done when the `$deps` slot is changed this way. Therefore it is advised to be cautious.

```
ps$deps
```

```
   id on           cond
1:  D  A <CondEqual[9]>
2:  B  D <CondAnyOf[9]>
```

9.4.2.3. Vector Parameters

Unlike in the old ParamHelpers package, there are no more vectorial parameters in paradox. Instead, it is now possible to create multiple copies of a single parameter using the `$rep` function. This creates a ParamSet consisting of multiple copies of the parameter, which can then (optionally) be added to another ParamSet.

```
ps2d = ParamDbl$new("x", lower = 0, upper = 1)$rep(2)
print(ps2d)
```

```
<ParamSet>
        id    class lower upper nlevels        default value
1: x_rep_1 ParamDbl     0     1     Inf <NoDefault[3]>
2: x_rep_2 ParamDbl     0     1     Inf <NoDefault[3]>
```

```
ps$add(ps2d)
print(ps)
```

```
<ParamSet>
        id    class lower upper nlevels        default parents value
1:       A ParamLgl    NA    NA       2 <NoDefault[3]>           TRUE
2:       B ParamInt     0    10      11 <NoDefault[3]>       D     1
3:       C ParamDbl     0     4     Inf <NoDefault[3]>
4:       D ParamFct    NA    NA       3              y       A
5:       E ParamUty    NA    NA     Inf <NoDefault[3]>
6: x_rep_1 ParamDbl     0     1     Inf <NoDefault[3]>
7: x_rep_2 ParamDbl     0     1     Inf <NoDefault[3]>
```

It is also possible to use a `ParamUty` to accept vectorial parameters, which also works for parameters of variable length. A `ParamSet` containing a `ParamUty` can be used for parameter checking, but not for sampling. To sample values for a method that needs a vectorial parameter, it is advised to use a parameter transformation function that creates a vector from atomic values.

Assembling a vector from repeated parameters is aided by the parameter's `$tags`: Parameters that were generated by the `$rep()` command automatically get tagged as belonging to a group of repeated parameters.

```
ps$tags
```

```
$A
character(0)

$B
[1] "tag1" "tag2"

$C
character(0)

$D
character(0)
```

```
$E
character(0)

$x_rep_1
[1] "x_rep"

$x_rep_2
[1] "x_rep"
```

9.4.3. Parameter Sampling

It is often useful to have a list of possible parameter values that can be systematically iterated through, for example to find parameter values for which an algorithm performs particularly well (tuning). `paradox` offers a variety of functions that allow creating evenly-spaced parameter values in a "grid" design as well as random sampling. In the latter case, it is possible to influence the sampling distribution in more or less fine detail.

A point to always keep in mind while sampling is that only numerical and factorial parameters that are bounded can be sampled from, i.e. not `ParamUty`. Furthermore, for most samplers `ParamInt` and `ParamDbl` must have finite lower and upper bounds.

9.4.3.1. Parameter Designs

Functions that sample the parameter space fundamentally return an object of the `Design` class. These objects contain the sampled data as a `data.table` under the `$data` slot, and also offer conversion to a list of parameter-values using the **`$transpose()`** function.

9.4.3.2. Grid Design

The `generate_design_grid()` function is used to create grid designs that contain all combinations of parameter values: All possible values for `ParamLgl` and `ParamFct`, and values with a given resolution for `ParamInt` and `ParamDbl`. The resolution can be given for all numeric parameters, or for specific named parameters through the `param_resolutions` parameter.

```
design = generate_design_grid(psSmall, 2)
print(design)
```

```
<Design> with 8 rows:
       A  B C
1:  TRUE  0 0
2:  TRUE  0 4
3:  TRUE 10 0
4:  TRUE 10 4
5: FALSE  0 0
6: FALSE  0 4
```

```
7: FALSE 10 0
8: FALSE 10 4
```

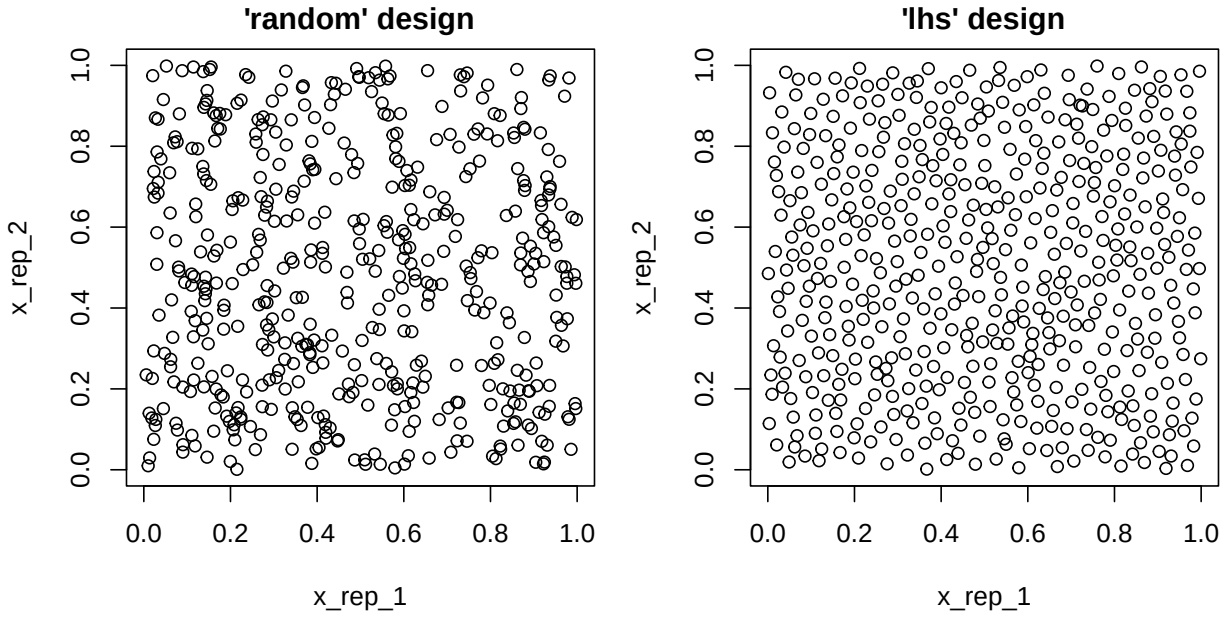
```
generate_design_grid(psSmall, param_resolutions = c(B = 1, C = 2))
```

```
<Design> with 4 rows:
   B C     A
1: 0 0  TRUE
2: 0 0 FALSE
3: 0 4  TRUE
4: 0 4 FALSE
```

9.4.3.3. Random Sampling

paradox offers different methods for random sampling, which vary in the degree to which they can be configured. The easiest way to get a uniformly random sample of parameters is generate_design_random(). It is also possible to create "latin hypercube" sampled parameter values using generate_design_lhs(), which utilizes the lhs package. LHS-sampling creates low-discrepancy sampled values that cover the parameter space more evenly than purely random values.

```
pvrand = generate_design_random(ps2d, 500)
pvlhs = generate_design_lhs(ps2d, 500)
```



9.4.3.4. Generalized Sampling: The `Sampler` Class

It may sometimes be desirable to configure parameter sampling in more detail. `paradox` uses the `Sampler` abstract base class for sampling, which has many different sub-classes that can be parameterized and combined to control the sampling process. It is even possible to create further sub-classes of the `Sampler` class (or of any of *its* subclasses) for even more possibilities.

Every `Sampler` object has a `sample()` function, which takes one argument, the number of instances to sample, and returns a `Design` object.

9.4.3.4.1. 1D-Samplers

There is a variety of samplers that sample values for a single parameter. These are `Sampler1DUnif` (uniform sampling), `Sampler1DCateg` (sampling for categorical parameters), `Sampler1DNormal` (normally distributed sampling, truncated at parameter bounds), and `Sampler1DRfun` (arbitrary 1D sampling, given a random-function). These are initialized with a single `Param`, and can then be used to sample values.

```
sampA = Sampler1DCateg$new(parA)
sampA$sample(5)
```

```
<Design> with 5 rows:
       A
1:  TRUE
2:  TRUE
3: FALSE
4: FALSE
5: FALSE
```

9.4.3.4.2. Hierarchical Sampler

The `SamplerHierarchical` sampler is an auxiliary sampler that combines many 1D-Samplers to get a combined distribution. Its name "hierarchical" implies that it is able to respect parameter dependencies. This suggests that parameters only get sampled when their dependencies are met.

The following example shows how this works: The `Int` parameter `B` depends on the `Lgl` parameter `A` being `TRUE`. `A` is sampled to be `TRUE` in about half the cases, in which case `B` takes a value between 0 and 10. In the cases where `A` is `FALSE`, `B` is set to `NA`.

```
psSmall$add_dep("B", "A", CondEqual$new(TRUE))
sampH = SamplerHierarchical$new(psSmall,
  list(Sampler1DCateg$new(parA),
    Sampler1DUnif$new(parB),
    Sampler1DUnif$new(parC))
)
sampled = sampH$sample(1000)
table(sampled$data[, c("A", "B")], useNA = "ifany")
```

```
       B
A         0   1   2   3   4   5   6   7   8   9  10 <NA>
  FALSE   0   0   0   0   0   0   0   0   0   0   0  493
  TRUE   51  49  50  42  47  47  44  52  35  49  41    0
```

9.4.3.4.3. Joint Sampler

Another way of combining samplers is the SamplerJointIndep. SamplerJointIndep also makes it possible to combine Samplers that are not 1D. However, SamplerJointIndep currently can not handle ParamSets with dependencies.

```
sampJ = SamplerJointIndep$new(
  list(Sampler1DUnif$new(ParamDbl$new("x", 0, 1)),
    Sampler1DUnif$new(ParamDbl$new("y", 0, 1)))
)
sampJ$sample(5)
```

```
<Design> with 5 rows:
           x          y
1: 0.9980689 0.29325189
2: 0.5696531 0.14916164
3: 0.7999309 0.87583963
4: 0.9762024 0.06155586
5: 0.4334808 0.60938294
```

9.4.3.4.4. SamplerUnif

The Sampler used in generate_design_random() is the SamplerUnif sampler, which corresponds to a HierarchicalSampler of Sampler1DUnif for all parameters.

9.4.4. Parameter Transformation

While the different Samplers allow for a wide specification of parameter distributions, there are cases where the simplest way of getting a desired distribution is to sample parameters from a simple distribution (such as the uniform distribution) and then transform them. This can be done by assigning a function to the `$trafo` slot of a ParamSet. The `$trafo` function is called with two parameters:

- The list of parameter values to be transformed as `x`
- The ParamSet itself as `param_set`

The `$trafo` function must return a list of transformed parameter values.

The transformation is performed when calling the `$transpose` function of the Design object returned by a Sampler with the `trafo` ParamSet to `TRUE` (the default). The following, for example, creates a parameter that is exponentially distributed:

```
psexp = ParamSet$new(list(ParamDbl$new("par", 0, 1)))
psexp$trafo = function(x, param_set) {
  x$par = -log(x$par)
  x
}
design = generate_design_random(psexp, 2)
print(design)
```

```
<Design> with 2 rows:
          par
1: 0.07302144
2: 0.15870426
```

```
design$transpose()  # trafo is TRUE
```

```
[[1]]
[[1]]$par
[1] 2.617002


[[2]]
[[2]]$par
[1] 1.840713
```

Compare this to `$transpose()` without transformation:

```
design$transpose(trafo = FALSE)
```

```
[[1]]
[[1]]$par
[1] 0.07302144


[[2]]
[[2]]$par
[1] 0.1587043
```

9.4.4.1. Transformation between Types

Usually the design created with one `ParamSet` is then used to configure other objects that themselves have a `ParamSet` which defines the values they take. The `ParamSet`s which can be used for random sampling, however, are restricted in some ways: They must have finite bounds, and they may not contain "untyped" (`ParamUty`) parameters. `$trafo` provides the glue for these situations. There

is relatively little constraint on the trafo function's return value, so it is possible to return values that have different bounds or even types than the original ParamSet. It is even possible to remove some parameters and add new ones.

Suppose, for example, that a certain method requires a *function* as a parameter. Let's say a function that summarizes its data in a certain way. The user can pass functions like `median()` or `mean()`, but could also pass quantiles or something completely different. This method would probably use the following ParamSet:

```
methodPS = ParamSet$new(
  list(
    ParamUty$new("fun",
      custom_check = function(x) checkmate::checkFunction(x, nargs = 1))
  )
)
print(methodPS)
```

```
<ParamSet>
    id    class lower upper nlevels        default value
1: fun ParamUty    NA    NA     Inf <NoDefault[3]>
```

If one wanted to sample this method, using one of four functions, a way to do this would be:

```
samplingPS = ParamSet$new(
  list(
    ParamFct$new("fun", c("mean", "median", "min", "max"))
  )
)

samplingPS$trafo = function(x, param_set) {
  # x$fun is a `character(1)`,
  # in particular one of 'mean', 'median', 'min', 'max'.
  # We want to turn it into a function!
  x$fun = get(x$fun, mode = "function")
  x
}
```

```
design = generate_design_random(samplingPS, 2)
print(design)
```

```
<Design> with 2 rows:
   fun
1: max
2: min
```

Note that the Design only contains the column "fun" as a character column. To get a single value as a *function*, the $transpose function is used.

```
xvals = design$transpose()
print(xvals[[1]])
```

```
$fun
function (..., na.rm = FALSE)  .Primitive("max")
```

We can now check that it fits the requirements set by methodPS, and that fun it is in fact a function:

```
methodPS$check(xvals[[1]])
```

```
[1] TRUE
```

```
xvals[[1]]$fun(1:10)
```

```
[1] 10
```

Imagine now that a different kind of parametrization of the function is desired: The user wants to give a function that selects a certain quantile, where the quantile is set by a parameter. In that case the $transpose function could generate a function in a different way. For interpretability, the parameter is called "quantile" before transformation, and the "fun" parameter is generated on the fly.

```
samplingPS2 = ParamSet$new(
  list(
    ParamDbl$new("quantile", 0, 1)
  )
)

samplingPS2$trafo = function(x, param_set) {
  # x$quantile is a `numeric(1)` between 0 and 1.
  # We want to turn it into a function!
  list(fun = function(input) quantile(input, x$quantile))
}
```

```
design = generate_design_random(samplingPS2, 2)
print(design)
```

```
<Design> with 2 rows:
     quantile
1: 0.03543698
2: 0.65563727
```

The Design now contains the column "quantile" that will be used by the $transpose function to create the fun parameter. We also check that it fits the requirement set by methodPS, and that it is a function.

```
xvals = design$transpose()
print(xvals[[1]])
```

```
$fun
function(input) quantile(input, x$quantile)
<environment: 0x562ae66408e0>
```

```
methodPS$check(xvals[[1]])
```

```
[1] TRUE
```

```
xvals[[1]]$fun(1:10)
```

```
3.543698%
 1.318933
```

9.4.5. Defining a Tuning Spaces

When running an optimization, it is important to inform the tuning algorithm about what hyperparameters are valid. Here the names, types, and valid ranges of each hyperparameter are important. All this information is communicated with objects of the class ParamSet, which is defined in paradox. While it is possible to create ParamSet-objects using its $new-constructor, it is much shorter and readable to use the ps-shortcut, which will be presented here. For an in-depth description of paradox and its classes, see Section 9.4.

Note, that ParamSet objects exist in two contexts. First, ParamSet-objects are used to define the space of valid parameter settings for a learner (and other objects). Second, they are used to define a search space for tuning. We are mainly interested in the latter. For example we can consider the minsplit parameter of the classif.rpart Learner. The ParamSet associated with the learner has a lower but *no* upper bound. However, for tuning the value, a lower *and* upper bound must be given because tuning search spaces need to be bounded. For Learner or PipeOp objects, typically "unbounded" ParamSets are used. Here, however, we will mainly focus on creating "bounded" ParamSets that can be used for tuning. See Section 9.4 for more details on using ParamSets to define parameter ranges for use-cases besides tuning.

9.4.5.1. Creating ParamSets

An empty "ParamSet") – not yet very useful – can be constructed using just the "ps") call:

```
search_space = ps()
print(search_space)
```

```
<ParamSet>
Empty.
```

ps takes named Domain arguments that are turned into parameters. A possible search space for the "classif.svm" learner could for example be:

```
search_space = ps(
  cost = p_dbl(lower = 0.1, upper = 10),
  kernel = p_fct(levels = c("polynomial", "radial"))
)
print(search_space)
```

```
<ParamSet>
       id    class lower upper nlevels        default value
1:   cost ParamDbl   0.1    10     Inf <NoDefault[3]>
2: kernel ParamFct    NA    NA       2 <NoDefault[3]>
```

There are five domain constructors that produce a parameters when given to ps:

Constructor	Description	Is bounded?	Underlying Class
p_dbl	Real valued parameter ("double")	When upper and lower are given	ParamDbl
p_int	Integer parameter	When upper and lower are given	ParamInt
p_fct	Discrete valued parameter ("factor")	Always	ParamFct
p_lgl	Logical / Boolean parameter	Always	ParamLgl
p_uty	Untyped parameter	Never	ParamUty

These domain constructors each take some of the following arguments:

- **lower**, **upper**: lower and upper bound of numerical parameters (p_dbl and p_int). These need to be given to get bounded parameter spaces valid for tuning.
- **levels**: Allowed categorical values for p_fct parameters. Required argument for p_fct. See below for more details on this parameter.
- **trafo**: transformation function, see below.
- **depends**: dependencies, see below.
- **tags**: Further information about a parameter, used for example by the hyperband tuner.
- **default**: Value corresponding to default behavior when the parameter is not given. Not used for tuning search spaces.

- **special_vals**: Valid values besides the normally accepted values for a parameter. Not used for tuning search spaces.
- **custom_check**: Function that checks whether a value given to p_uty is valid. Not used for tuning search spaces.

The lower and upper parameters are always in the first and second position respectively, except for p_fct where levels is in the first position. It is preferred to omit the labels (ex: upper = 0.1 becomes just 0.1). This way of defining a ParamSet is more concise than the equivalent definition above. Preferred:

```
search_space = ps(cost = p_dbl(0.1, 10), kernel = p_fct(c("polynomial", "radial")))
```

9.4.5.2. Transformations (trafo)

We can use the paradox function generate_design_grid to look at the values that would be evaluated by grid search. (We are using rbindlist() here because the result of $transpose() is a list that is harder to read. If we didn't use $transpose(), on the other hand, the transformations that we investigate here are not applied.) In generate_design_grid(search_space, 3), search_space is the ParamSet argument and 3 is the specified resolution in the parameter space. The resolution for categorical parameters is ignored; these parameters always produce a grid over all of their valid levels. For numerical parameters the endpoints of the params are always included in the grid, so if there were 3 levels for the kernel instead of 2 there would be 9 rows, or if the resolution was 4 in this example there would be 8 rows in the resulting table.

```
library("data.table")
rbindlist(generate_design_grid(search_space, 3)$transpose())
```

```
    cost     kernel
1:  0.10 polynomial
2:  0.10     radial
3:  5.05 polynomial
4:  5.05     radial
5: 10.00 polynomial
6: 10.00     radial
```

We notice that the cost parameter is taken on a linear scale. We assume, however, that the difference of cost between 0.1 and 1 should have a similar effect as the difference between 1 and 10. Therefore it makes more sense to tune it on a *logarithmic scale*. This is done by using a **transformation** (trafo). This is a function that is applied to a parameter after it has been sampled by the tuner. We can tune cost on a logarithmic scale by sampling on the linear scale [-1, 1] and computing 10^x from that value.

```
search_space = ps(
  cost = p_dbl(-1, 1, trafo = function(x) 10^x),
  kernel = p_fct(c("polynomial", "radial"))
)
```

```
rbindlist(generate_design_grid(search_space, 3)$transpose())
```

```
   cost     kernel
1:  0.1 polynomial
2:  0.1     radial
3:  1.0 polynomial
4:  1.0     radial
5: 10.0 polynomial
6: 10.0     radial
```

It is even possible to attach another transformation to the ParamSet as a whole that gets executed after individual parameter's transformations were performed. It is given through the `.extra_trafo` argument and should be a function with parameters `x` and `param_set` that takes a list of parameter values in `x` and returns a modified list. This transformation can access all parameter values of an evaluation and modify them with interactions. It is even possible to add or remove parameters. (The following is a bit of a silly example.)

```
search_space = ps(
  cost = p_dbl(-1, 1, trafo = function(x) 10^x),
  kernel = p_fct(c("polynomial", "radial")),
  .extra_trafo = function(x, param_set) {
    if (x$kernel == "polynomial") {
      x$cost = x$cost * 2
    }
    x
  }
)
rbindlist(generate_design_grid(search_space, 3)$transpose())
```

```
   cost     kernel
1:  0.2 polynomial
2:  0.1     radial
3:  2.0 polynomial
4:  1.0     radial
5: 20.0 polynomial
6: 10.0     radial
```

The available types of search space parameters are limited: continuous, integer, discrete, and logical scalars. There are many machine learning algorithms, however, that take parameters of other types, for example vectors or functions. These can not be defined in a search space ParamSet, and they are often given as ParamUty in the Learner's ParamSet. When trying to tune over these hyperparameters, it is necessary to perform a Transformation that changes the type of a parameter.

An example is the `class.weights` parameter of the Support Vector Machine (SVM), which takes a named vector of class weights with one entry for each target class. The trafo that would tune `class.weights` for the `mlr_tasks_spam`, `'tsk("spam")` dataset could be:

```
search_space = ps(
  class.weights = p_dbl(0.1, 0.9, trafo = function(x) c(spam = x, nonspam = 1 - x))
)
generate_design_grid(search_space, 3)$transpose()
```

```
[[1]]
[[1]]$class.weights
   spam nonspam
    0.1     0.9


[[2]]
[[2]]$class.weights
   spam nonspam
    0.5     0.5


[[3]]
[[3]]$class.weights
   spam nonspam
    0.9     0.1
```

(We are omitting `rbindlist()` in this example because it breaks the vector valued return elements.)

9.4.6. Automatic Factor Level Transformation

A common use-case is the necessity to specify a list of values that should all be tried (or sampled from). It may be the case that a hyperparameter accepts function objects as values and a certain list of functions should be tried. Or it may be that a choice of special numeric values should be tried. For this, the `p_fct` constructor's `level` argument may be a value that is not a `character` vector, but something else. If, for example, only the values `0.1`, `3`, and `10` should be tried for the `cost` parameter, even when doing random search, then the following search space would achieve that:

```
search_space = ps(
  cost = p_fct(c(0.1, 3, 10)),
  kernel = p_fct(c("polynomial", "radial"))
)
rbindlist(generate_design_grid(search_space, 3)$transpose())
```

```
   cost     kernel
1:  0.1 polynomial
2:  0.1     radial
3:  3.0 polynomial
4:  3.0     radial
5: 10.0 polynomial
6: 10.0     radial
```

This is equivalent to the following:

```
search_space = ps(
  cost = p_fct(c("0.1", "3", "10"),
    trafo = function(x) list(`0.1` = 0.1, `3` = 3, `10` = 10)[[x]]),
  kernel = p_fct(c("polynomial", "radial"))
)
rbindlist(generate_design_grid(search_space, 3)$transpose())
```

```
   cost     kernel
1:  0.1 polynomial
2:  0.1     radial
3:  3.0 polynomial
4:  3.0     radial
5: 10.0 polynomial
6: 10.0     radial
```

Note: Though the resolution is 3 here, in this case it doesn't matter because both `cost` and `kernel` are factors (the resolution for categorical variables is ignored, these parameters always produce a grid over all their valid levels).

This may seem silly, but makes sense when considering that factorial tuning parameters are always `character` values:

```
search_space = ps(
  cost = p_fct(c(0.1, 3, 10)),
  kernel = p_fct(c("polynomial", "radial"))
)
typeof(search_space$params$cost$levels)
```

```
[1] "character"
```

Be aware that this results in an "unordered" hyperparameter, however. Tuning algorithms that make use of ordering information of parameters, like genetic algorithms or model based optimization, will perform worse when this is done. For these algorithms, it may make more sense to define a `p_dbl` or `p_int` with a more fitting trafo.

The `class.weights` case from above can also be implemented like this, if there are only a few candidates of `class.weights` vectors that should be tried. Note that the `levels` argument of `p_fct` must be named if there is no easy way for `as.character()` to create names:

```
search_space = ps(
  class.weights = p_fct(
    list(
      candidate_a = c(spam = 0.5, nonspam = 0.5),
      candidate_b = c(spam = 0.3, nonspam = 0.7)
    )
  )
)
generate_design_grid(search_space)$transpose()
```

```
[[1]]
[[1]]$class.weights
   spam nonspam
    0.5     0.5


[[2]]
[[2]]$class.weights
   spam nonspam
    0.3     0.7
```

9.4.6.1. Parameter Dependencies (`depends`)

Some parameters are only relevant when another parameter has a certain value, or one of several values. The Support Vector Machine (SVM), for example, has the `degree` parameter that is only valid when `kernel` is `"polynomial"`. This can be specified using the `depends` argument. It is an expression that must involve other parameters and be of the form `<param> == <scalar>`, `<param> %in% <vector>`, or multiple of these chained by `&&`. To tune the `degree` parameter, one would need to do the following:

```
search_space = ps(
  cost = p_dbl(-1, 1, trafo = function(x) 10^x),
  kernel = p_fct(c("polynomial", "radial")),
  degree = p_int(1, 3, depends = kernel == "polynomial")
)
rbindlist(generate_design_grid(search_space, 3)$transpose(), fill = TRUE)
```

```
    cost     kernel degree
1:  0.1 polynomial      1
2:  0.1 polynomial      2
3:  0.1 polynomial      3
```

```
 4:  0.1     radial     NA
 5:  1.0 polynomial      1
 6:  1.0 polynomial      2
 7:  1.0 polynomial      3
 8:  1.0     radial     NA
 9: 10.0 polynomial      1
10: 10.0 polynomial      2
11: 10.0 polynomial      3
12: 10.0     radial     NA
```

9.4.6.2. Creating Tuning ParamSets from other ParamSets

Having to define a tuning `ParamSet` for a `Learner` that already has parameter set information may seem unnecessarily tedious, and there is indeed a way to create tuning `ParamSets` from a `Learner`'s `ParamSet`, making use of as much information as already available.

This is done by setting values of a `Learner`'s `ParamSet` to so-called `TuneTokens`, constructed with a `to_tune` call. This can be done in the same way that other hyperparameters are set to specific values. It can be understood as the hyperparameters being tagged for later tuning. The resulting `ParamSet` used for tuning can be retrieved using the `$search_space()` method.

```
learner = lrn("classif.svm")
learner$param_set$values$kernel = "polynomial" # for example
learner$param_set$values$degree = to_tune(lower = 1, upper = 3)

print(learner$param_set$search_space())
```

```
<ParamSet>
       id    class lower upper nlevels        default value
1: degree ParamInt     1     3       3 <NoDefault[3]>
```

```
rbindlist(generate_design_grid(
  learner$param_set$search_space(), 3)$transpose()
)
```

```
   degree
1:      1
2:      2
3:      3
```

It is possible to omit `lower` here, because it can be inferred from the lower bound of the `degree` parameter itself. For other parameters, that are already bounded, it is possible to not give any bounds at all, because their ranges are already bounded. An example is the logical `shrinking` hyperparameter:

```
learner$param_set$values$shrinking = to_tune()

print(learner$param_set$search_space())
```

```
<ParamSet>
          id    class lower upper nlevels        default value
1:    degree ParamInt     1     3       3 <NoDefault[3]>
2: shrinking ParamLgl    NA    NA       2           TRUE
```

```
rbindlist(generate_design_grid(
  learner$param_set$search_space(), 3)$transpose()
)
```

```
   degree shrinking
1:      1      TRUE
2:      1     FALSE
3:      2      TRUE
4:      2     FALSE
5:      3      TRUE
6:      3     FALSE
```

`"to_tune"`) can also be constructed with a `Domain` object, i.e. something constructed with a `p_***` call. This way it is possible to tune continuous parameters with discrete values, or to give trafos or dependencies. One could, for example, tune the `cost` as above on three given special values, and introduce a dependency of `shrinking` on it. Notice that a short form for `to_tune(<levels>)` is a short form of `to_tune(p_fct(<levels>))`.

> **Note**
>
> When introducing the dependency, we need to use the `degree` value from *before* the implicit trafo, which is the name or `as.character()` of the respective value, here `"val2"`!

```
learner$param_set$values$type = "C-classification" # needs to be set because of a bug in par
learner$param_set$values$cost = to_tune(c(val1 = 0.3, val2 = 0.7))
learner$param_set$values$shrinking = to_tune(p_lgl(depends = cost == "val2"))

print(learner$param_set$search_space())
```

```
<ParamSet>
          id    class lower upper nlevels        default parents value
1:      cost ParamFct    NA    NA       2 <NoDefault[3]>
2:    degree ParamInt     1     3       3 <NoDefault[3]>
3: shrinking ParamLgl    NA    NA       2 <NoDefault[3]>    cost
Trafo is set.
```

```
rbindlist(generate_design_grid(learner$param_set$search_space(), 3)$transpose(), fill = TRUE
```

```
   degree cost shrinking
1:      1  0.3        NA
2:      1  0.7      TRUE
3:      1  0.7     FALSE
4:      2  0.3        NA
5:      2  0.7      TRUE
6:      2  0.7     FALSE
7:      3  0.3        NA
8:      3  0.7      TRUE
9:      3  0.7     FALSE
```

The `"search_space()` picks up dependencies from the underlying ParamSet automatically. So if the `kernel` is tuned, then `degree` automatically gets the dependency on it, without us having to specify that. (Here we reset `cost` and `shrinking` to `NULL` for the sake of clarity of the generated output.)

```
learner$param_set$values$cost = NULL
learner$param_set$values$shrinking = NULL
learner$param_set$values$kernel = to_tune(c("polynomial", "radial"))

print(learner$param_set$search_space())
```

```
<ParamSet>
       id    class lower upper nlevels        default parents value
1: degree ParamInt     1     3       3 <NoDefault[3]>  kernel
2: kernel ParamFct    NA    NA       2 <NoDefault[3]>
```

```
rbindlist(generate_design_grid(learner$param_set$search_space(), 3)$transpose(), fill = TRUE
```

```
       kernel degree
1: polynomial      1
2: polynomial      2
3: polynomial      3
4:     radial     NA
```

It is even possible to define whole ParamSets that get tuned over for a single parameter. This may be especially useful for vector hyperparameters that should be searched along multiple dimensions. This ParamSet must, however, have an `.extra_trafo` that returns a list with a single element, because it corresponds to a single hyperparameter that is being tuned. Suppose the `class.weights` hyperparameter should be tuned along two dimensions:

```
learner$param_set$values$class.weights = to_tune(
  ps(spam = p_dbl(0.1, 0.9), nonspam = p_dbl(0.1, 0.9),
    .extra_trafo = function(x, param_set) list(c(spam = x$spam, nonspam = x$nonspam))
))
head(generate_design_grid(learner$param_set$search_space(), 3)$transpose(), 3)
```

```
[[1]]
[[1]]$kernel
[1] "polynomial"

[[1]]$degree
[1] 1

[[1]]$class.weights
   spam nonspam
    0.1     0.1


[[2]]
[[2]]$kernel
[1] "polynomial"

[[2]]$degree
[1] 1

[[2]]$class.weights
   spam nonspam
    0.1     0.5


[[3]]
[[3]]$kernel
[1] "polynomial"

[[3]]$degree
[1] 1

[[3]]$class.weights
   spam nonspam
    0.1     0.9
```

9.5. Logging

We use the lgr package for logging and progress output.

9.5.1. Changing mlr3 logging levels

To change the setting for mlr3 for the current session, you need to retrieve the logger (which is a R6 object) from lgr, and then change the threshold of the like this:

```
requireNamespace("lgr")

logger = lgr::get_logger("mlr3")
logger$set_threshold("<level>")
```

The default log level is "info". All available levels can be listed as follows:

```
getOption("lgr.log_levels")
```

```
fatal error  warn  info debug trace
  100   200   300   400   500   600
```

To increase verbosity, set the log level to a higher value, e.g. to "debug" with:

```
lgr::get_logger("mlr3")$set_threshold("debug")
```

To reduce the verbosity, reduce the log level to warn:

```
lgr::get_logger("mlr3")$set_threshold("warn")
```

lgr comes with a global option called "lgr.default_threshold" which can be set via options() to make your choice permanent across sessions.

Also note that the optimization packages such as mlr3tuning mlr3fselect use the logger of their base package bbotk. To disable the output from mlr3, but keep the output from mlr3tuning, reduce the verbosity for the logger mlr3 and optionally change the logger bbotk to the desired level.

```
lgr::get_logger("mlr3")$set_threshold("warn")
lgr::get_logger("bbotk")$set_threshold("info")
```

9.5.2. Redirecting output

Redirecting output is already extensively covered in the documentation and vignette of lgr. Here is just a short example that adds an additional appender to log events into a temporary file in JSON format:

```
tf = tempfile("mlr3log_", fileext = ".json")

# get the logger as R6 object
logger = lgr::get_logger("mlr")
```

```
5
6  # add Json appender
7  logger$add_appender(lgr::AppenderJson$new(tf), name = "json")
8
9  # signal a warning
10 logger$warn("this is a warning from mlr3")
11
12 # print the contents of the file
13 cat(readLines(tf))
14
15 # remove the appender again
16 logger$remove_appender("json")
```

9.5.3. Immediate Log Feedback

mlr3 uses future and encapsulation to make evaluations fast, stable, and reproducible. However, this may lead to logs being delayed, out of order, or, in case of some errors, not present at all.

When it is necessary to have immediate access to log messages, for example to investigate problems, one may therefore choose to disable future and encapsulation. This can be done by enabling the debug mode using `options(mlr.debug = TRUE)`; the `$encapsulate` slot of learners should also be set to `"none"` (default) or `"evaluate"`, but not `"callr"`. This should only be done to investigate problems, however, and not for production use, because

1. this disables parallelization, and
2. this leads to different RNG behavior and therefore to results that are not reproducible when the debug mode is set.

10. Model Interpretation

The goal of this chapter is to present key methods that allow in-depth posthoc analysis of an already trained model. The methods presented are model-agnostic, i.e. they can be applied to models of different classes. When using predictive models in practice, it is often the case that high performance on a validation set is not enough. Users more and more often want to know which variables are important and how they influence the model's predictions. For the end user, such knowledge allows better utilisation of models in the decision-making process, e.g. by analysing different possible decision options. In addition, if the model's behaviour turns out to be in line with the domain knowledge or the user's intuition then the user's confidence in the prediction will increase. For the modeller, an in-depth analysis of the model allows undesirable model behaviour to be detected and corrected.

Predictive models have numerous applications in virtually every area of life. The increasing availability of data and frameworks to create models has allowed the widespread adoption of these solutions. However, this does not always go together with enough testing of the models and the consequences of incorrect predictions can be severe. The bestseller book „Weapons of Math Destruction'' (O'Neil 2016) discusses examples of deployed black-boxes that have led to wrong-headed decisions, sometimes on a massive scale. So what can we do to make our models more thoroughly tested? The answer is methods that allow deeper interpretation of predictive models. In this chapter, we will provide illustrations of how to perform the most popular of these methods (Holzinger et al. 2022).

In principle, all generic frameworks for model interpretation apply to the models fitted with `mlr3` by just extracting the fitted models from the `Learner` objects.

However, two of the most popular frameworks additionally come with some convenience for `mlr3`, these are

- `iml` presented in Section 10.2, and
- `DALEX` presented in Section 10.3.

Both these packages offer similar functionality, but they differ in design choices. `iml` is based on the R6 class system and for this reason working with it is more similar in style to working with the `mlr3` package. `DALEX` is based on the S3 class system and is mainly focused on the ability to compare multiple different models on the same graph for comparison and on the explainable model analysis process.

10.1. Penguin Task

To understand what model interpretation packages can offer, we start with a thorough example. The goal of this example is to figure out the species of penguins given a set of features. The palmerpenguins::penguins (Horst, Hill, and Gorman 2020) data set will be used which is an alternative to the `iris` data set. The `penguins` data sets contain 8 variables of 344 penguins:

```
data("penguins", package = "palmerpenguins")
str(penguins)
```

```
tibble [344 x 8] (S3: tbl_df/tbl/data.frame)
 $ species          : Factor w/ 3 levels "Adelie","Chinstrap",..: 1 1 1 1 1 1 1 1 1 1 ...
 $ island           : Factor w/ 3 levels "Biscoe","Dream",..: 3 3 3 3 3 3 3 3 3 3 ...
 $ bill_length_mm   : num [1:344] 39.1 39.5 40.3 NA 36.7 39.3 38.9 39.2 34.1 42 ...
 $ bill_depth_mm    : num [1:344] 18.7 17.4 18 NA 19.3 20.6 17.8 19.6 18.1 20.2 ...
 $ flipper_length_mm: int [1:344] 181 186 195 NA 193 190 181 195 193 190 ...
 $ body_mass_g      : int [1:344] 3750 3800 3250 NA 3450 3650 3625 4675 3475 4250 ...
 $ sex              : Factor w/ 2 levels "female","male": 2 1 1 NA 1 2 1 2 NA NA ...
 $ year             : int [1:344] 2007 2007 2007 2007 2007 2007 2007 2007 2007 2007 ...
```

To get started run:

```
library("mlr3")
library("mlr3learners")
set.seed(1)
```

```
penguins = na.omit(penguins)
task_peng = as_task_classif(penguins, target = "species")
```

`penguins = na.omit(penguins)` is to omit the 11 cases with missing values. If not omitted, there will be an error when running the learner from the data points that have N/A for some features.

```
learner = lrn("classif.ranger")
learner$predict_type = "prob"
learner$train(task_peng)
learner$model
```

```
Ranger result

Call:
 ranger::ranger(dependent.variable.name = task$target_names, data = task$data(),      probabil

Type:                             Probability estimation
Number of trees:                  500
Sample size:                      333
```

```
Number of independent variables:  7
Mtry:                             2
Target node size:                 10
Variable importance mode:         none
Splitrule:                        gini
OOB prediction error (Brier s.):  0.01790106
```

```
x = penguins[which(names(penguins) != "species")]
```

As explained in Section Learners, specific learners can be queried with `mlr_learners`. In Section Train/Predict it is recommended for some classifiers to use the `predict_type` as `prob` instead of directly predicting a label. This is what is done in this example. `penguins[which(names(penguins) != "species")]` is the data of all the features and `y` will be the penguins`species`. `learner$train(task_peng)` trains the model and `learner$model` stores the model from the training command. `Predictor` holds the machine learning model and the data. All interpretation methods in `iml` need the machine learning model and the data to be wrapped in the `Predictor` object.

10.2. iml

Author: Shawn Storm

`iml` is an R package that interprets the behaviour and explains predictions of machine learning models. The functions provided in the `iml` package are model-agnostic which gives the flexibility to use any machine learning model.

This chapter provides examples of how to use `iml` with `mlr3`. For more information refer to the IML github and the IML book

Next is the core functionality of `iml`. In this example, three separate interpretation methods will be used: FeatureEffects, FeatureImp and Shapley

- `FeatureEffects` computes the effects for all given features on the model prediction. Different methods are implemented: Accumulated Local Effect (ALE) plots, Partial Dependence Plots (PDPs) and Individual Conditional Expectation (ICE) curves.
- `Shapley` computes feature contributions for single predictions with the Shapley value – an approach from cooperative game theory (Shapley Value).
- `FeatureImp` computes the importance of features by calculating the increase in the model's prediction error after permuting the feature (more here).

10.2.1. FeatureEffects

In addition to the commands above the following two need to be run:

```r
library("iml")

model = Predictor$new(learner, data = x, y = penguins$species)

num_features = c("bill_length_mm", "bill_depth_mm", "flipper_length_mm", "body_mass_g", "yea
effect = FeatureEffects$new(model)
plot(effect, features = num_features)
```

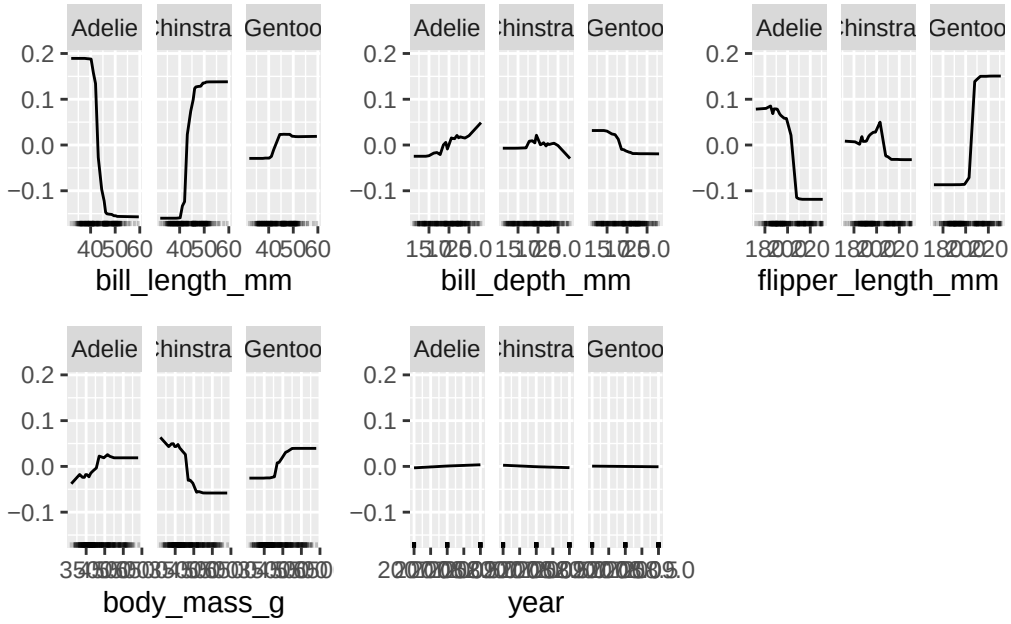


Figure 10.1.: Plot of the results from FeatureEffects. FeatureEffects computes and plots feature effects of prediction models

`effect` stores the object from the `FeatureEffect` computation and the results can then be plotted. In this example, all of the features provided by the `penguins` data set were used.

All features except for `year` provide meaningful interpretable information. It should be clear why `year` doesn't provide anything of significance. `bill_length_mm` shows for example that when the bill length is smaller than roughly 40mm, there is a high chance that the penguin is an Adelie.

10.2.2. Shapley

```r
x = penguins[which(names(penguins) != "species")]
model = Predictor$new(learner, data = penguins, y = "species")
x.interest = data.frame(penguins[1, ])
shapley = Shapley$new(model, x.interest = x.interest)
plot(shapley)
```

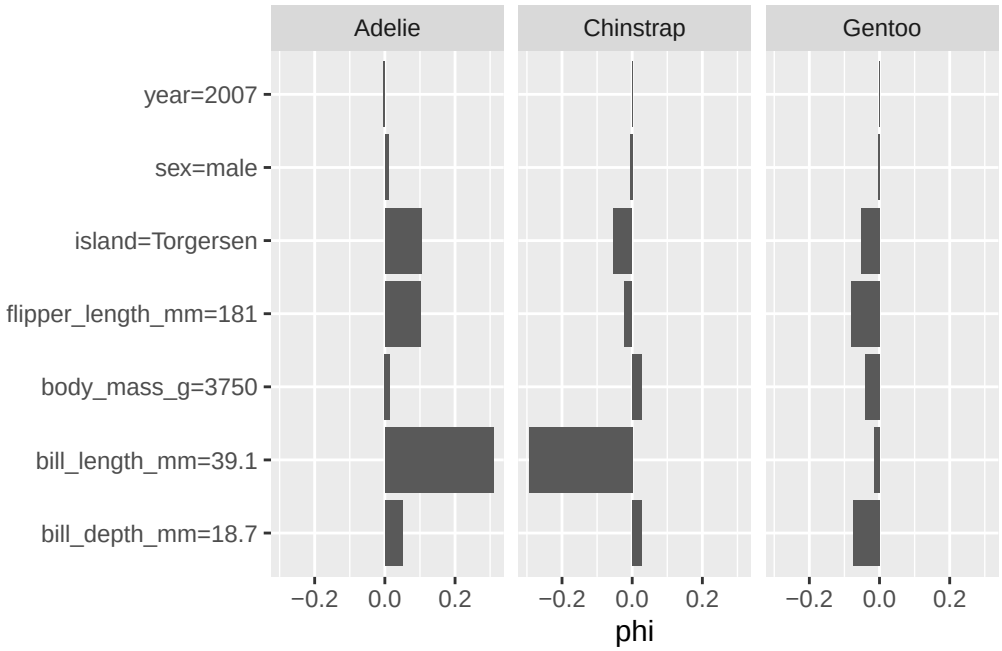


Figure 10.2.: Plot of the results from Shapley. ϕ gives the increase or decrease in probability given the values on the vertical axis

The ϕ provides insight into the probability given the values on the vertical axis. For example, a penguin is less likely to be Gentoo if the bill_depth=18.7 is and much more likely to be Adelie than Chinstrap.

10.2.3. FeatureImp

```
effect = FeatureImp$new(model, loss = "ce")
effect$plot(features = num_features)
```

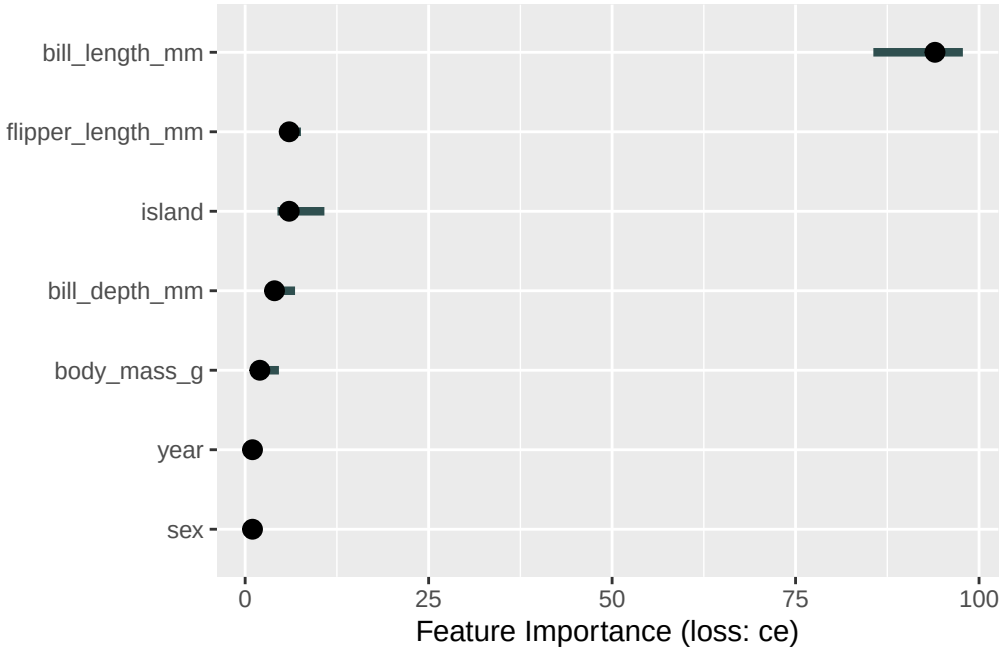


Figure 10.3.: Plot of the results from FeatureImp. FeatureImp visualizes the importance of features given the prediction model

`FeatureImp` shows the level of importance of the features when classifying penguins. It is clear to see that the `bill_length_mm` is of high importance and one should concentrate on the different boundaries of this feature when attempting to classify the three species.

10.2.4. Independent Test Data

It is also interesting to see how well the model performs on a test data set. For this section, exactly as was recommended in Section Train/Predict, 80% of the penguin data set will be used for the training set and 20% for the test set:

```
train_set = sample(task_peng$nrow, 0.8 * task_peng$nrow)
test_set = setdiff(seq_len(task_peng$nrow), train_set)
learner$train(task_peng, row_ids = train_set)
prediction = learner$predict(task_peng, row_ids = test_set)
```

First, we compare the feature importance on training and test set

```
# plot on training
model = Predictor$new(learner, data = penguins[train_set, ], y = "species")
effect = FeatureImp$new(model, loss = "ce")
plot_train = plot(effect, features = num_features)

# plot on test data
```

```
model = Predictor$new(learner, data = penguins[test_set, ], y = "species")
effect = FeatureImp$new(model, loss = "ce")
plot_test = plot(effect, features = num_features)

# combine into single plot
libr
plot
```

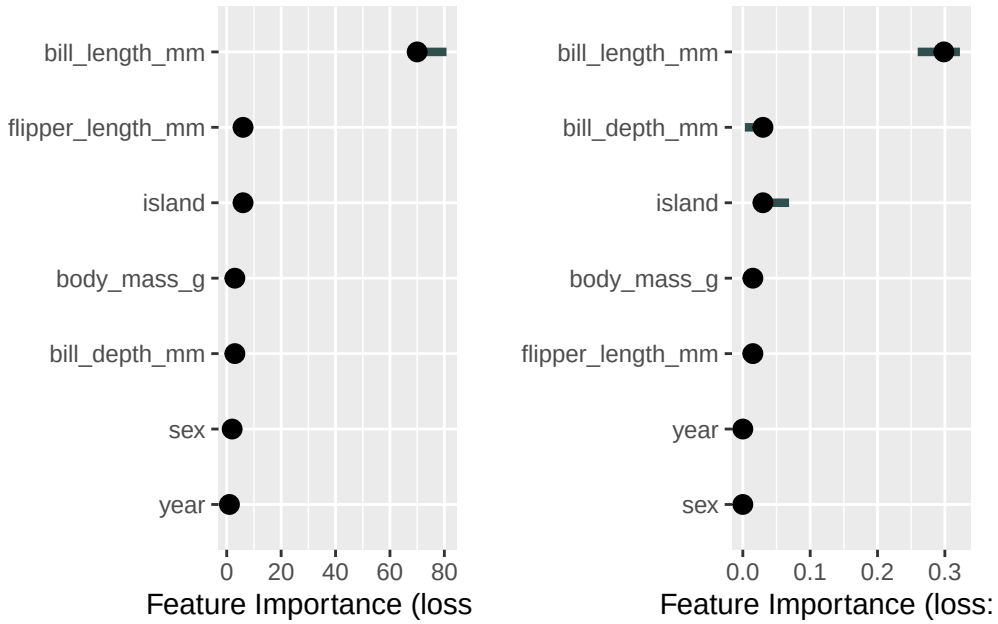


Figure 10.4.: FeatImp on train (left) and test (right)

The results of the train set for `FeatureImp` are very similar, which is expected. We follow a similar approach to compare the feature effects:

```
model = Predictor$new(learner, data = penguins[train_set, ], y = "species")
effect = FeatureEffects$new(model)
plot(effect, features = num_features)
```

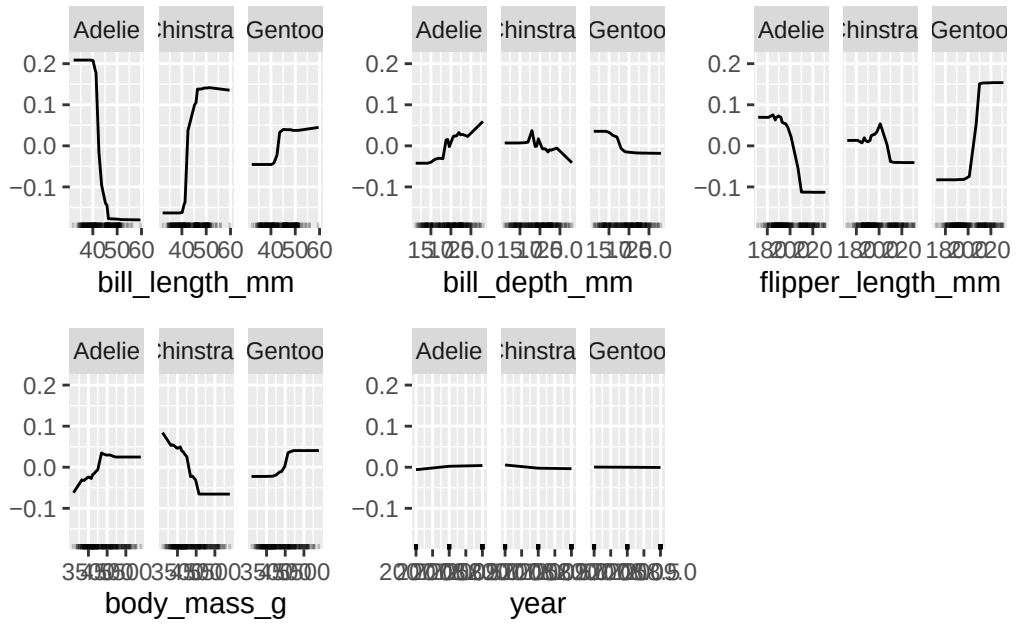


Figure 10.5.: FeatEffect train data set

```
model = Predictor$new(learner, data = penguins[test_set, ], y = "species")
effect = FeatureEffects$new(model)
plot(effect, features = num_features)
```

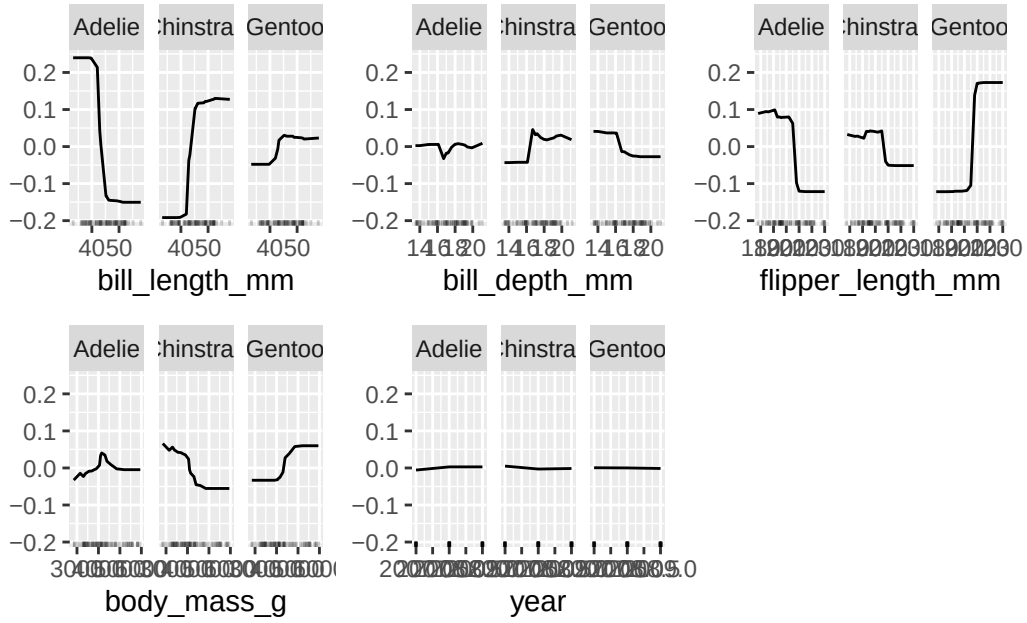


Figure 10.6.: FeatEffect test data set

As is the case with `FeatureImp`, the test data results show either an over- or underestimate of feature importance / feature effects compared to the results where the entire penguin data set was used. This would be a good opportunity for the reader to attempt to resolve the estimation by playing with the amount of features and the amount of data used for both the test and train data sets of `FeatureImp` and `FeatureEffects`. Be sure to not change the line `train_set = sample(task_peng$nrow, 0.8 * task_peng$nrow)` as it will randomly sample the data again.

10.3. DALEX

The `DALEX` (Biecek 2018) package belongs to DrWhy family of solutions created to support the responsible development of machine learning models. It implements the most common methods for explaining predictive models using posthoc model agnostic techniques. You can use it for any model built with the `mlr3` package as well as with other frameworks in `R`. The counterpart in `Python` is the library `dalex` (Baniecki et al. 2021).

The philosophy of working with `DALEX` package is based on the process of explanatory model analysis described in the EMA book (Biecek and Burzykowski 2021). In this chapter, we present code snippets and a general overview of this package. For illustrative purposes, we reuse the `learner` model built in the Section 10.1 on `palmerpenguins::penguins` data.

Once you become familiar with the philosophy of working with the `DALEX` package, you can also use other packages from this family such as `fairmodels` (Wiśniewski and Biecek 2022) for detection and mitigation of biases, `modelStudio` (Baniecki and Biecek 2019) for interactive model exploration, `modelDown` (Romaszko et al. 2019) for the automatic generation of IML model documentation in the form of a report, `survex` (Krzyziński et al. 2023) for the explanation of survival models, or `treeshap` for the analysis of tree-based models.

10.3.1. Explanatory model analysis

The analysis of a model is usually an interactive process starting with a shallow analysis – usually a single-number summary. Then in a series of subsequent steps, one can systematically deepen understanding of the model by exploring the importance of single variables or pairs of variables to an in-depth analysis of the relationship between selected variables to the model outcome. See Bücker et al. (2022) for a broader discussion of what the model exploration process looks like.

This explanatory model analysis (EMA) process can focus on a single observation, in which case we speak of local model analysis, or for a set of observations, in which case we speak of global data analysis. Below, we will present these two scenarios in separate subsections. See Figure 10.7 for an overview of key functions that will be discussed.

Predictive models in R have different internal structures. To be able to analyse them systematically, an intermediate object – a wrapper – is needed to provide a consistent interface for accessing the model. Working with explanations in the `DALEX` package always starts with the creation of such a wrapper with the use of the `DALEX::explain()` function. This function has several arguments that allow the model created by the various frameworks to be parameterised accordingly. For models created in the `mlr3` package, it is more convenient to use the `DALEXtra::explain_mlr3()`.

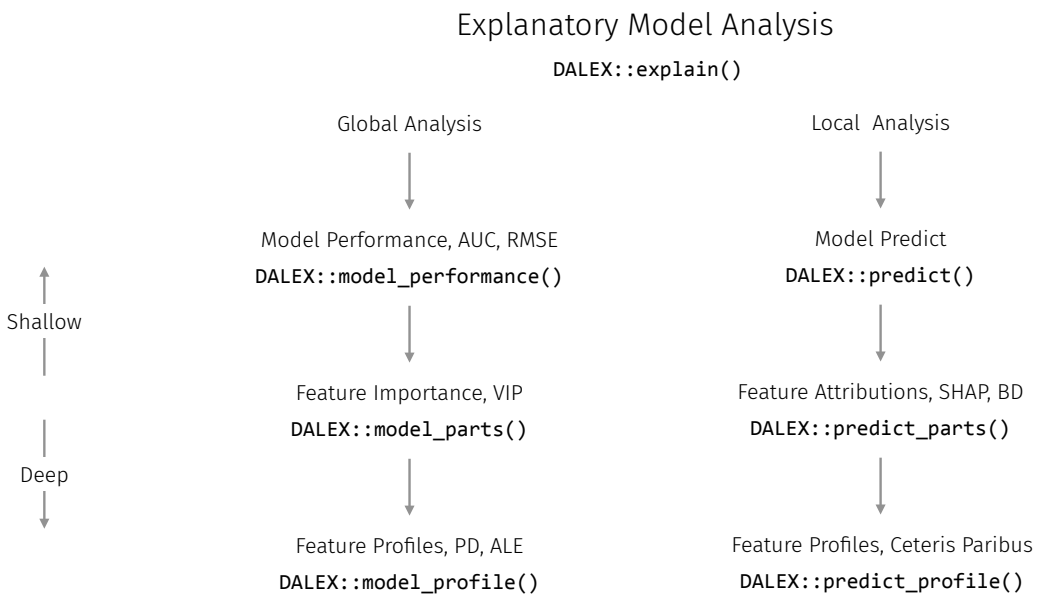


Figure 10.7.: Taxonomy of methods for model exploration presented in this chapter. Left part overview methods for global level exploration while the right part is related to local level model exploration.

```
library("DALEX")
library("DALEXtra")

ranger_exp = DALEX::explain(learner,
  data = penguins[test_set, ],
  y = penguins[test_set, "species"],
  label = "Ranger Penguins",
  colorize = FALSE)
```

```
Preparation of a new explainer is initiated
  -> model label       :  Ranger Penguins
  -> data              :  67  rows  8  cols
  -> data              :  tibble converted into a data.frame
  -> target variable   :  Argument 'y' was a data frame. Converted to a vector. (  WARNING  )
  -> target variable   :  67  values
  -> predict function  :  yhat.LearnerClassif  will be used (  default  )
  -> predicted values  :  No value for predict function target column. (  default  )
  -> model_info        :  package mlr3 , ver. 0.14.1 , task multiclass (  default  )
  -> predicted values  :  predict function returns multiple columns:  3  (  default  )
  -> residual function :  difference between 1 and probability of true class (  default  )
  -> residuals         :  numerical, min =  0 , mean =  0.07756016 , max =  0.5380321
  A new explainer has been created!
```

The `DALEX::explain()` function performs a series of internal checks so the output is a bit verbose.

Turn the `verbose = FALSE` argument to make it less wordy.

10.3.2. Global level exploration

The global model analysis aims to understand how a model behaves on average on a set of observations, most commonly a test set. In the DALEX package, functions for global analysis have names starting with the prefix `model_`.

10.3.2.1. Model Performance

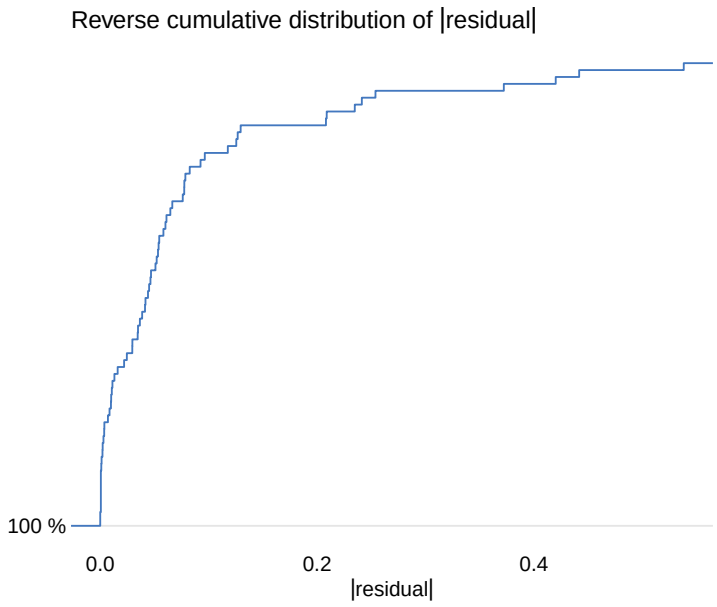
As shown in Figure Figure 10.7, it starts by evaluating the performance of a model. This can be done with a variety of tools, in the DALEX package the default is to use the `DALEX::model_performance` function. Since the `explain` function checks what type of task is being analysed, it can select the appropriate performance measures for it. In our illustration, we have a multi-label classification, so measures such as micro-aggregated F1, macro-aggregated F1 etc. are calculated in the following snippet. One of the calculated measures is cross entropy and it will be used later in the following sections.

Each explanation can be drawn with the generic `plot()` function, for multi-label classification the distribution of residuals is drawn by default.

```
perf_penguin = model_performance(ranger_exp)
perf_penguin
```

```
Measures for:  multiclass
micro_F1   : 1
macro_F1   : 1
w_macro_F1 : 1
accuracy   : 1
w_macro_auc: 1
cross_entro: 6.034954

Residuals:
          0%          10%          20%          30%          40%          50%
0.0000000000 0.0005846154 0.0036863492 0.0111489133 0.0315985873 0.0440341048
         60%          70%          80%          90%         100%
0.0535907937 0.0683762754 0.0956176783 0.2191798413 0.5380321429
```

```
library("ggplot2")
old_theme = set_theme_dalex("ema")
plot(perf_penguin)
```



The task of classifying the penguin species is rather easy, which is why there are so many values of 1 in the performance assessment of this model.

10.3.2.2. Permutational Variable Importance

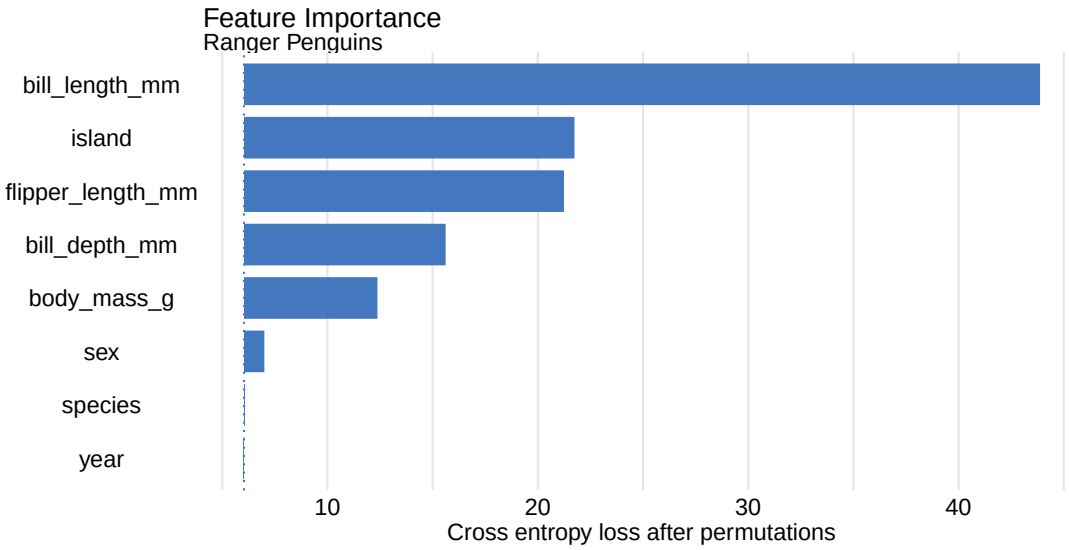
A popular technique for assessing variable importance in a model-agnostic manner is the permutation variable importance. It is based on the difference (or ratio) in the selected loss function after the selected variable or set of variables has been permuted. Read more about this technique in Variable-importance Measures chapter.

The `DALEX::model_parts()` function calculates the importance of variables and its results can be visualized with the generic `plot()` function.

```
ranger_effect = model_parts(ranger_exp)
head(ranger_effect)
```

```
       variable mean_dropout_loss           label
1  _full_model_          6.034954 Ranger Penguins
2          year          5.988560 Ranger Penguins
3       species          6.034954 Ranger Penguins
4           sex          7.002289 Ranger Penguins
5   body_mass_g         12.377824 Ranger Penguins
6 bill_depth_mm         15.617252 Ranger Penguins
```

```
plot(ranger_effect, show_boxplots = FALSE)
```



The bars start in loss (here cross-entropy loss) for the selected data and end in a loss for the data after the permutation of the selected variable. The more important the variable, the more the model will lose after its permutation.

10.3.2.3. Partial Dependence

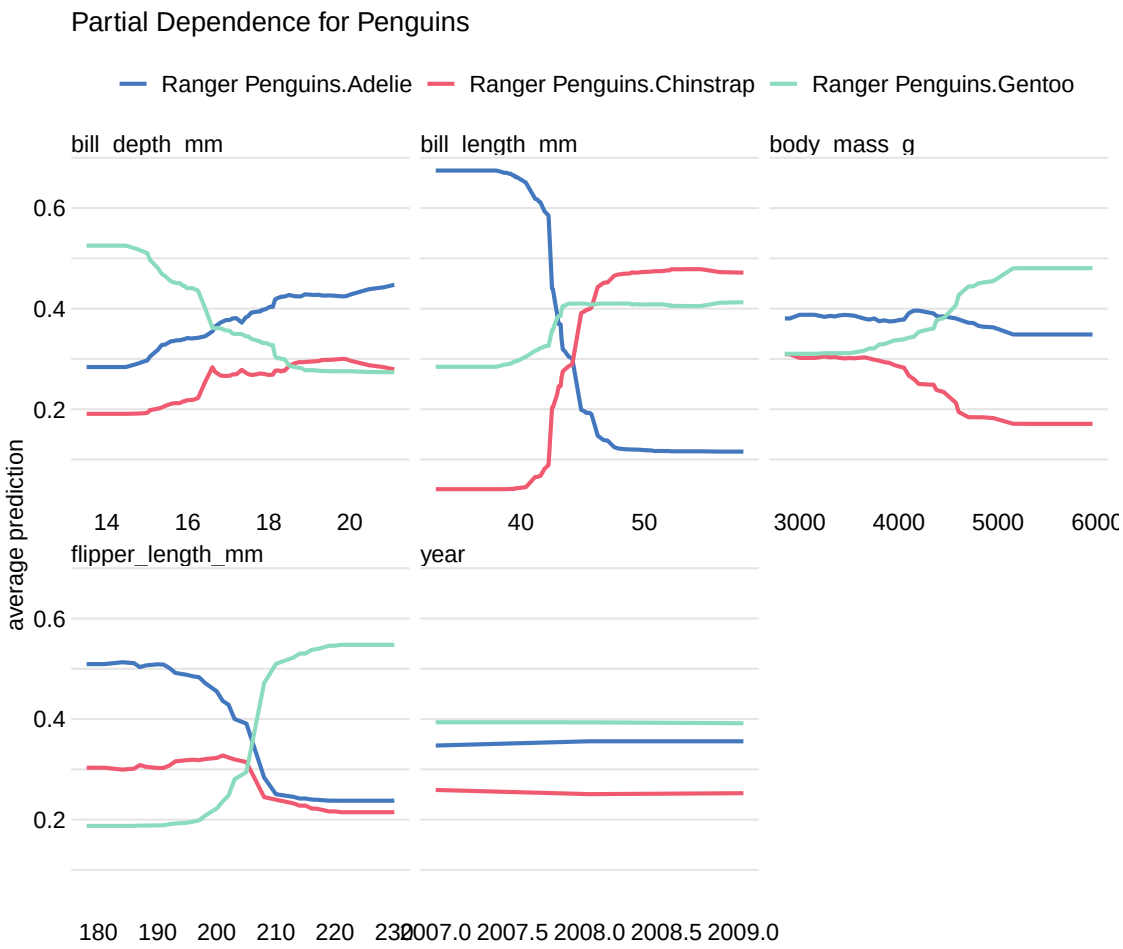
Once we know which variables are most important, we can use Partial Dependence Plots to show how the model, on average, changes with changes in selected variables.

The `DALEX::model_profile()` function calculates the partial dependence profiles. The `type` argument of this function also allows *Marginal profiles* and *Accumulated Local profiles* to be calculated. Again, the result of the explanation can be model_profile with the generic function `plot()`.

```
ranger_profiles = model_profile(ranger_exp)
ranger_profiles
```

```
Top profiles    :
        _vname_                    _label_    _x_     _yhat_ _ids_
1 bill_depth_mm    Ranger Penguins.Adelie 13.500 0.2839077     0
2 bill_depth_mm Ranger Penguins.Chinstrap 13.500 0.1908264     0
3 bill_depth_mm    Ranger Penguins.Gentoo 13.500 0.5252659     0
4 bill_depth_mm    Ranger Penguins.Adelie 13.566 0.2839077     0
5 bill_depth_mm Ranger Penguins.Chinstrap 13.566 0.1908264     0
6 bill_depth_mm    Ranger Penguins.Gentoo 13.566 0.5252659     0
```

```
plot(ranger_profiles) +
  theme(legend.position = "top") +
  ggtitle("Partial Dependence for Penguins","")
```



For the multi-label classification model, profiles are drawn for each class separately by indicating them with different colours. We already know which variable is the most important, so now we can read how the model result changes with the change of this variable. In our example, based on `bill_length_mm` we can separate *Adelie* from *Chinstrap* and based on `flipper_length_mm` we can separate *Adelie* from *Gentoo*.

10.3.3. Local level explanation

The local model analysis aims to understand how a model behaves for a single observation. In the DALEX package, functions for local analysis have names starting with the prefix `predict_`.

We will carry out the following examples using Steve the penguin of the `Adelie` species as an example.

```
steve = penguins[1,]
steve
```

```
# A tibble: 1 x 8
```

```
  species island    bill_length_mm bill_depth_mm flipper_l~1 body_~2 sex    year
  <fct>   <fct>              <dbl>         <dbl>       <int>   <int> <fct> <int>
1 Adelie  Torgersen           39.1          18.7         181    3750 male   2007
# ... with abbreviated variable names 1: flipper_length_mm, 2: body_mass_g
```

10.3.3.1. Model Prediction

As shown in Figure Figure 10.7, the local analysis starts with the calculation of a model prediction.

For Steve, the species was correctly predicted as `Adelie` with high probability.

```
predict(ranger_exp, steve)
```

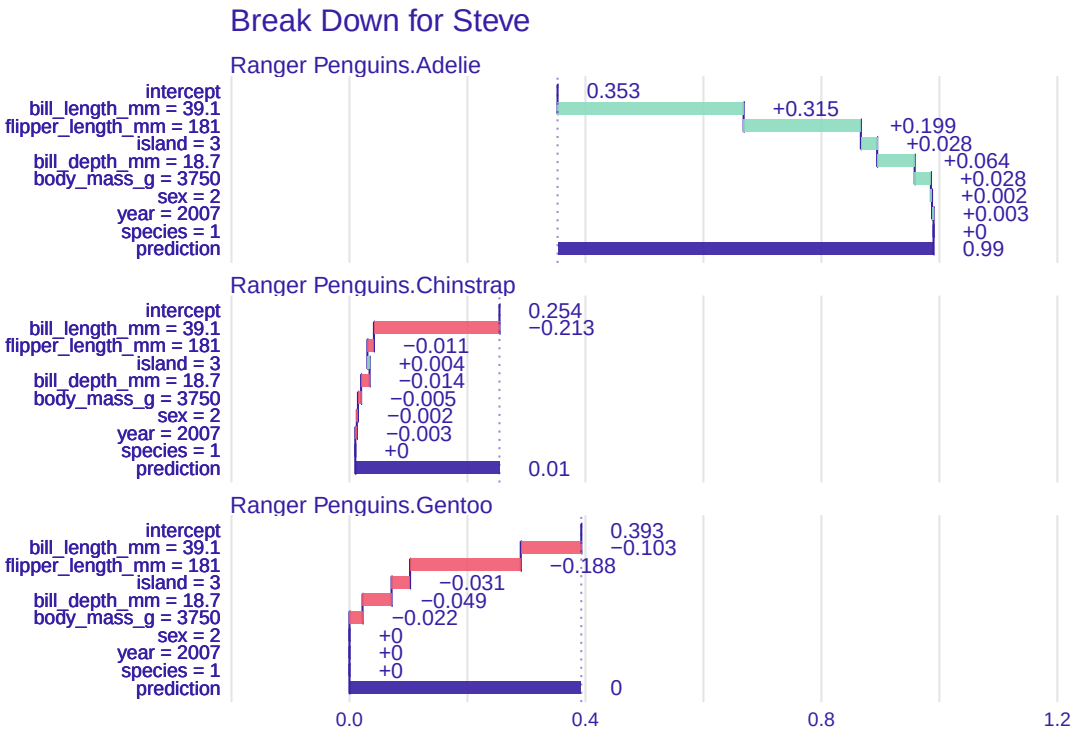
```
        Adelie   Chinstrap Gentoo
[1,] 0.9900897 0.009910317      0
```

10.3.3.2. Break Down

A popular technique for assessing the contributions of variables to model prediction is Break Down (see Introduction to Break Down chapter for more information about this method).

The function `DALEX::predict_parts()` function calculates the attributions of variables and its results can be visualized with the generic `plot()` function.

```
ranger_attributions = predict_parts(ranger_exp, new_observation = steve)
plot(ranger_attributions) + ggtitle("Break Down for Steve")
```



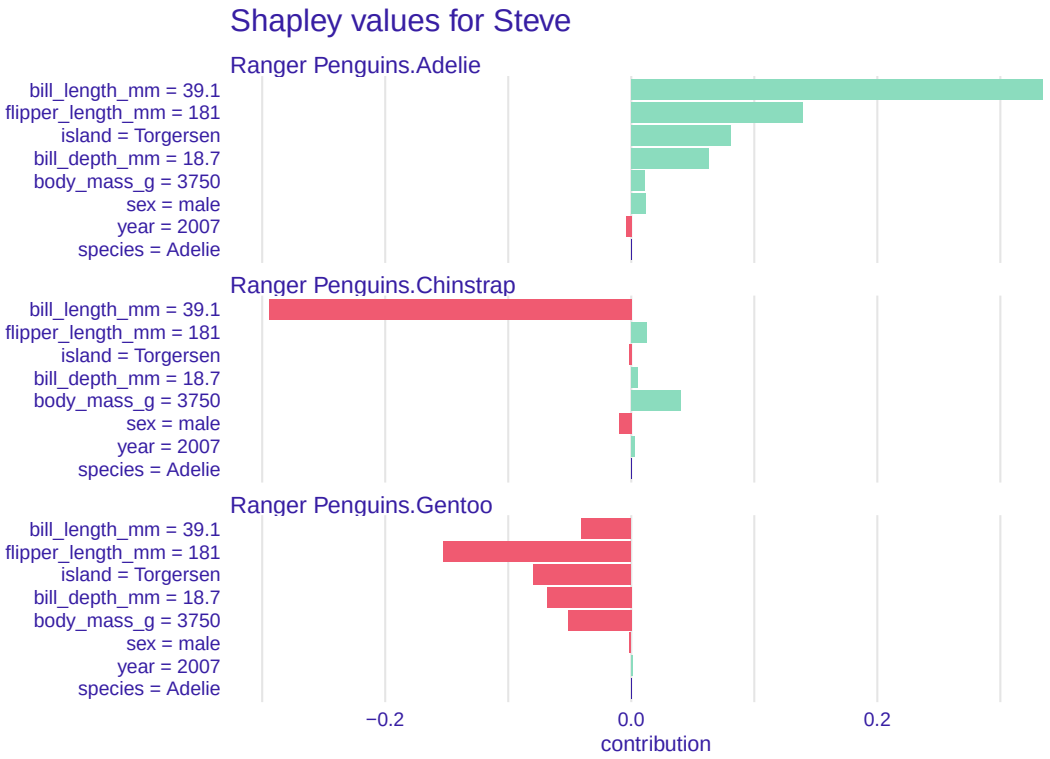
Looking at the plots above, we can read that the biggest contributors to the final prediction were for Steve the variables bill length and flipper.

10.3.3.3. Shapley Values

By far the most popular technique for local model exploration (Holzinger et al. 2022) is Shapley values and the most popular algorithm for estimating these values is the SHAP algorithm. Find a detailed description of the method and algorithm in the chapter SHapley Additive exPlanations (SHAP).

The function `DALEX::predict_parts()` calculates SHAP attributions, you just need to set `type = "shap"`. Its results can be visualized with a generic `plot()` function.

```
ranger_shap = predict_parts(ranger_exp, new_observation = steve,
              type = "shap")
plot(ranger_shap, show_boxplots = FALSE) +
              ggtitle("Shapley values for Steve", "")
```



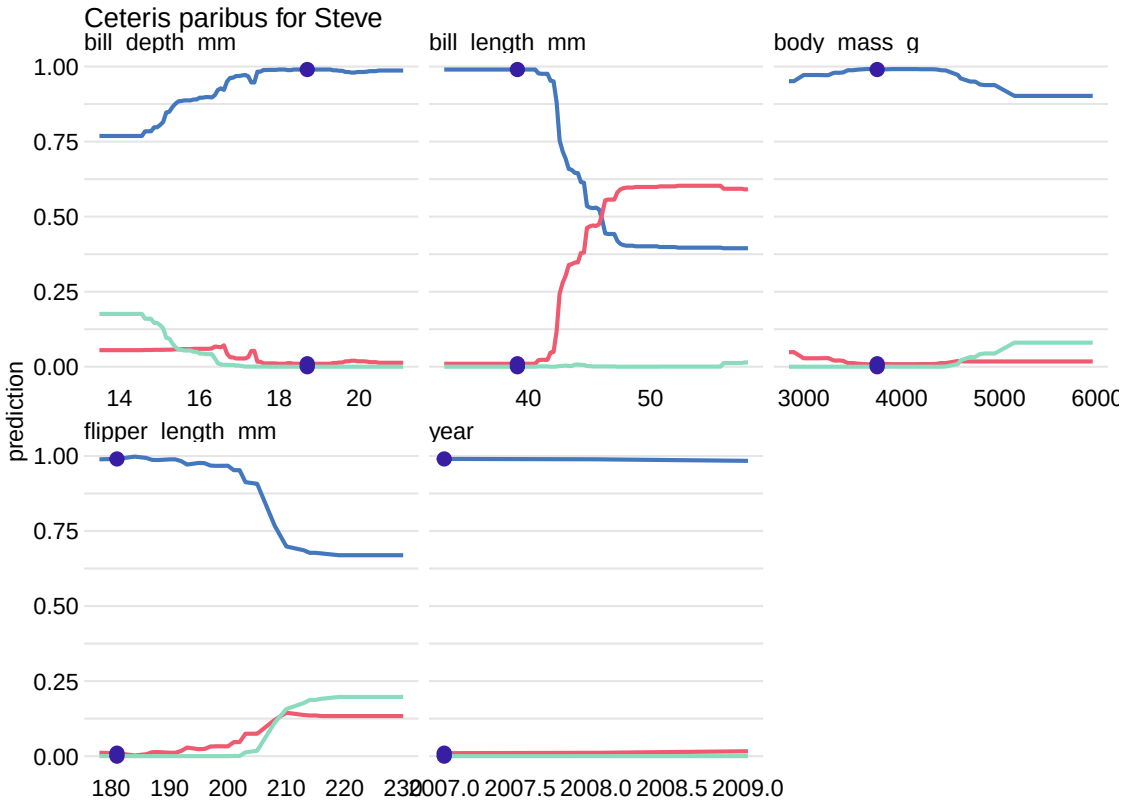
The results for Break Down and SHAP methods are generally similar. Differences will emerge if there are many complex interactions in the model.

10.3.3.4. Ceteris Paribus

In the previous section, we've introduced a global explanation – Partial Dependence plots. Ceteris Paribus plots are the local level version of that plot. Read more about this technique in the chapter Ceteris Paribus and note that these profiles are also called Individual Conditional Expectations (ICE). They show the response of a model when only one variable is changed while others stay unchanged.

The function `DALEX::predict_profile()` calculates Ceteris paribus profiles which can be visualized with the generic `plot()` function.

```
ranger_ceteris = predict_profile(ranger_exp, steve)
plot(ranger_ceteris) + ggtitle("Ceteris paribus for Steve", " ")
```



Blue dot stands for the prediction for Steve. Only a big change in bill length could convince the model of Steve's different species.

10.4. Exercises

Model explanation allows us to confront our expert knowledge related to the problem with relations learned by the model. Following tasks are based on predictions of the value of football players based on data from the FIFA game. It is a graceful example, as most people have some intuition about how a footballer's age or skill can affect their value. The latest FIFA statistics can be downloaded from kaggle.com, but also one can use the 2020 data avaliable in the `DALEX` packages(see `DALEX::fifa` dataset). The following exercises can be performed in both the `iml` and `DALEX` packages and we have provided solutions for both.

1. Prepare a `mlr3` regression task for `fifa` data. Select only variables describing the age and skills of footballers. Train any predictive model for this task, e.g. `regr.ranger`.

2. Use the permutation importance method to calculate variable importance ranking. Which variable is the most important? Is it surprising?

3. Use the Partial Dependence profile to draw the global behavior of the model for this variable. Is it aligned with your expectations?

4 Choose one of the football players. You can choose some well-known striker (e.g. Robert Lewandowski) or a well-known goalkeeper (e.g. Manuel Neuer). The following tasks are worth repeating for several different choices.

5. For the selected footballer, calculate and plot the Shapley values. Which variable is locally the most important and has the strongest influence on the valuation of the footballer?
6. For the selected footballer, calculate the Ceteris Paribus / Individual Conditional Expectatons profiles to draw the local behaviour of the model for this variable. Is it different from the global behaviour?

11. Extending

TODO (150-200 WORDS)

This chapter gives instructions on how to extend `mlr3` and its extension packages with custom objects.

The approach is always the same:

1. determine the base class you want to inherit from,
2. extend the class with your custom functionality,
3. test your implementation
4. (optionally) add new object to the respective `Dictionary`.

The chapter Create a new learner illustrates the steps needed to create a custom learner in `mlr3`.

> ! **This section of the book might be complex for some readers.**

11.1. Adding new Learners

Although many learners are already included in the `mlr3` ecosystem, there might be a situation in which your algorithm of choice is not implemented. Here, we show how to create a custom mlr3learner step-by-step using `mlr3extralearners::create_learner`. If you intend to add a learner to mlr3extralearners, **it is strongly recommended** to **first** open a learner request issue to inform the `mlr3` team about your idea. This allows to discuss the implementation details and potential peculiarities of the learner before putting actual work in.

This section gives insights on how a mlr3learner is constructed and how to troubleshoot issues. See the Learner FAQ subsection for help.

Summary of steps for adding a new learner

1. Check that the learner does not already exist here.
2. Install `mlr3extralearners` and if you want to create a PR, also fork and clone it.
3. Run `mlr3extralearners::create_learner()`.
4. Add the learner's `ParamSet`.
5. Manually add `.train` and `.predict` private methods to the learner.
6. Implement supported optional extractors and hotstarting if applicable.
7. Fill out the missing parts in the learner's description. To add references you first need to create an entry in bibentries.R

8. Check that unit tests and parameter tests pass (these are automatically created).
9. Run cleaning functions.
10. Open a pull request with the "new learner" template.

> **Warning**
>
> Do not copy/paste the code shown in this section. Use `create_learner()` to start.

11.1.1. Setting-up mlr3extralearners

In order to use `mlr3extralearners::create_learner` you must have mlr3extralearners installed. Note that mlr3extralearners is not on CRAN and has to be installed from GitHub. To ensure that you have the latest version, run `remotes::install_github("mlr-org/mlr3extralearners")` before proceeding.

If you want to create a pull request to mlr3extralearners you also need to

1. Fork the repository
2. Clone a local copy of your forked repository.

11.1.2. Calling create_learner

The learner `classif.rpart` will be used as a running example throughout this section.

```
library("mlr3extralearners")
create_learner(
  path = "path/to/a/folder",
  classname = "Rpart",
  type = "classif",
  key = "rpart",
  algorithm = "Decision Tree",
  package = "rpart",
  caller = "rpart",
  feature_types = c("logical", "integer", "numeric", "factor", "ordered"),
  predict_types = c("response", "prob"),
  properties = c("importance", "missings", "multiclass", "twoclass", "weights"),
  gh_name = "RaphaelS1",
  label = "Regression and Partition Tree",
  data_formats = "data.table"
)
```

The full documentation for the function arguments is in `mlr3extralearners::create_learner`, in this example we are doing the following:

1. `path = "path/to/a/folder"` - This determines where the templates are being generated. If the path is the root of an R package, the learner is created in the ./R directory and the test

files in ./tests/testthat. Otherwise, all files are being created in the folder pointed to by path. Already existing files will not be modified.
2. `classname = "Rpart"` - Set the R6 class name to LearnerClassifRpart (classif is below)
3. `algorithm = "Decision Tree"` - Create the title as "Classification Decision Tree Learner", where "Classification" is determined automatically from `type` and "Learner" is added for all learners.
4. `type = "classif"` - Setting the learner as a classification learner, automatically filling the title, class name, id (`"classif.rpart"`) and task type.
5. `key = "rpart"` - Used with `type` to create the unique ID of the learner, `"classif.rpart"`.
6. `package = "rpart"` - Setting the package from which the learner is implemented, this fills in things like the training function (along with `caller`) and the `man` field.
7. `caller = "rpart"` - This tells the `.train` function, and the description which function is called to run the algorithm, with `package` this automatically fills `rpart::rpart`.
8. `feature_types = c("logical", "integer", "numeric", "factor", "ordered")` - Sets the type of features that can be handled by the learner. See meta information.
9. `predict_types = c("response", "prob"),` - Sets the available prediction types as response (pointwise prediction) and prob (probabilities). See meta information.
10. `properties = c("importance", "missings", "multiclass", "twoclass", "weights")` - Sets the properties the learner supports. By including `"importance"` a public method called `importance` will be created that must be manually filled. See meta information and optional extractors.
11. `gh_name = "RaphaelS1"` - Fills the '@author' tag with my GitHub handle, this is required as it identifies the maintainer of the learner.

The sections below show an exemplary execution of `mlr3extralearners::create_learner`.

11.1.3. `learner_package_type_key.R`

The first generated file which must be updated after running `create_learner()` is the one following the structure `learner_<package>_<type>_<key>.R`; in this example `learner_rpart_classif_rpart.R`.

For our example, the resulting script looks like this:

```
#' @title Classification Decision Tree Learner
#' @author RaphaelS1
#' @name mlr_learners_classif.rpart
#'
#' @description
#' FIXME: BRIEF DESCRIPTION OF THE LEARNER.
#' Calls [rpart::rpart()] from FIXME: (CRAN VS NO CRAN): \CRANpkg{rpart} | 'rpart'.
#'
#' @section Custom mlr3 parameters:
#' FIXME: DEVIATIONS FROM UPSTREAM PARAMETERS. DELETE IF NOT APPLICABLE.
#'
#' @section Custom mlr3 defaults:
#' FIXME: DEVIATIONS FROM UPSTREAM DEFAULTS. DELETE IF NOT APPLICABLE.
#'
```

```
#' @section Installation:
#' FIXME: CUSTOM INSTALLATION INSTRUCTIONS. DELETE IF NOT APPLICABLE.
#'
#' @templateVar id classif.rpart
#' @template learner
#'
#' @references
#' FIXME: ADD REFERENCES
#'
#' @template seealso_learner
#' @template example
#' @export
LearnerClassifRpart = R6Class("LearnerClassifRpart",
  inherit = LearnerClassif,
  public = list(
    #' @description
    #' Creates a new instance of this [R6][R6::R6Class] class.
    initialize = function() {
      # FIXME: MANUALLY ADD PARAMETERS BELOW AND THEN DELETE THIS LINE
      param_set = ps()

      # FIXME: MANUALLY UPDATE PARAM VALUES BELOW IF APPLICABLE THEN DELETE THIS LINE.
      param_set$values = list()

      super$initialize(
        id = "classif.rpart",
        packages = "rpart",
        feature_types = c("logical", "integer", "numeric", "factor", "ordered"),
        predict_types = c("response", "prob"),
        param_set = param_set,
        properties = c("importance", "missings", "multiclass", "twoclass", "weights"),
        man = "mlr3extralearners::mlr_learners_classif.rpart",
        label = "Regression and Partition Tree"
      )
    },
    # FIXME: ADD IMPORTANCE METHOD IF APPLICABLE AND DELETE OTHERWISE
    # SEE mlr3extralearners::LearnerRegrRandomForest FOR AN EXAMPLE
    #' @description
    #' The importance scores are extracted from the slot FIXME:.
    #' @return Named `numeric()`.
    importance = function() {
      pars = self$param_set$get_values(tags = "importance")
      # FIXME: Implement importance
    }
  ),
  private = list(
```

```
    .train = function(task) {
      # get parameters for training
      pars = self$param_set$get_values(tags = "train")

      # FIXME: IF LEARNER DOES NOT HAVE 'weights' PROPERTY THEN DELETE THESE LINES.
      if ("weights" %in% task$properties) {
        # Add weights to learner
      }

      # FIXME: CREATE OBJECTS FOR THE TRAIN CALL
      # AT LEAST "data" AND "formula" ARE REQUIRED
      formula = task$formula()
      data = task$data()

      # FIXME: HERE IS SPACE FOR SOME CUSTOM ADJUSTMENTS BEFORE PROCEEDING TO THE
      # TRAIN CALL. CHECK OTHER LEARNERS FOR WHAT CAN BE DONE HERE
      # USE THE mlr3misc::invoke FUNCTION (IT'S SIMILAR TO do.call())

      invoke(
        rpart::rpart,
        formula = formula,
        data = data,
        .args = pars
      )
    },
    .predict = function(task) {
      # get parameters with tag "predict"
      pars = self$param_set$get_values(tags = "predict")

      # get newdata and ensure same ordering in train and predict
      newdata = ordered_features(task, self)

      # Calculate predictions for the selected predict type.
      type = self$predict_type

      pred = invoke(predict, self$model, newdata = newdata, type = type, .args = pars)

      # FIXME: ADD PREDICTIONS TO LIST BELOW
      list()
    }
  )
)

.extralrns_dict$add("classif.rpart", LearnerClassifRpart)
```

Now we have to do the following (the description will be addressed later):

1. Add the learner's parameters to the ParamSet.
2. Optionally change default values for the parameters.
3. Fill in the private `.train` method, which takes a (filtered) `Task` and returns a model.
4. Fill in the private `.predict` method, which operates on the model in `self$model` (stored during `$train()`) and a (differently subsetted) `Task` to return a named list of predictions.
5. As we included "importance" in `properties`, we have to add the public method `importance()` which returns a named numeric vectors with the decreasingly sorted importance scores (values) for the different features (names).

11.1.4. Meta-information

In the constructor (`initialize()`) the constructor of the super class (e.g. `LearnerClassif`) is called with meta information about the learner which should be constructed. This includes:

- `id`: The ID of the new learner. Usually consists of `<type>.<key>`, for example: `"classif.rpart"`.
- `packages`: The upstream package name(s) of the implemented learner.
- `param_set`: A set of hyperparameters and their descriptions provided as a `paradox::ParamSet`. For each hyperparameter the appropriate class needs to be chosen. When using the `paradox::ps` shortcut, a short constructor of the form `p_***` can be used:
  - `paradox::ParamLgl` / `paradox::p_lgl` for scalar logical hyperparameters.
  - `paradox::ParamInt` / `paradox::p_int` for scalar integer hyperparameters.
  - `paradox::ParamDbl` / `paradox::p_dbl` for scalar numeric hyperparameters.
  - `paradox::ParamFct` / `paradox::p_fct` for scalar factor hyperparameters (this includes characters).
  - `paradox::ParamUty` / `paradox::p_uty` for everything else (e.g. vector paramters or list parameters).
- `predict_types`: Set of predict types the learner supports. These differ depending on the type of the learner. See `mlr_reflections$learner_predict_types` for the full list of predict types supported by `mlr3`.
  - `LearnerClassif`
    - `response`: Only predicts a class label for each observation.
    - `prob`: Also predicts the posterior probability for each class for each observation.
  - `LearnerRegr`
    - `response`: Only predicts a numeric response for each observation.
    - `se`: Also predicts the standard error for each value of response.
  - `LearnerSurv`
    - `lp` - Linear predictor calculated as the fitted coefficients multiplied by the test data.
    - `distr` - Predicted survival distribution, either discrete or continuous. Implemented in `distr6`.
    - `crank` - Continuous risk ranking.
    - `response` - Predicted survival time.
  - `LearnerDens`
    - `pdf`- Predicts the probability density function.

    - `cdf` - Predicts the cumulative distribution function.
    - `distr` - Predicts a distribution as implemented in `distr6`.
  - `LearnerClust`
    - `partition` - Assigns the observation to a partition.
    - `prob` - Returns a probability for each partition.

- `feature_types`: Set of feature types the learner is able to handle. See `mlr_reflections$task_feature_type` for feature types supported by `mlr3`.
- `properties`: Set of properties of the learner. See `mlr_reflections$learner_properties` for the full list of learner properties supported by `mlr3`. The list of properties includes:
  - `"twoclass"`: The learner works on binary classification problems.
  - `"multiclass"`: The learner works on multi-class classification problems.
  - `"missings"`: The learner can natively handle missing values.
  - `"weights"`: The learner can work on tasks which have observation weights / case weights.
  - `"importance"`: The learner supports extracting importance values for features.
  - `"selected_features"`: The learner supports extracting the features which were selected by the model.
  - `"oob_error"`: The learner supports extracting the out of bag error.
  - `"loglik"`: The learner supports extracting the log-likelihood of the learner.
  - `"hotstart_forward"`: The learner allows to continue training the model e.g. by adding more trees to a random forest.
  - `"hotstart_backward"`: The learner allows to "undo" some of the training, e.g. by removing some trees from a model.
- `man`: The roxygen identifier of the learner. This is used within the `$help()` method of the super class to open the help page of the learner.
- `label`: The label of the learner. This should briefly describe the learner (similar to the description's title) and is for example used for printing.

11.1.5. ParamSet

The `ParamSet` is the set of hyperparameters used in model training and predicting, this is given as a `paradox::ParamSet`. The set consists of a list of hyperparameters, where each has a specific class for the hyperparameter type (see above). In addition, each parameter has one or more tags, that determine in which method they are used.

Beyond that there are other tags that serve specific purposes:

- The tag `"threads"` should be used (if applicable) to tag the parameter that determines the number of threads used for the learner's internal parallelization. This parameter can be set using `set_threads`.
- The tag `"required"` should be used to tag parameters that must be provided for the algorithm to be executable.
- In case optional extractors are available, the can (although this is rarely the case) also have parameters and can be tagged accordingly.
- If hotstarting is available, the fidelity parameter should be tagged with `"hotstart"`.

For `classif.rpart` the `param_set` can be defined as follows

```
param_set = ps(
  minsplit = p_int(lower = 1L, default = 20L, tags = "train"),
  minbucket = p_int(lower = 1L, tags = "train"),
  cp = p_dbl(lower = 0, upper = 1, default = 0.01, tags = "train"),
  maxcompete = p_int(lower = 0L, default = 4L, tags = "train"),
  maxsurrogate = p_int(lower = 0L, default = 5L, tags = "train"),
  maxdepth = p_int(lower = 1L, upper = 30L, default = 30L, tags = "train"),
  usesurrogate = p_int(lower = 0L, upper = 2L, default = 2L, tags = "train"),
  surrogatestyle = p_int(lower = 0L, upper = 1L, default = 0L, tags = "train"),
  xval = p_int(lower = 0L, default = 0L, tags = "train"),
  keep_model = p_lgl(default = FALSE, tags = "train")
)
param_set$values = list(xval = 0L)
```

Within mlr3 packages we suggest to stick to the shorthand notation above for consistency, however the `param_set` can be written with the underlying R6 classes as shown here

```
param_set = ParamSet$new(list(
  ParamInt$new(id = "minsplit", default = 20L, lower = 1L, tags = "train"),
  ParamInt$new(id = "minbucket", lower = 1L, tags = "train"),
  ParamDbl$new(id = "cp", default = 0.01, lower = 0, upper = 1, tags = "train"),
  ParamInt$new(id = "maxcompete", default = 4L, lower = 0L, tags = "train"),
  ParamInt$new(id = "maxsurrogate", default = 5L, lower = 0L, tags = "train"),
  ParamInt$new(id = "maxdepth", default = 30L, lower = 1L, upper = 30L, tags = "train"),
  ParamInt$new(id = "usesurrogate", default = 2L, lower = 0L, upper = 2L, tags = "train"),
  ParamInt$new(id = "surrogatestyle", default = 0L, lower = 0L, upper = 1L, tags = "train"),
  ParamInt$new(id = "xval", default = 0L, lower = 0L, tags = "train"),
  ParamLgl$new(id = "keep_model", default = FALSE, tags = "train")
))
param_set$values = list(xval = 0L)
```

You should read though the learner documentation to find the full list of available parameters. Just looking at some of these in this example:

- `"cp"` is numeric, has a feasible range of `[0,1]` and defaults to `0.01`. The parameter is used during `"train"`.
- `"xval"` is integer has a lower bound of `0`, a default of `0` and the parameter is used during `"train"`.
- `"keep_model"` is logical with a default of `FALSE` and is used during `"train"`.

In some rare cases you may want to change the default parameter values. You can do this by changing the `param_set$values`. You can see we have done this for `"classif.rpart"` where the default for `xval` is changed to `0`. Note that the default in the ParamSet is recorded as our changed default (0), and not the original (10). It is strongly recommended to only change the defaults if absolutely required, when this is the case add the following to the learner documentation:

```
#' @section Custom mlr3 defaults:
#' - `<parameter>`:
#'   - Actual default: <value>
#'   - Adjusted default: <value>
#'   - Reason for change: <text>
```

11.1.6. Train function

The train function takes a Task as input and must return a model. Let's say we want to translate the following call of `rpart::rpart()` into code that can be used inside the `.train()` method.

First, we write something down that works completely without mlr3:

```
data = iris
model = rpart::rpart(Species ~ ., data = iris, xval = 0)
```

We need to pass the formula notation `Species ~ .`, the data and the hyperparameters. To get the hyperparameters, we call `self$param_set$get_values(tag = "train")` and thereby query all parameters that are using during `"train"`. Then, the dataset is extracted from the Task. Because the learner has the property `"weights"`, we insert the weights of the task if there are any.

Last, we call the upstream function `rpart::rpart()` with the data and pass all hyperparameters via argument `.args` using the `mlr3misc::invoke()` function. The latter is simply an optimized version of `do.call()` that we use within the mlr3 ecosystem.

```
.train = function(task) {
  pars = self$param_set$get_values(tags = "train")
  if ("weights" %in% task$properties) {
    pars$weights = task$weights$weight
  }
  formula = task$formula()
  data = task$data()
  invoke(
    rpart::rpart,
    formula = formula,
    data = data,
    .args = pars
  )
}
```

11.1.7. Predict function

The internal predict method `.predict()` also operates on a Task as well as on the fitted model that has been created by the `train()` call previously and has been stored in `self$model`.

The return value is a `Prediction` object. We proceed analogously to what we did in the previous section. We start with a version without any `mlr3` objects and continue to replace objects until we have reached the desired interface:

```
# inputs:
task = tsk("iris")
self = list(model = rpart::rpart(task$formula(), data = task$data()))

data = iris
response = predict(self$model, newdata = data, type = "class")
prob = predict(self$model, newdata = data, type = "prob")
```

The `"rpart::predict.rpart()"` function predicts class labels if argument `type` is set to to `"class"`, and class probabilities if set to `"prob"`.

Next, we transition from `data` to a `Task` again and construct a list with the return type requested by the user, this is stored in the `$predict_type` slot of a learner class. Note that the `Task` is automatically passed to the prediction object, so all you need to do is return the predictions! Make sure the list names are identical to the task predict types.

The final `.predict()` method is below, we could omit the `pars` line as there are no parameters with the `"predict"` tag but we keep it here to be consistent:

```
.predict = function(task) {
  pars = self$param_set$get_values(tags = "predict")
  # get newdata and ensure same ordering in train and predict
  newdata = ordered_features(task, self)
  if (self$predict_type == "response") {
    response = invoke(
      predict,
      self$model,
      newdata = newdata,
      type = "class",
      .args = pars
    )

    return(list(response = response))
  } else {
    prob = invoke(
      predict,
      self$model,
      newdata = newdata,
      type = "prob",
      .args = pars
    )
    return(list(prob = prob))
  }
}
```

> **Warning**
>
> You cannot rely on the column order of the data returned by `task$data()` as the order of columns may be different from the order of the columns during `$.train`. The `newdata` line ensures the ordering is the same by calling the same order as in train!

11.1.8. Optional Extractors

Specific learner implementations are free to implement additional getters to ease the access of certain parts of the model in the inherited subclasses. The blueprint for these methods is only included in the generated learner template, if the property is set when calling `create_learner()`. The comments in the templates will include references to other learners that have this property and can be used as guiding examples. To determine whether these methods are applicable, one has to determine whether the learner supports this method in principle **and** whether it is implemented in the upstream package.

For the following operations, extractors are standardized:

- `importance(...)` - Returns the feature importance score as numeric vector. The higher the score, the more important the variable. The returned vector is named with feature names and sorted in decreasing order. Note that the model might omit features it has not used at all. The learner must be tagged with property `"importance"`.
- `selected_features(...)` - Returns a subset of selected features as character(). The learner must be tagged with property `"selected_features"`.
- `oob_error(...)` - Returns the out-of-bag error of the model as `numeric(1)`. The learner must be tagged with property `"oob_error"`.
- `loglik(...)` - Extracts the log-likelihood (c.f. `stats::logLik()`). The learner must be tagged with property `"loglik"`.

In this case, we only have to implement the `importance()` method.

```
importance = function() {
  if (is.null(self$model)) {
    stopf("No model stored")
  }

  importance = sort(self$model$variable.importance, decreasing = TRUE)
  if (is.null(importance)) {
    importance = mlr3misc::set_names(numeric())
  }
  return(importance)
}
```

11.1.9. Hotstarting

Some learners support resuming or continuing from an already fitted model. We assume that hotstarting is only possible if a single hyperparameter (also called the fidelity parameter, usually controlling the complexity or expensiveness) is altered and all other hyperparameters are identical. The fidelity parameters should be tagged with `"hotstart"`. Examples are:

- Random Forest: Starting from a model with n trees, a random forest with n + k trees can be obtained by adding k trees (`"hotstart_forward"`) and a random forest with n - k trees can be obtained by removing k trees (`"hotstart_backward"`).
- Gradient Boosting: When having fitted a model with n iterations, we only need k iterations to obtain a model with n + k iterations. (`"hotstart_forward"`).

For more information see HotstartStack.

11.1.10. Control objects/functions of learners

Some learners rely on a "control" object/function such as `glmnet::glmnet.control()`. Accounting for such depends on how the underlying package works:

- If the package forwards the control parameters via `...` and makes it possible to just pass control parameters as additional parameters directly to the train call, there is no need to distinguish both `"train"` and `"control"` parameters.
- If the control parameters need to be passed via a separate argument, one can e.g. use `formalArgs(glmnet::glmnet.control)` to get the names of the control parameters and then extract them from the `pars` like shown below.

```
pars = self$param_set$get_values(tags = "train")
ii = names(pars) %in% formalArgs(glmnet::glmnet.control)
pars_ctrl = pars[ii]
pars_train = pars[!ii]

invoke([...], .args = pars_train, control = pars_ctrl)
```

11.1.11. Adding the description

Once the learner is implemented - and is not only intended for personal use - it's description should be filled out. Most steps should be clear from the instructions given in the template. For the section '@references', the entry first has to be added to the file `bibentries.R`, essentially by converting the bibtex file to a R `bibentry` function call.

11.1.12. Testing the learner

Once your learner is created, you are ready to start testing if it works, there are three types of tests: manual, unit and parameter.

11.1.12.1. Train and Predict

For a bare-bone check you can just try to run a simple `train()` call locally.

```
task = tsk("iris") # assuming a Classif learner
lrn = lrn("classif.rpart")
lrn$train(task)
p = lrn$predict(task)
p$confusion
```

If it runs without erroring, that's a very good start!

11.1.12.2. Autotest

To ensure that your learner is able to handle all kinds of different properties and feature types, we have written an "autotest" that checks the learner for different combinations of such.

The "autotest" setup is generated automatically by `create_learner()`. It will have a name with the form `test_package_type_key.R`, in our case this will actually be `test_rpart_classif_rpart.R`. This will create the following script, for which no changes are required to pass (assuming the learner was correctly created):

```
test_that("autotest", {
  learner = lrn("classif.rpart")
  expect_learner(learner)
  # note that you can skip tests using the exclude argument
  result = run_autotest(learner)
  expect_true(result, info = result$error)
})
```

For some learners that have required parameters, it is needed to set some values for required parameters after construction so that the learner can be run in the first place.

You can also exclude some specific test arrangements within the "autotest" via the argument `exclude` in the `run_autotest()` function. Currently the `run_autotest()` function lives in inst/testthat of the `mlr3` and still lacks documentation. This should change in the near future.

To finally run the test suite, call `devtools::test()` or hit `CTRL + Shift + T` if you are using RStudio.

11.1.12.3. Checking Parameters

Some learners have a high number of parameters and it is easy to miss out on some during the creation of a new learner. In addition, if the maintainer of the upstream package changes something with respect to the arguments of the algorithm, the learner is in danger to break. Also, new arguments could be added upstream and manually checking for new additions all the time is tedious.

Therefore we have written a "Parameter Check" that runs regularly for every learner. This "Parameter Check" compares the parameters of the mlr3 ParamSet against all arguments available in the upstream function that is called during `$train()` and `$predict()`. Again the file is automatically created by `create_learner()`. This will be named like `test_paramtest_package_type_key.R`, so in our example `test_paramtest_rpart_classif_rpart.R`. When the `.train` function calls multiple functions (e.g. a control function as described above), a list of functions can be passed to the parameter test.

The test comes with an `exclude` argument that should be used to *exclude and explain* why certain arguments of the upstream function are not within the ParamSet of the mlr3learner. This will likely be required for all learners as common arguments like `x`, `target` or `data` are handled by the mlr3 interface and are therefore not included within the ParamSet.

However, there might be more parameters that need to be excluded, for example:

- Type dependent parameters, i.e. parameters that only apply for classification or regression learners.
- Parameters that are actually deprecated by the upstream package and which were therefore not included in the mlr3 ParamSet.

All excluded parameters should have a comment justifying their exclusion.

In our example, the final paramtest script looks like:

```
test_that("classif.rpart train", {
  learner = lrn("classif.rpart")
  # this can also be a list of functions
  fun = rpart::rpart
  exclude = c(
    "formula", # handled internally
    "model", # handled internally
    "data", # handled internally
    "weights", # handled by task
    "subset", # handled by task
    "na.action", # handled internally
    "method", # handled internally
    "x", # handled internally
    "y", # handled internally
    "parms", # handled internally
    "control", # handled internally
    "cost" # handled internally
  )

  paramtest = run_paramtest(learner, fun, exclude, tag = "train")
  expect_paramtest(paramtest)
})

test_that("classif.rpart predict", {
  learner = lrn("classif.rpart")
```

```
  fun = rpart:::predict.rpart
  exclude = c(
    "object", # handled internally
    "newdata", # handled internally
    "type", # handled internally
    "na.action" # handled internally
  )

  paramtest = run_paramtest(learner, fun, exclude, tag = "predict")
  expect_paramtest(paramtest)
})
```

11.1.13. Package Cleaning

Once all tests are passing, run the following functions to ensure that the package remains clean and tidy

1. `devtools::document(roclets = c('rd', 'collate', 'namespace'))`
2. If you haven't done this before run: `remotes::install_github('mlr-org/styler.mlr')`
3. `styler::style_pkg(style = styler.mlr::mlr_style)`
4. `usethis::use_tidy_description()`
5. `lintr::lint_package()`

Please fix any errors indicated by `lintr` before creating a pull request. Finally ensure that all `FIXME` are resolved and deleted in the generated files.

You are now ready to add your learner to the `mlr3` ecosystem! Simply open a pull request to https://github.com/mlr-org/mlr3extralearners/pulls with the new learner template and complete the checklist in there. Creating this request will trigger an automated workflow that checks whether various conditions (such as `rcmdcheck::rcmdcheck()`) are satisfied. Once the pull request is approved and merged, your learner will automatically appear on the package website.

11.1.14. Thanks and Maintenance

Thank you for contributing to the `mlr3` ecosystem!

When you created the learner you would have given your GitHub handle, meaning that you are now listed as the learner author and maintainer. This means that if the learner breaks it is your responsibility to fix the learner - you can view the status of your learner here.

11.1.15. Learner FAQ

Question 1

How to deal with Parameters which have no default?

Answer

If the learner does not work without providing a value, set a reasonable default in `param_set$values`, add tag `"required"` to the parameter and document your default properly.

Question 2

Where to add the package of the upstream package in the DESCRIPTION file?

Add it to the "Suggests" section.

Question 3

How to handle arguments from external "control" functions such as `glmnet::glmnet_control()`?

Answer

See "Control objects/functions of learners".

Question 4

How to document if my learner uses a custom default value that differs to the default of the upstream package?

Answer

If you set a custom default for the mlr3learner that does not cope with the one of the upstream package (think twice if this is really needed!), add this information to the help page of the respective learner.

You can use the following skeleton for this:

```
#' @section Custom mlr3 defaults:
#' * `<parameter>`:
#'   * Actual default: <value>
#'   * Adjusted default: <value>
#'   * Reason for change: <text>
```

Question 5

When should the `"required"` tag be used when defining Params and what is its purpose?

Answer

The `"required"` tag should be used when the following conditions are met:

- The upstream function cannot be run without setting this parameter, i.e. it would throw an error.
- The parameter has no default in the upstream function.

In `mlr3` we follow the principle that every learner should be constructable without setting custom parameters. Therefore, if a parameter has no default in the upstream function, a custom value is usually set for this parameter in the mlr3learner (remember to document such changes in the help page of the learner).

Even though this practice ensures that no parameter is unset in an mlr3learner and partially removes the usefulness of the `"required"` tag, the tag is still useful in the following scenario:

If a user sets custom parameters after construction of the learner

```
lrn = lrn("<id>")
lrn$param_set$values = list("<param>" = <value>)
```

Here, all parameters besides the ones set in the list would be unset. See `paradox::ParamSet` for more information. If a parameter is tagged as `"required"` in the ParamSet, the call above would error and prompt the user that required parameters are missing.

Question 6

What is this error when I run `devtools::load_all()`

```
> devtools::load_all(".")
Loading mlr3extralearners
Warning message:
.onUnload failed in unloadNamespace() for 'mlr3extralearners', details:
  call: vapply(hooks, function(x) environment(x)$pkgname, NA_character_)
  error: values must be length 1,
 but FUN(X[[1]]) result is length 0
```

Answer

This is not an error but a warning and you can safely ignore it!

11.2. Adding new Measures

In this section we showcase how to implement a custom performance measure.

A good starting point is writing down the loss function independently of `mlr3` (we also did this in the `mlr3measures` package). Here, we illustrate writing measure by implementing the root of the mean squared error for regression problems:

```
root_mse = function(truth, response) {
  mse = mean((truth - response)^2)
  sqrt(mse)
}

root_mse(c(0, 0.5, 1), c(0.5, 0.5, 0.5))
```

```
[1] 0.4082483
```

In the next step, we embed the `root_mse()` function into a new `R6` class inheriting from base classes `MeasureRegr`/`Measure`. For classification measures, use `MeasureClassif`. We keep it simple here and only explain the most important parts of the `Measure` class:

```
MeasureRootMSE = R6::R6Class("MeasureRootMSE",
  inherit = mlr3::MeasureRegr,
  public = list(
```

```
    initialize = function() {
      super$initialize(
        # custom id for the measure
        id = "root_mse",

        # additional packages required to calculate this measure
        packages = character(),

        # properties, see below
        properties = character(),

        # required predict type of the learner
        predict_type = "response",

        # feasible range of values
        range = c(0, Inf),

        # minimize during tuning?
        minimize = TRUE
      )
    }
  ),

  private = list(
    # custom scoring function operating on the prediction object
    .score = function(prediction, ...) {
      root_mse = function(truth, response) {
        mse = mean((truth - response)^2)
        sqrt(mse)
      }

      root_mse(prediction$truth, prediction$response)
    }
  )
)
```

This class can be used as template for most performance measures. If something is missing, you might want to consider having a deeper dive into the following arguments:

- `properties`: If you tag you measure with the property `"requires_task"`, the `Task` is automatically passed to your `.score()` function (don't forget to add the argument `Task` in the signature). The same is possible with `"requires_learner"` if you need to operate on the `Learner` and `"requires_train_set"` if you want to access the set of training indices in the score function.
- `aggregator`: This function (defaulting to `mean()`) controls how multiple performance scores, i.e. from different resampling iterations, are aggregated into a single numeric value if `average` is set to micro averaging. This is ignored for macro averaging.

- `predict_sets`: Prediction sets (subset of `("train", "test")`) to operate on. Defaults to the "test" set.

Finally, if you want to use your custom measure just like any other measure shipped with `mlr3` and access it via the `mlr_measures` dictionary, you can easily add it:

```
mlr3::mlr_measures$add("root_mse", MeasureRootMSE)
```

Typically it is a good idea to put the measure together with the call to `mlr_measures$add()` in a new R file and just source it in your project.

```
## source("measure_root_mse.R")
msr("root_mse")
```

```
<MeasureRootMSE:root_mse>
* Packages: mlr3
* Range: [0, Inf]
* Minimize: TRUE
* Average: macro
* Parameters: list()
* Properties: -
* Predict type: response
```

11.3. Adding new PipeOps

This section showcases how the `mlr3pipelines` package can be extended to include custom `PipeOp`s. To run the following examples, we will need a `Task`; we are using the well-known "Iris" task:

```
library("mlr3")
task = tsk("iris")
task$data()
```

```
        Species Petal.Length Petal.Width Sepal.Length Sepal.Width
  1:     setosa          1.4         0.2          5.1         3.5
  2:     setosa          1.4         0.2          4.9         3.0
  3:     setosa          1.3         0.2          4.7         3.2
  4:     setosa          1.5         0.2          4.6         3.1
  5:     setosa          1.4         0.2          5.0         3.6
 ---
146: virginica          5.2         2.3          6.7         3.0
147: virginica          5.0         1.9          6.3         2.5
148: virginica          5.2         2.0          6.5         3.0
149: virginica          5.4         2.3          6.2         3.4
150: virginica          5.1         1.8          5.9         3.0
```

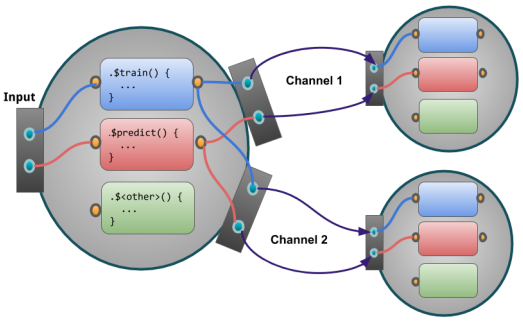
mlr3pipelines is fundamentally built around R6. When planning to create custom PipeOp objects, it can only help to familiarize yourself with it.

In principle, all a PipeOp must do is inherit from the PipeOp R6 class and implement the `.train()` and `.predict()` functions. There are, however, several auxiliary subclasses that can make the creation of *certain* operations much easier.

11.3.1. General Case Example: `PipeOpCopy`

A very simple yet useful PipeOp is `PipeOpCopy`, which takes a single input and creates a variable number of output channels, all of which receive a copy of the input data. It is a simple example that showcases the important steps in defining a custom PipeOp. We will show a simplified version here, **`PipeOpCopyTwo`**, that creates exactly two copies of its input data.

The following figure visualizes how our PipeOp is situated in the `Pipeline` and the significant in- and outputs.



11.3.1.1. First Steps: Inheriting from PipeOp

The first part of creating a custom PipeOp is inheriting from PipeOp. We make a mental note that we need to implement a `.train()` and a `.predict()` function, and that we probably want to have an `initialize()` as well:

```
PipeOpCopyTwo = R6::R6Class("PipeOpCopyTwo",
  inherit = mlr3pipelines::PipeOp,
  public = list(
    initialize = function(id = "copy.two") {
      ....
    },
  ),
  private == list(
    .train = function(inputs) {
      ....
    },

    .predict = function(inputs) {
      ....
```

```
    }
  )
)
```

Note, that **private** methods, e.g. `.train` and `.predict` etc are prefixed with a `.`.

11.3.1.2. Channel Definitions

We need to tell the `PipeOp` the layout of its channels: How many there are, what their names are going to be, and what types are acceptable. This is done on initialization of the `PipeOp` (using a `super$initialize` call) by giving the `input` and `output` `data.table` objects. These must have three columns: a `"name"` column giving the names of input and output channels, and a `"train"` and `"predict"` column naming the class of objects we expect during training and prediction as input / output. A special value for these classes is `"*"`, which indicates that any class will be accepted; our simple copy operator accepts any kind of input, so this will be useful. We have only one input, but two output channels.

By convention, we name a single channel `"input"` or `"output"`, and a group of channels [`"input1"`, `"input2"`, ...], unless there is a reason to give specific different names. Therefore, our `input` `data.table` will have a single row `<"input", "*", "*">`, and our `output` table will have two rows, `<"output1", "*", "*">` and `<"output2", "*", "*">`.

All of this is given to the `PipeOp` creator. Our `initialize()` will thus look as follows:

```
initialize = function(id = "copy.two") {
  input = data.table::data.table(name = "input", train = "*", predict = "*")
  # the following will create two rows and automatically fill the `train`
  # and `predict` cols with "*"
  output = data.table::data.table(
    name = c("output1", "output2"),
    train = "*", predict = "*"
  )
  super$initialize(id,
    input = input,
    output = output
  )
}
```

11.3.1.3. Train and Predict

Both `.train()` and `.predict()` will receive a `list` as input and must give a `list` in return. According to our `input` and `output` definitions, we will always get a list with a single element as input, and will need to return a list with two elements. Because all we want to do is create two copies, we will just create the copies using `c(inputs, inputs)`.

Two things to consider:

- The `.train()` function must always modify the `self$state` variable to something that is not `NULL` or `NO_OP`. This is because the `$state` slot is used as a signal that `PipeOp` has been trained on data, even if the state itself is not important to the `PipeOp` (as in our case). Therefore, our `.train()` will set `self$state = list()`.
- It is not necessary to "clone" our input or make deep copies, because we don't modify the data. However, if we were changing a reference-passed object, for example by changing data in a `Task`, we would have to make a deep copy first. This is because a `PipeOp` may never modify its input object by reference.

Our `.train()` and `.predict()` functions are now:

```
.train = function(inputs) {
  self$state = list()
  c(inputs, inputs)
}
```

```
.predict = function(inputs) {
  c(inputs, inputs)
}
```

11.3.1.4. Putting it Together

The whole definition thus becomes

```
PipeOpCopyTwo = R6::R6Class("PipeOpCopyTwo",
  inherit = mlr3pipelines::PipeOp,
  public = list(
    initialize = function(id = "copy.two") {
      super$initialize(id,
        input = data.table::data.table(name = "input", train = "*", predict = "*"),
        output = data.table::data.table(name = c("output1", "output2"),
                              train = "*", predict = "*")
      )
    }
  ),
  private = list(
    .train = function(inputs) {
      self$state = list()
      c(inputs, inputs)
    },

    .predict = function(inputs) {
      c(inputs, inputs)
    }
  )
```

```
)
```

We can create an instance of our PipeOp, put it in a graph, and see what happens when we train it on something:

```
library("mlr3pipelines")
poct = PipeOpCopyTwo$new()
gr = Graph$new()
gr$add_pipeop(poct)

print(gr)
```

```
Graph with 1 PipeOps:
       ID         State sccssors prdcssors
 copy.two <<UNTRAINED>>
```

```
result = gr$train(task)

str(result)
```

```
List of 2
 $ copy.two.output1:Classes 'TaskClassif', 'TaskSupervised', 'Task', 'R6' <TaskClassif:iris>
 $ copy.two.output2:Classes 'TaskClassif', 'TaskSupervised', 'Task', 'R6' <TaskClassif:iris>
```

11.3.2. Special Case: Preprocessing

Many PipeOps perform an operation on exactly one Task, and return exactly one Task. They may even not care about the "Target" / "Outcome" variable of that task, and only do some modification of some input data. However, it is usually important to them that the Task on which they perform prediction has the same data columns as the Task on which they train. For these cases, the auxiliary base class PipeOpTaskPreproc exists. It inherits from PipeOp itself, and other PipeOps should use it if they fall in the kind of use-case named above.

When inheriting from PipeOpTaskPreproc, one must either implement the private methods `.train_task()` and `.predict_task()`, or the methods `.train_dt()`, `.predict_dt()`, depending on whether wants to operate on a Task object or on its data as `data.tables`. In the second case, one can optionally also overload the `.select_cols()` method, which chooses which of the incoming Task's features are given to the `.train_dt()` / `.predict_dt()` functions.

The following will show two examples: `PipeOpDropNA`, which removes a Task's rows with missing values during training (and implements `.train_task()` and `.predict_task()`), and PipeOpScale, which scales a Task's numeric columns (and implements `.train_dt()`, `.predict_dt()`, and `.select_cols()`).

11.3.2.1. Example: `PipeOpDropNA`

Dropping rows with missing values may be important when training a model that can not handle them.

Because `mlr3` `"Task", text = "Tasks")` only contain a view to the underlying data, it is not necessary to modify data to remove rows with missing values. Instead, the rows can be removed using the `Task`'s `$filter` method, which modifies the `Task` in-place. This is done in the private method `.train_task()`. We take care that we also set the `$state` slot to signal that the `PipeOp` was trained.

The private method `.predict_task()` does not need to do anything; removing missing values during prediction is not as useful, since learners that cannot handle them will just ignore the respective rows. Furthermore, `mlr3` expects a `Learner` to always return just as many predictions as it was given input rows, so a `PipeOp` that removes `Task` rows during training can not be used inside a `GraphLearner`.

When we inherit from `PipeOpTaskPreproc`, it sets the `input` and `output` `data.table`s for us to only accept a single `Task`. The only thing we do during `initialize()` is therefore to set an `id` (which can optionally be changed by the user).

The complete `PipeOpDropNA` can therefore be written as follows. Note that it inherits from `PipeOpTaskPreproc`, unlike the `PipeOpCopyTwo` example from above:

```
PipeOpDropNA = R6::R6Class("PipeOpDropNA",
  inherit = mlr3pipelines::PipeOpTaskPreproc,
  public = list(
    initialize = function(id = "drop.na") {
      super$initialize(id)
    }
  ),

  private = list(
    .train_task = function(task) {
      self$state = list()
      featuredata = task$data(cols = task$feature_names)
      exclude = apply(is.na(featuredata), 1, any)
      task$filter(task$row_ids[!exclude])
    },

    .predict_task = function(task) {
      # nothing to be done
      task
    }
  )
)
```

To test this `PipeOp`, we create a small task with missing values:

```
smalliris = iris[(1:5) * 30, ]
smalliris[1, 1] = NA
smalliris[2, 2] = NA
sitask = as_task_classif(smalliris, target = "Species")
print(sitask$data())
```

```
      Species Petal.Length Petal.Width Sepal.Length Sepal.Width
1:     setosa          1.6         0.2           NA         3.2
2: versicolor          3.9         1.4          5.2          NA
3: versicolor          4.0         1.3          5.5         2.5
4:  virginica          5.0         1.5          6.0         2.2
5:  virginica          5.1         1.8          5.9         3.0
```

We test this by feeding it to a new `Graph` that uses `PipeOpDropNA`.

```
gr = Graph$new()
gr$add_pipeop(PipeOpDropNA$new())

filtered_task = gr$train(sitask)[[1]]
print(filtered_task$data())
```

```
      Species Petal.Length Petal.Width Sepal.Length Sepal.Width
1: versicolor          4.0         1.3          5.5         2.5
2:  virginica          5.0         1.5          6.0         2.2
3:  virginica          5.1         1.8          5.9         3.0
```

11.3.2.2. Example: `PipeOpScaleAlways`

An often-applied preprocessing step is to simply **center** and/or **scale** the data to mean 0 and standard deviation 1. This fits the `PipeOpTaskPreproc` pattern quite well. Because it always replaces all columns that it operates on, and does not require any information about the task's target, it only needs to overload the `.train_dt()` and `.predict_dt()` functions. This saves some boilerplate-code from getting the correct feature columns out of the task, and replacing them after modification.

Because scaling only makes sense on numeric features, we want to instruct `PipeOpTaskPreproc` to give us only these numeric columns. We do this by overloading the `.select_cols()` function: It is called by the class to determine which columns to pass to `.train_dt()` and `.predict_dt()`. Its input is the `Task` that is being transformed, and it should return a `character` vector of all features to work with. When it is not overloaded, it uses all columns; instead, we will set it to only give us numeric columns. Because the `levels()` of the data table given to `.train_dt()` and `.predict_dt()` may be different from the `Task`'s levels, these functions must also take a `levels` argument that is a named list of column names indicating their levels. When working with numeric data, this argument can be ignored, but it should be used instead of `levels(dt[[column]])` for factorial or character columns.

This is the first PipeOp where we will be using the $state slot for something useful: We save the centering offset and scaling coefficient and use it in $.predict()!

For simplicity, we are not using hyperparameters and will always scale and center all data. Compare this PipeOpScaleAlways operator to the one defined inside the mlr3pipelines package, PipeOpScale.

```
PipeOpScaleAlways = R6::R6Class("PipeOpScaleAlways",
  inherit = mlr3pipelines::PipeOpTaskPreproc,
  public = list(
    initialize = function(id = "scale.always") {
      super$initialize(id = id)
    }
  ),

  private = list(
    .select_cols = function(task) {
      task$feature_types[type == "numeric", id]
    },

    .train_dt = function(dt, levels, target) {
      sc = scale(as.matrix(dt))
      self$state = list(
        center = attr(sc, "scaled:center"),
        scale = attr(sc, "scaled:scale")
      )
      sc
    },

    .predict_dt = function(dt, levels) {
      t((t(dt) - self$state$center) / self$state$scale)
    }
  )
)
```

(Note for the observant: If you check `PipeOpScale.R` from the mlr3pipelines package, you will notice that is uses "`get("type")`" and "`get("id")`" instead of "`type`" and "`id`", because the static code checker on CRAN would otherwise complain about references to undefined variables. This is a "problem" with `data.table` and not exclusive to mlr3pipelines.)

We can, again, create a new Graph that uses this PipeOp to test it. Compare the resulting data to the original "iris" Task data printed at the beginning:

```
gr = Graph$new()
gr$add_pipeop(PipeOpScaleAlways$new())

result = gr$train(task)

```

```
result[[1]]$data()
```

```
       Species Petal.Length Petal.Width Sepal.Length Sepal.Width
  1:    setosa   -1.3357516  -1.3110521  -0.89767388  1.01560199
  2:    setosa   -1.3357516  -1.3110521  -1.13920048 -0.13153881
  3:    setosa   -1.3923993  -1.3110521  -1.38072709  0.32731751
  4:    setosa   -1.2791040  -1.3110521  -1.50149039  0.09788935
  5:    setosa   -1.3357516  -1.3110521  -1.01843718  1.24503015
 ---
146: virginica    0.8168591   1.4439941   1.03453895 -0.13153881
147: virginica    0.7035638   0.9192234   0.55148575 -1.27867961
148: virginica    0.8168591   1.0504160   0.79301235 -0.13153881
149: virginica    0.9301544   1.4439941   0.43072244  0.78617383
150: virginica    0.7602115   0.7880307   0.06843254 -0.13153881
```

11.3.3. Special Case: Preprocessing with Simple Train

It is possible to make even further simplifications for many PipeOps that perform mostly the same operation during training and prediction. The point of Task preprocessing is often to modify the training data in mostly the same way as prediction data (but in a way that *may* depend on training data).

Consider constant feature removal, for example: The goal is to remove features that have no variance, or only a single factor level. However, what features get removed must be decided during *training*, and may only depend on training data. Furthermore, the actual process of removing features is the same during training and prediction.

A simplification to make is therefore to have a private method `.get_state(task)` which sets the `$state` slot during training, and a private method `.transform(task)`, which gets called both during training *and* prediction. This is done in the PipeOpTaskPreprocSimple class. Just like PipeOpTaskPreproc, one can inherit from this and overload these functions to get a PipeOp that performs preprocessing with very little boilerplate code.

Just like PipeOpTaskPreproc, PipeOpTaskPreprocSimple offers the possibility to instead overload the `.get_state_dt(dt, levels)` and `.transform_dt(dt, levels)` methods (and optionally, again, the `.select_cols(task)` function) to operate on `data.table` feature data instead of the whole Task.

Even some methods that do not use PipeOpTaskPreprocSimple *could* work in a similar way: The `PipeOpScaleAlways` example from above will be shown to also work with this paradigm.

11.3.3.1. Example: `PipeOpDropConst`

A typical example of a preprocessing operation that does almost the same operation during training and prediction is an operation that drops features depending on a criterion that is evaluated during training. One simple example of this is dropping constant features. Because the mlr3 Task class offers a flexible view on underlying data, it is most efficient to drop columns from the task directly

using its `$select()` function, so the `.get_state_dt(dt, levels)` / `.transform_dt(dt, levels)` functions will *not* get used; instead we overload the `.get_state(task)` and `.transform(task)` methods.

The `.get_state()` function's result is saved to the `$state` slot, so we want to return something that is useful for dropping features. We choose to save the names of all the columns that have nonzero variance. For brevity, we use `length(unique(column)) > 1` to check whether more than one distinct value is present; a more sophisticated version could have a tolerance parameter for numeric values that are very close to each other.

The `.transform()` method is evaluated both during training *and* prediction, and can rely on the `$state` slot being present. All it does here is call the `Task$select` function with the columns we chose to keep.

The full `PipeOp` could be written as follows:

```
PipeOpDropConst = R6::R6Class("PipeOpDropConst",
  inherit = mlr3pipelines::PipeOpTaskPreprocSimple,
  public = list(
    initialize = function(id = "drop.const") {
      super$initialize(id = id)
    }
  ),

  private = list(
    .get_state = function(task) {
      data = task$data(cols = task$feature_names)
      nonconst = sapply(data, function(column) length(unique(column)) > 1)
      list(cnames = colnames(data)[nonconst])
    },

    .transform = function(task) {
      task$select(self$state$cnames)
    }
  )
)
```

This can be tested using the first five rows of the "Iris" `Task`, for which one feature (`"Petal.Width"`) is constant:

```
irishead = task$clone()$filter(1:5)
irishead$data()
```

```
   Species Petal.Length Petal.Width Sepal.Length Sepal.Width
1:  setosa          1.4         0.2          5.1         3.5
2:  setosa          1.4         0.2          4.9         3.0
3:  setosa          1.3         0.2          4.7         3.2
4:  setosa          1.5         0.2          4.6         3.1
5:  setosa          1.4         0.2          5.0         3.6
```

```
gr = Graph$new()$add_pipeop(PipeOpDropConst$new())
dropped_task = gr$train(irishead)[[1]]

dropped_task$data()
```

```
   Species Petal.Length Sepal.Length Sepal.Width
1:  setosa          1.4          5.1         3.5
2:  setosa          1.4          4.9         3.0
3:  setosa          1.3          4.7         3.2
4:  setosa          1.5          4.6         3.1
5:  setosa          1.4          5.0         3.6
```

We can also see that the `$state` was correctly set. Calling `$.predict()` with this graph, even with different data (the whole Iris `Task`!) will still drop the `"Petal.Width"` column, as it should.

```
gr$pipeops$drop.const$state
```

```
$cnames
[1] "Petal.Length" "Sepal.Length" "Sepal.Width"

$affected_cols
[1] "Petal.Length" "Petal.Width"  "Sepal.Length" "Sepal.Width"

$intasklayout
             id    type
1: Petal.Length numeric
2:  Petal.Width numeric
3: Sepal.Length numeric
4:  Sepal.Width numeric

$outtasklayout
             id    type
1: Petal.Length numeric
2: Sepal.Length numeric
3:  Sepal.Width numeric

$outtaskshell
Empty data.table (0 rows and 4 cols): Species,Petal.Length,Sepal.Length,Sepal.Width
```

```
dropped_predict = gr$predict(task)[[1]]

dropped_predict$data()
```

```
      Species Petal.Length Sepal.Length Sepal.Width
```

```
  1:    setosa          1.4          5.1         3.5
  2:    setosa          1.4          4.9         3.0
  3:    setosa          1.3          4.7         3.2
  4:    setosa          1.5          4.6         3.1
  5:    setosa          1.4          5.0         3.6
 ---
146: virginica          5.2          6.7         3.0
147: virginica          5.0          6.3         2.5
148: virginica          5.2          6.5         3.0
149: virginica          5.4          6.2         3.4
150: virginica          5.1          5.9         3.0
```

11.3.3.2. Example: `PipeOpScaleAlwaysSimple`

This example will show how a `PipeOpTaskPreprocSimple` can be used when only working on feature data in form of a `data.table`. Instead of calling the `scale()` function, the `center` and `scale` values are calculated directly and saved to the `$state` slot. The `.transform_dt()` function will then perform the same operation during both training and prediction: subtract the `center` and divide by the `scale` value. As in the `PipeOpScaleAlways` example above, we use `.select_cols()` so that we only work on numeric columns.

```
PipeOpScaleAlwaysSimple = R6::R6Class("PipeOpScaleAlwaysSimple",
  inherit = mlr3pipelines::PipeOpTaskPreprocSimple,
  public = list(
    initialize = function(id = "scale.always.simple") {
      super$initialize(id = id)
    }
  ),

  private = list(
    .select_cols = function(task) {
      task$feature_types[type == "numeric", id]
    },

    .get_state_dt = function(dt, levels, target) {
      list(
        center = sapply(dt, mean),
        scale = sapply(dt, sd)
      )
    },

    .transform_dt = function(dt, levels) {
      t((t(dt) - self$state$center) / self$state$scale)
    }
  )
)
```

We can compare this PipeOp to the one above to show that it behaves the same.

```
gr = Graph$new()$add_pipeop(PipeOpScaleAlways$new())
result_posa = gr$train(task)[[1]]

gr = Graph$new()$add_pipeop(PipeOpScaleAlwaysSimple$new())
result_posa_simple = gr$train(task)[[1]]
```

```
result_posa$data()
```

```
       Species Petal.Length Petal.Width Sepal.Length Sepal.Width
  1:    setosa   -1.3357516  -1.3110521  -0.89767388  1.01560199
  2:    setosa   -1.3357516  -1.3110521  -1.13920048 -0.13153881
  3:    setosa   -1.3923993  -1.3110521  -1.38072709  0.32731751
  4:    setosa   -1.2791040  -1.3110521  -1.50149039  0.09788935
  5:    setosa   -1.3357516  -1.3110521  -1.01843718  1.24503015
 ---
146: virginica    0.8168591   1.4439941   1.03453895 -0.13153881
147: virginica    0.7035638   0.9192234   0.55148575 -1.27867961
148: virginica    0.8168591   1.0504160   0.79301235 -0.13153881
149: virginica    0.9301544   1.4439941   0.43072244  0.78617383
150: virginica    0.7602115   0.7880307   0.06843254 -0.13153881
```

```
result_posa_simple$data()
```

```
       Species Petal.Length Petal.Width Sepal.Length Sepal.Width
  1:    setosa   -1.3357516  -1.3110521  -0.89767388  1.01560199
  2:    setosa   -1.3357516  -1.3110521  -1.13920048 -0.13153881
  3:    setosa   -1.3923993  -1.3110521  -1.38072709  0.32731751
  4:    setosa   -1.2791040  -1.3110521  -1.50149039  0.09788935
  5:    setosa   -1.3357516  -1.3110521  -1.01843718  1.24503015
 ---
146: virginica    0.8168591   1.4439941   1.03453895 -0.13153881
147: virginica    0.7035638   0.9192234   0.55148575 -1.27867961
148: virginica    0.8168591   1.0504160   0.79301235 -0.13153881
149: virginica    0.9301544   1.4439941   0.43072244  0.78617383
150: virginica    0.7602115   0.7880307   0.06843254 -0.13153881
```

11.3.4. Hyperparameters

mlr3pipelines uses the [paradox](https://paradox.mlr-org.com) package to define parameter spaces for PipeOps. Parameters for PipeOps can modify their behavior in certain ways, e.g. switch centering or scaling off in the PipeOpScale operator. The unified interface makes it possible to have parameters for whole Graphs that modify the individual PipeOp's behavior. The Graphs,

when encapsulated in GraphLearners, can even be tuned using the tuning functionality in mlr3tuning.

Hyperparameters are declared during initialization, when calling the PipeOp's $initialize() function, by giving a param_set argument. The param_set must be a ParamSet from the paradox package; see the tuning chapter or Section 9.4 for more information on how to define parameter spaces. After construction, the ParamSet can be accessed through the $param_set slot. While it is *possible* to modify this ParamSet, using e.g. the $add() and $add_dep() functions, *after* adding it to the PipeOp, it is strongly advised against.

Hyperparameters can be set and queried through the $values slot. When setting hyperparameters, they are automatically checked to satisfy all conditions set by the $param_set, so it is not necessary to type check them. Be aware that it is always possible to *remove* hyperparameter values.

When a PipeOp is initialized, it usually does not have any parameter values—$values takes the value list(). It is possible to set initial parameter values in the $initialize() constructor; this must be done *after* the super$initialize() call where the corresponding ParamSet must be supplied. This is because setting $values checks against the current $param_set, which would fail if the $param_set was not set yet.

When using an underlying library function (the scale function in PipeOpScale, say), then there is usually a "default" behaviour of that function when a parameter is not given. It is good practice to use this default behaviour whenever a parameter is not set (or when it was removed). This can easily be done when using the mlr3misc library's mlr3misc::invoke() function, which has functionality similar to "do.call()".

11.3.4.1. Hyperparameter Example: PipeOpScale

How to use hyperparameters can best be shown through the example of PipeOpScale, which is very similar to the example above, PipeOpScaleAlways. The difference is made by the presence of hyperparameters. PipeOpScale constructs a ParamSet in its $initialize function and passes this on to the super$initialize function:

```
PipeOpScale$public_methods$initialize
```

```
function (id = "scale", param_vals = list())
.__PipeOpScale__initialize(self = self, private = private, super = super,
    id = id, param_vals = param_vals)
<environment: namespace:mlr3pipelines>
```

The user has access to this and can set and get parameters. Types are automatically checked:

```
pss = po("scale")
print(pss$param_set)
```

```
<ParamSet:scale>
               id    class lower upper nlevels        default value
1:         center ParamLgl    NA    NA       2           TRUE
2:          scale ParamLgl    NA    NA       2           TRUE
3:         robust ParamLgl    NA    NA       2 <NoDefault[3]> FALSE
4: affect_columns ParamUty    NA    NA     Inf  <Selector[1]>
```

```
pss$param_set$values$center = FALSE
print(pss$param_set$values)
```

```
$robust
[1] FALSE

$center
[1] FALSE
```

```
pss$param_set$values$scale = "TRUE" # bad input is checked!
```

```
Error in self$assert(xs): Assertion on 'xs' failed: scale: Must be of type 'logical flag', not
```

How PipeOpScale handles its parameters can be seen in its `$.train_dt` method: It gets the relevant parameters from its `$values` slot and uses them in the `mlr3misc::invoke()` call. This has the advantage over calling `scale()` directly that if a parameter is not given, its default value from the `"scale()"` function will be used.

```
PipeOpScale$private_methods$.train_dt
```

```
function (dt, levels, target)
.__PipeOpScale__.train_dt(self = self, private = private, super = super,
    dt = dt, levels = levels, target = target)
<environment: namespace:mlr3pipelines>
```

Another change that is necessary compared to `PipeOpScaleAlways` is that the attributes `"scaled:scale"` and `"scaled:center"` are not always present, depending on parameters, and possibly need to be set to default values 1 or 0, respectively.

It is now even possible (if a bit pointless) to call PipeOpScale with both `scale` and `center` set to `FALSE`, which returns the original dataset, unchanged.

```
pss$param_set$values$scale = FALSE
pss$param_set$values$center = FALSE

gr = Graph$new()
```

```
gr$add_pipeop(pss)

result = gr$train(task)

result[[1]]$data()
```

```
        Species Petal.Length Petal.Width Sepal.Length Sepal.Width
  1:     setosa          1.4         0.2          5.1         3.5
  2:     setosa          1.4         0.2          4.9         3.0
  3:     setosa          1.3         0.2          4.7         3.2
  4:     setosa          1.5         0.2          4.6         3.1
  5:     setosa          1.4         0.2          5.0         3.6
 ---
146: virginica          5.2         2.3          6.7         3.0
147: virginica          5.0         1.9          6.3         2.5
148: virginica          5.2         2.0          6.5         3.0
149: virginica          5.4         2.3          6.2         3.4
150: virginica          5.1         1.8          5.9         3.0
```

11.4. Adding new Tuners

In this section, we show how to implement a custom tuner for `mlr3tuning`. The main task of a tuner is to iteratively propose new hyperparameter configurations that we want to evaluate for a given task, learner and validation strategy. The second task is to decide which configuration should be returned as a tuning result - usually it is the configuration that led to the best observed performance value. If you want to implement your own tuner, you have to implement an R6-Object that offers an `.optimize` method that implements the iterative proposal and you are free to implement `.assign_result` to differ from the before-mentioned default process of determining the result.

Before you start with the implementation make yourself familiar with the main R6-Objects in `bbotk` (Black-Box Optimization Toolkit). This package does not only provide basic black box optimization algorithms and but also the objects that represent the optimization problem (`OptimInstance`) and the log of all evaluated configurations (`Archive`).

There are two ways to implement a new tuner: a) If your new tuner can be applied to any kind of optimization problem it should be implemented as a `Optimizer`. Any `Optimizer` can be easily transformed to a `Tuner`. b) If the new custom tuner is only usable for hyperparameter tuning, for example because it needs to access the task, learner or resampling objects it should be directly implemented in `mlr3tuning` as a `Tuner`.

11.4.1. Adding a new Tuner

This is a summary of steps for adding a new tuner. The fifth step is only required if the new tuner is added via `bbotk`.

1. Check the tuner does not already exist as a [Optimizer](https://bbotk.mlr-org.com/reference/Optimizer.htm or [Tuner](https://mlr3tuning.mlr-org.com/reference/Tuner.html) in the GitHub repositories.
2. Use one of the existing optimizers / tuners as a template.
3. Overwrite the `.optimize` private method of the optimizer / tuner.
4. Optionally, overwrite the default `.assign_result` private method.
5. Use the `mlr3tuning::TunerFromOptimizer` class to transform the `Optimizer` to a `Tuner`.
6. Add unit tests for the tuner and optionally for the optimizer.
7. Open a new pull request for the [Tuner](https://mlr3tuning.mlr-org.com/reference/Tuner.html) and optionally a second one for the [Optimizer](https://bbotk.mlr-org.com/reference/Optimizer.html).

11.4.2. Template

If the new custom tuner is implemented via `bbotk`, use one of the existing optimizer as a template e.g. `bbotk::OptimizerRandomSearch`. There are currently only two tuners that are not based on a `Optimizer`: `mlr3hyperband::TunerHyperband` and `mlr3tuning::TunerIrace`. Both are rather complex but you can still use the documentation and class structure as a template. The following steps are identical for optimizers and tuners.

Rewrite the meta information in the documentation and create a new class name. Scientific sources can be added in `R/bibentries.R` which are added under `@source` in the documentation. The example and dictionary sections of the documentation are auto-generated based on the `@templateVar id <tuner_id>`. Change the parameter set of the optimizer / tuner and document them under `@section Parameters`. Do not forget to change `mlr_optimizers$add()` / `mlr_tuners$add()` in the last line which adds the optimizer / tuner to the dictionary.

11.4.3. Optimize method

The `$.optimize()` private method is the main part of the tuner. It takes an instance, proposes new points and calls the `$eval_batch()` method of the instance to evaluate them. Here you can go two ways: Implement the iterative process yourself or call an external optimization function that resides in another package.

11.4.3.1. Writing a custom iteration

Usually, the proposal and evaluation is done in a `repeat`-loop which you have to implement. Please consider the following points:

- You can evaluate one or multiple points per iteration
- You don't have to care about termination, as `$eval_batch()` won't allow more evaluations then allowed by the `bbotk::Terminator`. This implies, that code after the `repeat`-loop will not be executed.
- You don't have to care about keeping track of the evaluations as every evaluation is automatically stored in `inst$archive`.
- If you want to log additional information for each evaluation of the `Objective` in the `Archive` you can simply add columns to the `data.table` object that is passed to `$eval_batch()`.

11.4.3.2. Calling an external optimization function

Optimization functions from external packages usually take an objective function as an argument. In this case, you can pass `inst$objective_function` which internally calls `$eval_batch()`. Check out `OptimizerGenSA` for an example.

11.4.4. Assign result method

The default `$.assign_result()` private method simply obtains the best performing result from the archive. The default method can be overwritten if the new tuner determines the result of the optimization in a different way. The new function must call the `$assign_result()` method of the instance to write the final result to the instance. See `mlr3tuning::TunerIrace` for an implementation of `$.assign_result()`.

11.4.5. Transform optimizer to tuner

This step is only needed if you implement via `bbotk`. The `mlr3tuning::TunerFromOptimizer` class transforms a `Optimizer` to a `Tuner`. Just add the `Optimizer` to the `optimizer` field. See `mlr3tuning::TunerRandomSearch` for an example.

11.4.6. Add unit tests

The new custom tuner should be thoroughly tested with unit tests. `Tuner`s can be tested with the `test_tuner()` helper function. If you added the Tuner via a `Optimizer`, you should additionally test the `Optimizer` with the `test_optimizer()` helper function.

References

Baniecki, Hubert, and Przemyslaw Biecek. 2019. "modelStudio: Interactive Studio with Explanations for ML Predictive Models." *Journal of Open Source Software* 4 (43): 1798. https://doi.org/10.21105/joss.01798.

Baniecki, Hubert, Wojciech Kretowicz, Piotr Piątyszek, Jakub Wiśniewski, and Przemysław Biecek. 2021. "dalex: Responsible Machine Learning with Interactive Explainability and Fairness in Python." *Journal of Machine Learning Research* 22 (214): 1–7. http://jmlr.org/papers/v22/20-1473.html.

Bengio, Yoshua, and Yves Grandvalet. 2003. "No Unbiased Estimator of the Variance of k-Fold Cross-Validation." *Advances in Neural Information Processing Systems* 16.

Bergstra, James, and Yoshua Bengio. 2012. "Random Search for Hyper-Parameter Optimization." *Journal of Machine Learning Research* 13 (10): 281–305. http://jmlr.org/papers/v13/bergstra12a.html.

Biecek, Przemyslaw. 2018. "DALEX: Explainers for complex predictive models in R." *Journal of Machine Learning Research* 19 (84): 1–5. http://jmlr.org/papers/v19/18-416.html.

Biecek, Przemyslaw, and Tomasz Burzykowski. 2021. *Explanatory Model Analysis*. Chapman; Hall/CRC, New York. https://ema.drwhy.ai/.

Binder, Martin, Florian Pfisterer, Michel Lang, Lennart Schneider, Lars Kotthoff, and Bernd Bischl. 2021. "mlr3pipelines - Flexible Machine Learning Pipelines in R." *Journal of Machine Learning Research* 22 (184): 1–7. http://jmlr.org/papers/v22/21-0281.html.

Bischl, Bernd, Martin Binder, Michel Lang, Tobias Pielok, Jakob Richter, Stefan Coors, Janek Thomas, et al. 2021. "Hyperparameter Optimization: Foundations, Algorithms, Best Practices and Open Challenges." https://doi.org/10.48550/ARXIV.2107.05847.

Bischl, Bernd, Michel Lang, Lars Kotthoff, Julia Schiffner, Jakob Richter, Erich Studerus, Giuseppe Casalicchio, and Zachary M. Jones. 2016. "mlr: Machine Learning in R." *Journal of Machine Learning Research* 17 (170): 1–5. http://jmlr.org/papers/v17/15-066.html.

Bischl, Bernd, Olaf Mersmann, Heike Trautmann, and Claus Weihs. 2012. "Resampling Methods for Meta-Model Validation with Recommendations for Evolutionary Computation." *Evolutionary Computation* 20 (2): 249–75.

Bishop, Christopher M. 2006. *Pattern Recognition and Machine Learning*. Springer.

Bommert, Andrea, Xudong Sun, Bernd Bischl, Jörg Rahnenführer, and Michel Lang. 2020. "Benchmark for Filter Methods for Feature Selection in High-Dimensional Classification Data." *Computational Statistics & Data Analysis* 143: 106839. https://doi.org/https://doi.org/10.1016/j.csda.2019.106839.

Breiman, Leo. 1996. "Bagging Predictors." *Machine Learning* 24 (2): 123–40.

Brenning, Alexander. 2012. "Spatial Cross-Validation and Bootstrap for the Assessment of Prediction Rules in Remote Sensing: The R Package Sperrorest." In *2012 IEEE International Geoscience and Remote Sensing Symposium*. IEEE. https://doi.org/10.1109/igarss.2012.6352393.

Bücker, Michael, Gero Szepannek, Alicja Gosiewska, and Przemyslaw Biecek. 2022. "Transparency, Auditability, and Explainability of Machine Learning Models in Credit Scoring." *Journal of the Operational Research Society* 73 (1): 70–90. https://doi.org/10.1080/01605682.2021.1922098.

Chandrashekar, Girish, and Ferat Sahin. 2014. "A Survey on Feature Selection Methods." *Computers and Electrical Engineering* 40 (1): 16–28. https://doi.org/https://doi.org/10.1016/j.compeleceng.2013.11.024.

Collett, David. 2014. *Modelling Survival Data in Medical Research*. 3rd ed. CRC.

Davis, Jesse, and Mark Goadrich. 2006. "The Relationship Between Precision-Recall and ROC Curves." In *Proceedings of the 23rd International Conference on Machine Learning*, 233–40.

Demšar, Janez. 2006. "Statistical Comparisons of Classifiers over Multiple Data Sets." *Journal of Machine Learning Research* 7 (1): 1–30. https://jmlr.org/papers/v7/demsar06a.html.

Feurer, Matthias, and Frank Hutter. 2019. "Hyperparameter Optimization." In *Automated Machine Learning: Methods, Systems, Challenges*, edited by Frank Hutter, Lars Kotthoff, and Joaquin Vanschoren, 3–33. Cham: Springer International Publishing. https://doi.org/10.1007/978-3-030-05318-5_1.

Guyon, Isabelle, and André Elisseeff. 2003. "An Introduction to Variable and Feature Selection." *Journal of Machine Learning Research* 3 (Mar): 1157–82.

Hand, David J, and Robert J Till. 2001. "A Simple Generalisation of the Area Under the ROC Curve for Multiple Class Classification Problems." *Machine Learning* 45: 171–86.

Hansen, Nikolaus, and Anne Auger. 2011. "CMA-ES: Evolution Strategies and Covariance Matrix Adaptation." In *Proceedings of the 13th Annual Conference Companion on Genetic and Evolutionary Computation*, 991–1010.

Hastie, Trevor, Jerome Friedman, and Robert Tibshirani. 2001. *The Elements of Statistical Learning*. Springer New York. https://doi.org/10.1007/978-0-387-21606-5.

Holzinger, Andreas, Anna Saranti, Christoph Molnar, Przemyslaw Biecek, and Wojciech Samek. 2022. "Explainable AI Methods - a Brief Overview." *International Workshop on Extending Explainable AI Beyond Deep Models and Classifiers*, 13–38. https://doi.org/10.1007/978-3-031-04083-2_2.

Horst, Allison Marie, Alison Presmanes Hill, and Kristen B Gorman. 2020. *palmerpenguins: Palmer Archipelago (Antarctica) penguin data*. https://doi.org/10.5281/zenodo.3960218.

James, Gareth, Daniela Witten, Trevor Hastie, and Robert Tibshirani. 2014. *An Introduction to Statistical Learning: With Applications in r*. Springer Publishing Company, Incorporated.

Japkowicz, Nathalie, and Mohak Shah. 2011. *Evaluating Learning Algorithms: A Classification Perspective*. Cambridge University Press.

Karl, Florian, Tobias Pielok, Julia Moosbauer, Florian Pfisterer, Stefan Coors, Martin Binder, Lennart Schneider, et al. 2022. "Multi-Objective Hyperparameter Optimization - an Overview." https://doi.org/10.48550/ARXIV.2206.07438.

Kim, Ji-Hyun. 2009. "Estimating Classification Error Rate: Repeated Cross-Validation, Repeated Hold-Out and Bootstrap." *Computational Statistics & Data Analysis* 53 (11): 3735–45.

Krzyziński, Mateusz, Mikołaj Spytek, Hubert Baniecki, and Przemysław Biecek. 2023. "SurvSHAP(t): Time-dependent explanations of machine learning survival models." *Knowledge-Based Systems* 262: 110234. https://doi.org/https://doi.org/10.1016/j.knosys.2022.110234.

Lang, Michel. 2017. "checkmate: Fast Argument Checks for Defensive R Programming." *The R Journal* 9 (1): 437–45. https://doi.org/10.32614/RJ-2017-028.

Lang, Michel, Martin Binder, Jakob Richter, Patrick Schratz, Florian Pfisterer, Stefan Coors, Quay Au, Giuseppe Casalicchio, Lars Kotthoff, and Bernd Bischl. 2019. "mlr3: A Modern Object-Oriented Machine Learning Framework in R." *Journal of Open Source Software*, December. https://doi.org/10.21105/joss.01903.

Legendre, Pierre. 1993. "Spatial Autocorrelation: Trouble or New Paradigm?" *Ecology* 74 (6): 1659–73. https://doi.org/10.2307/1939924.

Li, Lisha, Kevin Jamieson, Giulia DeSalvo, Afshin Rostamizadeh, and Ameet Talwalkar. 2017.

"Hyperband: A Novel Bandit-Based Approach to Hyperparameter Optimization." *The Journal of Machine Learning Research* 18 (1): 6765–6816.

López-Ibáñez, Manuel, Jérémie Dubois-Lacoste, Leslie Pérez Cáceres, Mauro Birattari, and Thomas Stützle. 2016. "The Irace Package: Iterated Racing for Automatic Algorithm Configuration." *Operations Research Perspectives* 3: 43–58.

Lovelace, Robin, Jakub Nowosad, and Jannes Muenchow. 2019. *Geocomputation with R*. CRC Press.

Meyer, Hanna, Christoph Reudenbach, Tomislav Hengl, Marwan Katurji, and Thomas Nauss. 2018. "Improving Performance of Spatio-Temporal Machine Learning Models Using Forward Feature Selection and Target-Oriented Validation." *Environmental Modelling & Software* 101 (March): 1–9. https://doi.org/10.1016/j.envsoft.2017.12.001.

Molinaro, Annette M, Richard Simon, and Ruth M Pfeiffer. 2005. "Prediction Error Estimation: A Comparison of Resampling Methods." *Bioinformatics* 21 (15): 3301–7.

Muenchow, J., A. Brenning, and M. Richter. 2012. "Geomorphic Process Rates of Landslides Along a Humidity Gradient in the Tropical Andes." *Geomorphology* 139-140: 271–84. https://doi.org/https://doi.org/10.1016/j.geomorph.2011.10.029.

O'Neil, Cathy. 2016. *Weapons of Math Destruction: How Big Data Increases Inequality and Threatens Democracy*. New York, NY: Crown Publishing Group.

R Core Team. 2019. *R: A Language and Environment for Statistical Computing*. Vienna, Austria: R Foundation for Statistical Computing. https://www.R-project.org/.

Romaszko, Kamil, Magda Tatarynowicz, Mateusz Urbański, and Przemysław Biecek. 2019. "modelDown: Automated Website Generator with Interpretable Documentation for Predictive Machine Learning Models." *Journal of Open Source Software* 4 (38): 1444. https://doi.org/10.21105/joss.01444.

Schratz, Patrick, Jannes Muenchow, Eugenia Iturritxa, Jakob Richter, and Alexander Brenning. 2019. "Hyperparameter Tuning and Performance Assessment of Statistical and Machine-Learning Algorithms Using Spatial Data." *Ecological Modelling* 406 (August): 109–20. https://doi.org/10.1016/j.ecolmodel.2019.06.002.

Silverman, Bernard W. 1986. *Density Estimation for Statistics and Data Analysis*. Vol. 26. CRC press.

Simon, Richard. 2007. "Resampling Strategies for Model Assessment and Selection." In *Fundamentals of Data Mining in Genomics and Proteomics*, edited by Werner Dubitzky, Martin Granzow, and Daniel Berrar, 173–86. Boston, MA: Springer US. https://doi.org/10.1007/978-0-387-47509-7_8.

Sonabend, Raphael, Franz J Király, Andreas Bender, Bernd Bischl, and Michel Lang. 2021. "mlr3proba: An R Package for Machine Learning in Survival Analysis." *Bioinformatics*, February. https://doi.org/10.1093/bioinformatics/btab039.

Tsallis, Constantino, and Daniel A Stariolo. 1996. "Generalized Simulated Annealing." *Physica A: Statistical Mechanics and Its Applications* 233 (1-2): 395–406.

Wiśniewski, Jakub, and Przemysław Biecek. 2022. "The r Journal: Fairmodels: A Flexible Tool for Bias Detection, Visualization, and Mitigation in Binary Classification Models." *The R Journal* 14: 227–43. https://doi.org/10.32614/RJ-2022-019.

Wolpert, David H. 1992. "Stacked Generalization." *Neural Networks* 5 (2): 241–59. https://doi.org/https://doi.org/10.1016/S0893-6080(05)80023-1.

Xiang, Yang, Sylvain Gubian, Brian Suomela, and Julia Hoeng. 2013. "Generalized Simulated Annealing for Global Optimization: The GenSA Package." *R J.* 5 (1): 13.

A. Solutions to exercises

A.1. Solutions to Chapter 2

1. Use the built in `sonar` task and the `classif.rpart` learner along with the partition function to train a model.

```
set.seed(124)
task = tsk("sonar")
learner = lrn("classif.rpart", predict_type = "prob")
measure = msr("classif.ce")
splits = partition(task, ratio=0.8)

learner$train(task, splits$train)
```

Once the model is trained, generate the predictions on the test set, define the performance measure (`classif.ce`), and score the predictions.

```
preds = learner$predict(task, splits$test)

measure = msr("classif.ce")
preds$score(measure)
```

```
classif.ce
 0.2195122
```

2. Generate a confusion matrix from the built in function.

```
preds$confusion
```

```
        truth
response  M  R
       M 20  7
       R  2 12
```

Since the rows represent predictions (response) and the columns represent the ground truth values, the TP, FP, TN, and FN rates are as follows:

- True Positive (TP) = 20

- False Positive (FP) = 2
- True Negative (TN) = 12
- False Positive (FN) = 7

3. Since in this case we want the model to predict the negative class more often, we will raise the threshold (note the `predict_type` for the learner must be `prob` for this to work).

```
# raise threshold from 0.5 default to 0.6
preds$set_threshold(0.6)

preds$confusion
```

```
        truth
response  M  R
       M 14  4
       R  8 15
```

One reason we might want the false positive rate to be lower than the false negative rate is if we felt it was worse for a positive prediction to be incorrect (meaning the true label was the negative label) than it was for a negative prediction to be incorrect (meaning the true label was the positive label).

A.2. Solutions to Chapter 3

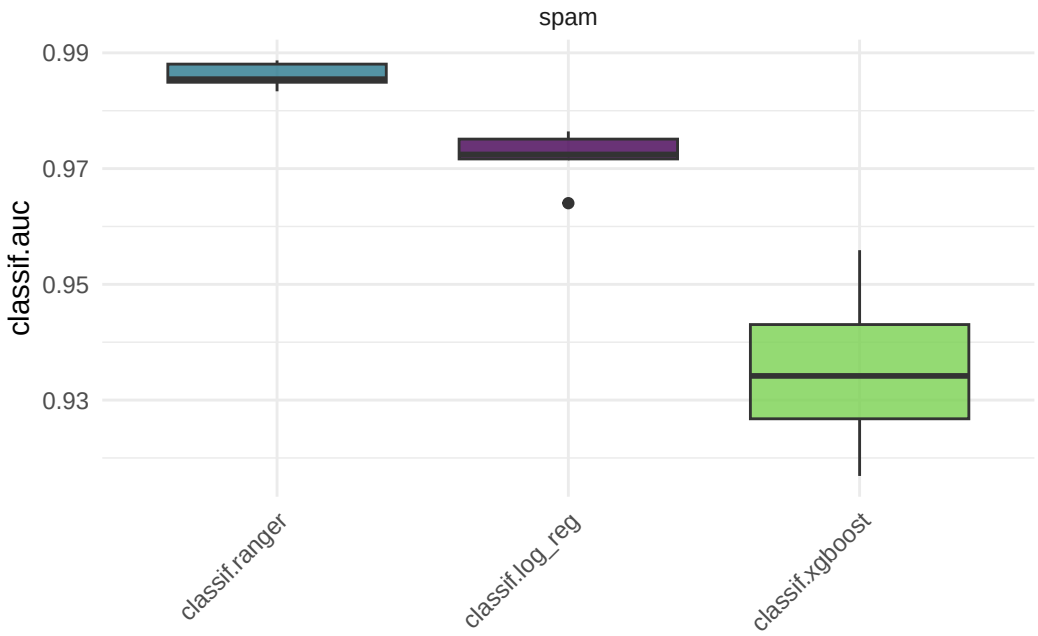
1. Use the `spam` task and 5-fold cross-validation to benchmark Random Forest (`classif.ranger`), Logistic Regression (`classif.log_reg`), and XGBoost (`classif.xgboost`) with regards to AUC. Which learner appears to do best? How confident are you in your conclusion? How would you improve upon this?

```
grid = benchmark_grid(
  tasks = tsk("spam"),
  learners = lrns(c("classif.ranger", "classif.log_reg", "classif.xgboost"), predict_type =
  resamplings = rsmp("cv", folds = 5)
)

bmr = benchmark(grid)
```

```
Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred
```

```
Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred

Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred
```

```
mlr3viz::autoplot(bmr, measure = msr("classif.auc"))
```



This is only a small example for a benchmark workflow, but without tuning (see Chapter 4), the results are naturally not suitable to make any broader statements about the superiority of either learner for this task.

2. A colleague claims to have achieved a 93.1% classification accuracy using the `classif.rpart` learner on the `penguins_simple` task. You want to reproduce their results and ask them about their resampling strategy. They said they used 3-fold cross-validation, and they assigned rows using the task's `row_id` modulo 3 to generate three evenly sized folds. Reproduce their results using the custom CV strategy.

```
task = tsk("penguins_simple")

resampling_customcv = rsmp("custom_cv")

resampling_customcv$instantiate(task = task, f = factor(task$row_ids %% 3))

rr = resample(
  task = task,
  learner = lrn("classif.rpart"),
  resampling = resampling_customcv
```

```
)

rr$aggregate(msr("classif.acc"))
```

```
classif.acc
  0.9309309
```

A.3. Solutions to Chapter 4

1. Tune the `mtry`, `sample.fraction`, `num.trees` hyperparameters of a random forest model (`regr.ranger`) on the `Motor Trend` data set (`mtcars`). Use a simple random search with 50 evaluations and select a suitable batch size. Evaluate with a 3-fold cross-validation and the root mean squared error.

```
set.seed(4)
learner = lrn("regr.ranger",
  mtry.ratio      = to_tune(0, 1),
  sample.fraction = to_tune(1e-1, 1),
  num.trees       = to_tune(1, 2000)
)

instance = ti(
  task = tsk("mtcars"),
  learner = learner,
  resampling = rsmp("cv", folds = 3),
  measures = msr("regr.rmse"),
  terminator = trm("evals", n_evals = 50)
)

tuner = tnr("random_search", batch_size = 10)

tuner$optimize(instance)
```

```
   mtry.ratio sample.fraction num.trees learner_param_vals  x_domain regr.rmse
1:  0.3558625       0.9108463       192          <list[4]> <list[3]>  2.757883
```

2. Evaluate the performance of the model created in Question 1 with nested resampling. Use a holdout validation for the inner resampling and a 3-fold cross-validation for the outer resampling. Print the unbiased performance estimate of the model.

```
set.seed(4)
learner = lrn("regr.ranger",
  mtry.ratio      = to_tune(0, 1),
  sample.fraction = to_tune(1e-1, 1),
```

```
  num.trees       = to_tune(1, 2000)
)

at = auto_tuner(
  method = tnr("random_search", batch_size = 10),
  learner = learner,
  resampling = rsmp("holdout"),
  measures = msr("regr.rmse"),
  terminator = trm("evals", n_evals = 50)
)

task = tsk("mtcars")
outer_resampling = rsmp("cv", folds = 3)
rr = resample(task, at, outer_resampling, store_models = TRUE)

rr$aggregate()
```

```
regr.mse
12.16805
```

A.4. Solutions to Chapter 5

1. Calculate a correlation filter on the `Motor Trend` data set (`mtcars`).

```
library("mlr3verse")
filter = flt("correlation")

task = tsk("mtcars")
filter$calculate(task)

as.data.table(filter)
```

```
    feature     score
 1:      wt 0.8676594
 2:     cyl 0.8521620
 3:    disp 0.8475514
 4:      hp 0.7761684
 5:    drat 0.6811719
 6:      vs 0.6640389
 7:      am 0.5998324
 8:    carb 0.5509251
 9:    gear 0.4802848
10:    qsec 0.4186840
```

2. Use the filter from the first exercise to select the five best features in the `mtcars` data set.

```
keep = names(head(filter$scores, 5))
task$select(keep)
task$feature_names
```

```
[1] "cyl"  "disp" "drat" "hp"   "wt"
```

3. Apply a backward selection to the penguins data set with a classification tree learner `"classif.rpart"` and holdout resampling by the measure classification accuracy. Compare the results with those in Section 5.2.1.

```
library("mlr3fselect")

instance = fselect(
  method = "sequential",
  strategy = "sbs",
  task =  tsk("penguins"),
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msr("classif.acc")
)
as.data.table(instance$result)[, .(bill_depth, bill_length, body_mass, classif.acc)]
```

```
   bill_depth bill_length body_mass classif.acc
1:       TRUE        TRUE      TRUE   0.9565217
```

```
instance$result_feature_set
```

```
[1] "bill_depth"  "bill_length" "body_mass"   "island"      "sex"
[6] "year"
```

Answer the following questions:

a. Do the selected features differ?

Yes, the backward selection selects more features.

b. Which feature selection method achieves a higher classification accuracy?

In this example, the backwards example performs slightly better, but this depends heavily on the random seed and could look different in another run.

c. Are the accuracy values in b) directly comparable? If not, what has to be changed to make them comparable?

No, they are not comparable because the holdout sampling called with `rsmp("holdout")` creates a different holdout set for the two runs. A fair comparison would create a single resampling instance and use it for both feature selections (see Chapter 3 for details):

```
resampling = rsmp("holdout")
resampling$instantiate(tsk("penguins"))

sfs = fselect(
  method = "sequential",
  strategy = "sfs",
  task =  tsk("penguins"),
  learner = lrn("classif.rpart"),
  resampling = resampling,
  measure = msr("classif.acc")
)
sbs = fselect(
  method = "sequential",
  strategy = "sbs",
  task =  tsk("penguins"),
  learner = lrn("classif.rpart"),
  resampling = resampling,
  measure = msr("classif.acc")
)
as.data.table(sfs$result)[, .(bill_depth, bill_length, body_mass, classif.acc)]
```

```
   bill_depth bill_length body_mass classif.acc
1:      FALSE        TRUE     FALSE    0.973913
```

```
as.data.table(sbs$result)[, .(bill_depth, bill_length, body_mass, classif.acc)]
```

```
   bill_depth bill_length body_mass classif.acc
1:       TRUE        TRUE      TRUE    0.973913
```

Alternatively, one could automate the feature selection and perform a benchmark between the two wrapped learners.

4. Automate the feature selection as in Section 5.2.6 with the `spam` data set and a logistic regression learner (`"classif.log_reg"`). Hint: Remember to call `library("mlr3learners")` for the logistic regression learner.

```
library("mlr3fselect")
library("mlr3learners")

at = auto_fselector(
  method = fs("random_search"),
  learner = lrn("classif.log_reg"),
  resampling = rsmp("holdout"),
  measure = msr("classif.acc"),
  terminator = trm("evals", n_evals = 50)
```

```
)

grid = benchmark_grid(
  task = tsk("spam"),
  learner = list(at, lrn("classif.log_reg")),
  resampling = rsmp("cv", folds = 3)
)

bmr = benchmark(grid)

aggr = bmr$aggregate(msrs(c("classif.acc", "time_train")))
as.data.table(aggr)[, .(learner_id, classif.acc, time_train)]
```

```
                learner_id classif.acc time_train
1: classif.log_reg.fselector   0.9219717      6.399
2:           classif.log_reg   0.9243633      0.119
```

A.5. Solutions to Chapter 6

A.6. Solutions to Chapter 8

A.7. Solutions to Chapter 9

A.8. Solutions to Chapter 10

1. Prepare a `mlr3` regression task for `fifa` data. Select only variables describing the age and skills of footballers. Train any predictive model for this task, e.g. `regr.ranger`.

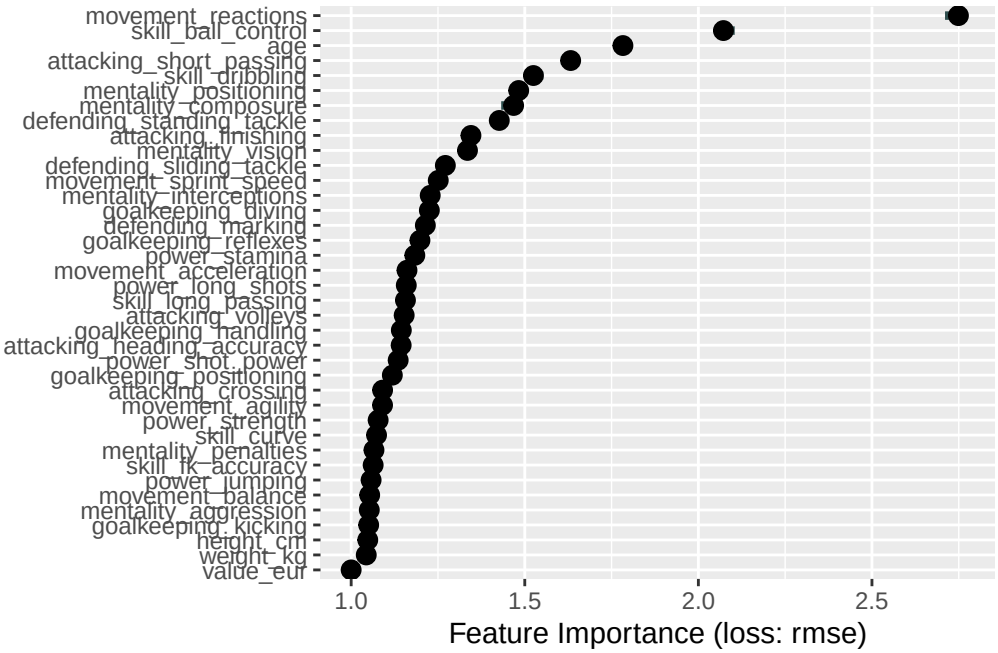
```
library("DALEX")
library("ggplot2")
data("fifa", package = "DALEX")
old_theme = set_theme_dalex("ema")

library("mlr3")
library("mlr3learners")
set.seed(1)

fifa20 <- fifa[,5:42]
task_fifa = as_task_regr(fifa20, target = "value_eur", id = "fifa20")

learner = lrn("regr.ranger")
learner$train(task_fifa)
learner$model
```

```
Ranger result

Call:
 ranger::ranger(dependent.variable.name = task$target_names, data = task$data(),      case.wei

Type:                             Regression
Number of trees:                  500
Sample size:                      5000
Number of independent variables:  37
Mtry:                             6
Target node size:                 5
Variable importance mode:         none
Splitrule:                        variance
OOB prediction error (MSE):       1.022805e+13
R squared (OOB):                  0.869943
```

2. Use the permutation importance method to calculate variable importance ranking. Which variable is the most important? Is it surprising?

With `iml`

```
library(iml)
model = Predictor$new(learner,
                      data = fifa20,
                      y = fifa$value_eur)

effect = FeatureImp$new(model,
                      loss = "rmse")
effect$plot()
```

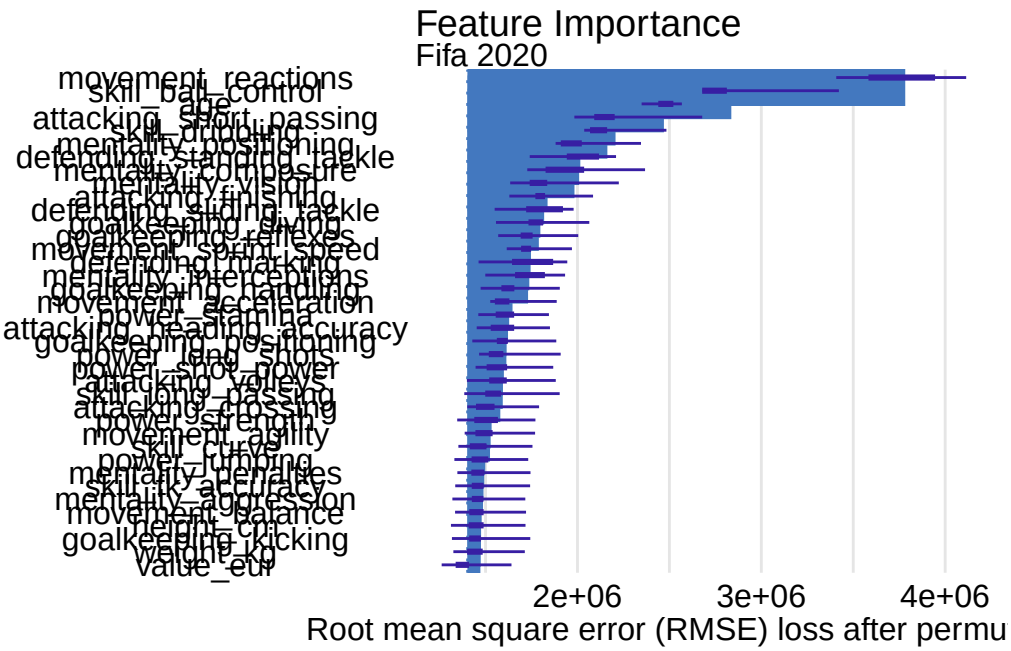


With `DALEX`

```
library("DALEX")
ranger_exp = DALEX::explain(learner,
  data = fifa20,
  y = fifa$value_eur,
  label = "Fifa 2020",
  verbose = FALSE)

ranger_effect = model_parts(ranger_exp, B = 5)
head(ranger_effect)
```

```
             variable mean_dropout_loss     label
1        _full_model_           1402526 Fifa 2020
2           value_eur           1402526 Fifa 2020
3           weight_kg           1471865 Fifa 2020
4 goalkeeping_kicking           1472795 Fifa 2020
5           height_cm           1474859 Fifa 2020
6    movement_balance           1475618 Fifa 2020
```

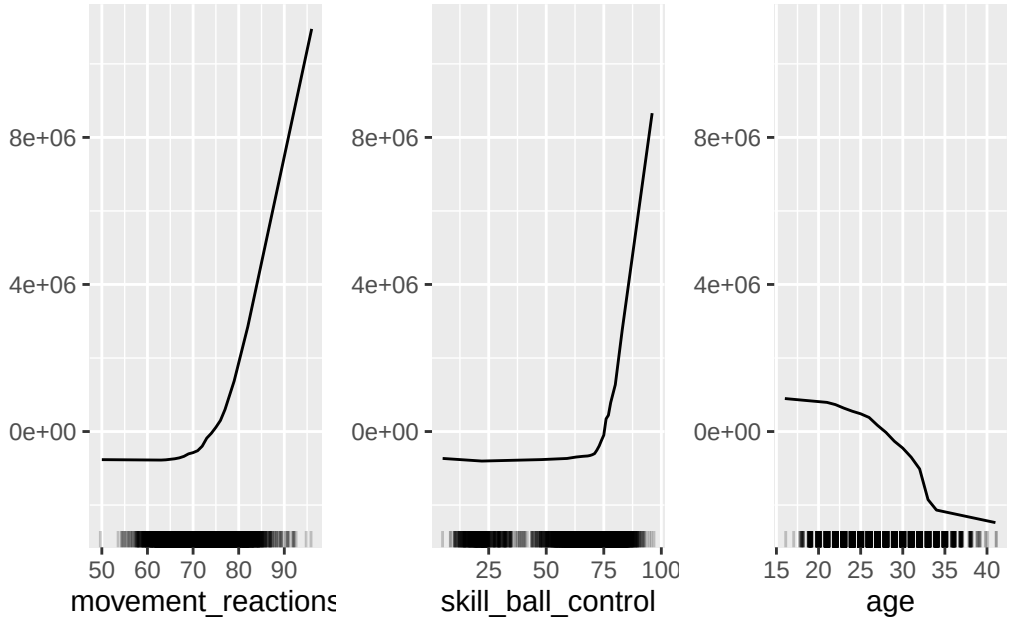
```
plot(ranger_effect)
```



3. Use the Partial Dependence profile to draw the global behavior of the model for this variable. Is it aligned with your expectations?

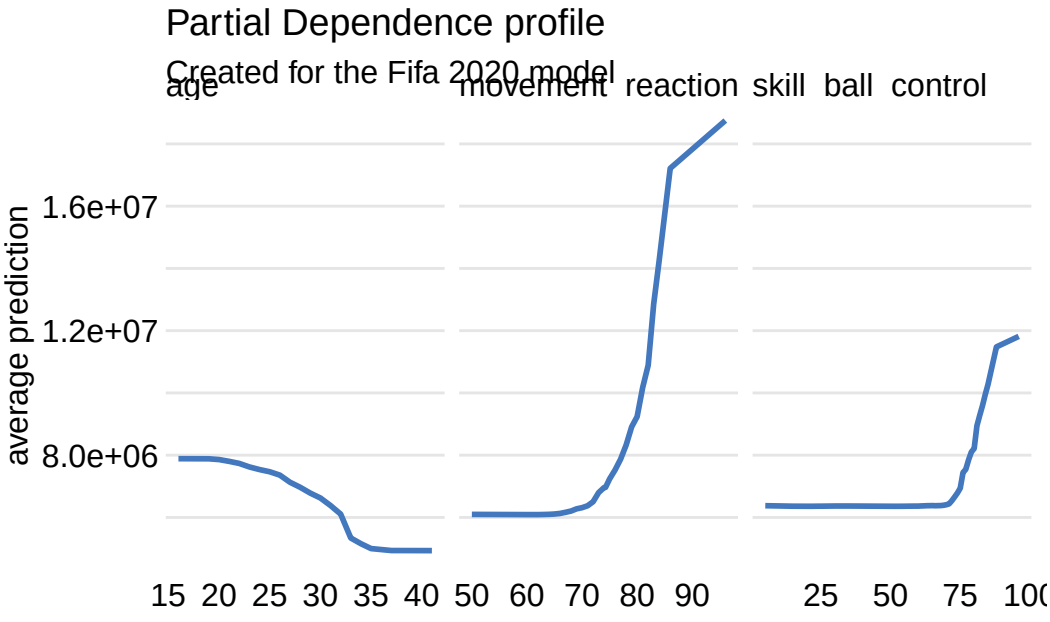
With `iml`

```
num_features = c("movement_reactions", "skill_ball_control", "age")

effect = FeatureEffects$new(model)
plot(effect, features = num_features)
```



With DALEX

```
num_features = c("movement_reactions", "skill_ball_control", "age")

ranger_profiles = model_profile(ranger_exp, variables = num_features)
plot(ranger_profiles)
```



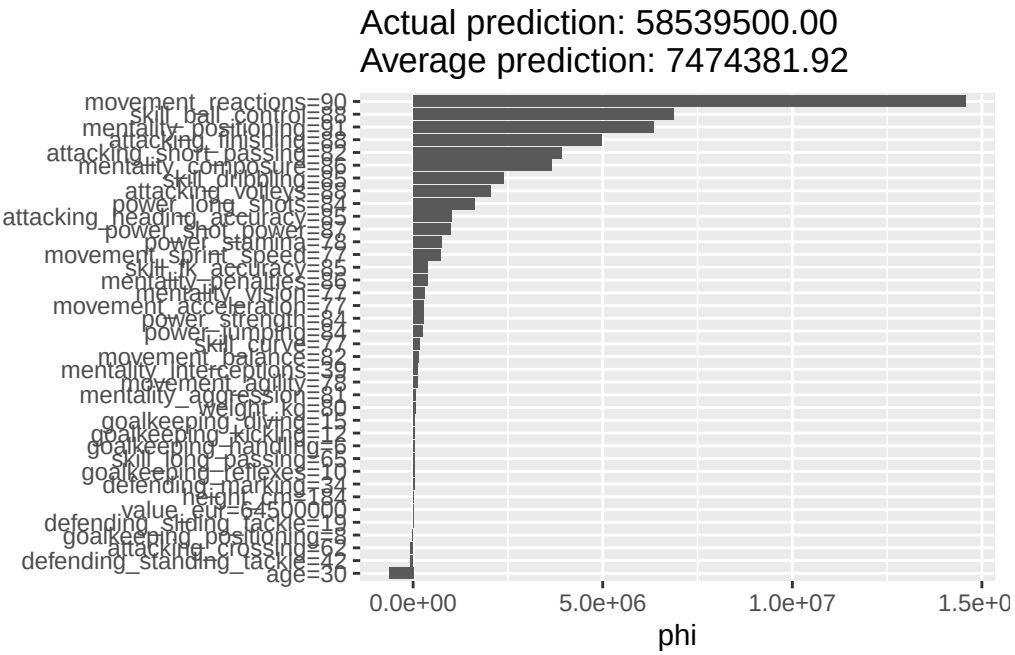
4 Choose one of the football players. You can choose some well-known striker (e.g. Robert Lewandowski) or a well-known goalkeeper (e.g. Manuel Neuer). The following tasks are worth repeating for several different choices.

```
player_1 <- fifa["R. Lewandowski", 5:42]
```

5. For the selected footballer, calculate and plot the Shapley values. Which variable is locally the most important and has the strongest influence on the valuation of the footballer?

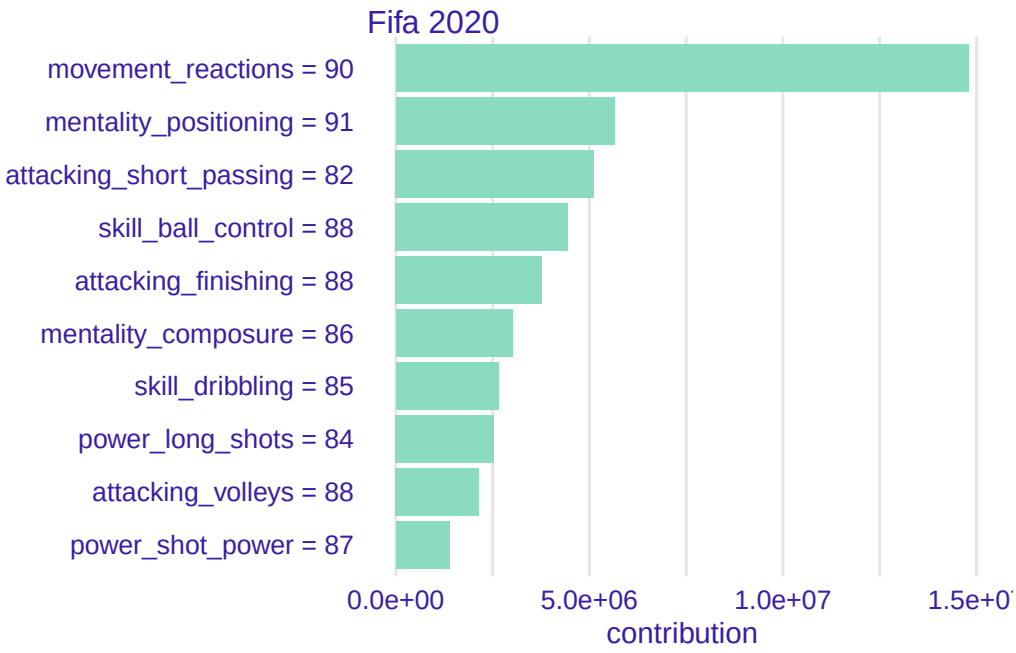
With `iml`

```
shapley = Shapley$new(model, x.interest = player_1)
plot(shapley)
```



With `DALEX`

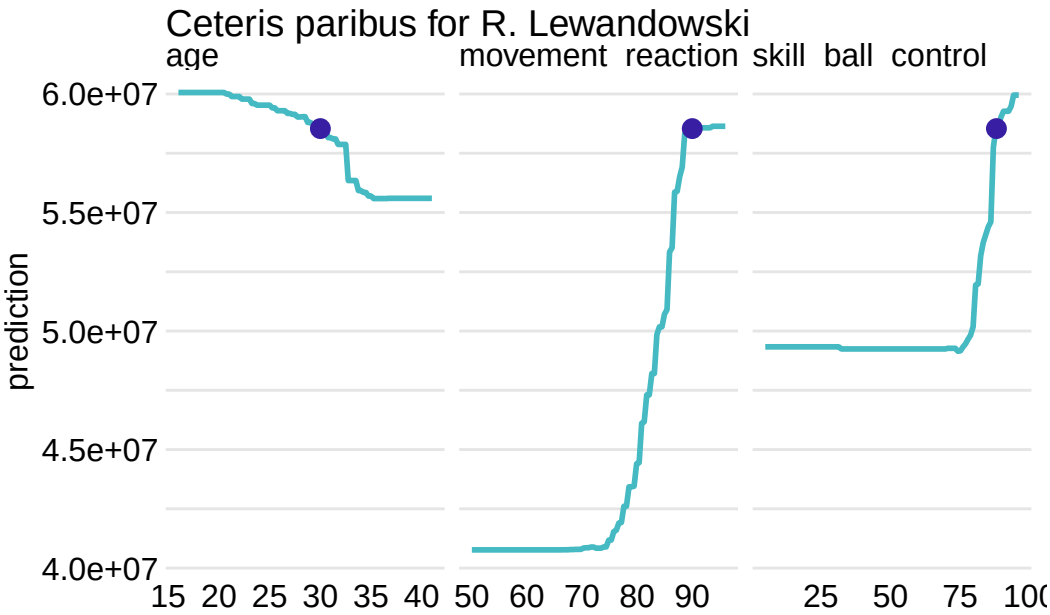
```
ranger_shap = predict_parts(ranger_exp,
              new_observation = player_1,
              type = "shap", B = 1)
plot(ranger_shap, show_boxplots = FALSE)
```



6. For the selected footballer, calculate the Ceteris Paribus / Individual Conditional Expectation profiles to draw the local behavior of the model for this variable. Is it different from the global behavior?

With `DALEX`

```
num_features = c("movement_reactions", "skill_ball_control", "age")

ranger_ceteris = predict_profile(ranger_exp, player_1)
plot(ranger_ceteris, variables = num_features) +
  ggtitle("Ceteris paribus for R. Lewandowski", " ")
```



A.9. Solutions to Chapter 11

B. Glossary

Term	Definition
Resampling	Repeatedly splitting data into training and test sets.

C. Tasks

The key features of the tasks that we use throughout the book are explained below as well as a plot of the target variable(s).

C.1. Regression Tasks

C.1.1. mtcars

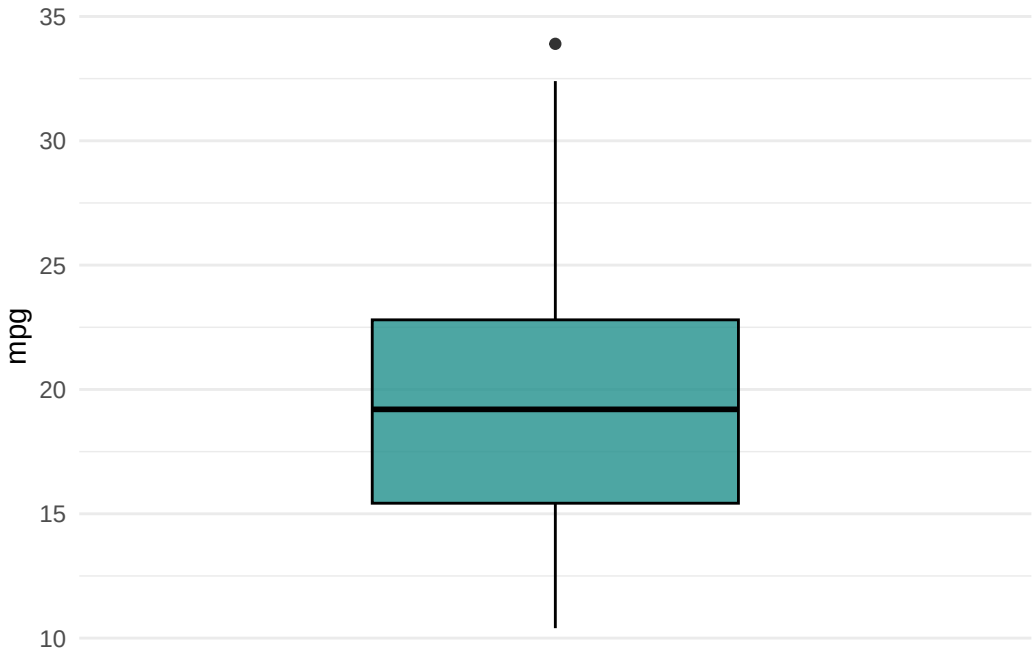
```
tsk("mtcars")
```

```
<TaskRegr:mtcars> (32 x 11): Motor Trends
* Target: mpg
* Properties: -
* Features (10):
  - dbl (10): am, carb, cyl, disp, drat, gear, hp, qsec, vs, wt
```

```
tsk("mtcars")$head()
```

```
    mpg am carb cyl disp drat gear  hp  qsec vs    wt
1: 21.0  1    4   6  160 3.90    4 110 16.46  0 2.620
2: 21.0  1    4   6  160 3.90    4 110 17.02  0 2.875
3: 22.8  1    1   4  108 3.85    4  93 18.61  1 2.320
4: 21.4  0    1   6  258 3.08    3 110 19.44  1 3.215
5: 18.7  0    2   8  360 3.15    3 175 17.02  0 3.440
6: 18.1  0    1   6  225 2.76    3 105 20.22  1 3.460
```

```
autoplot(tsk("mtcars"))
```



See more at `?mlr_tasks_mtcars`.

C.2. Classification Tasks

C.2.1. penguins

```
tsk("penguins")
```

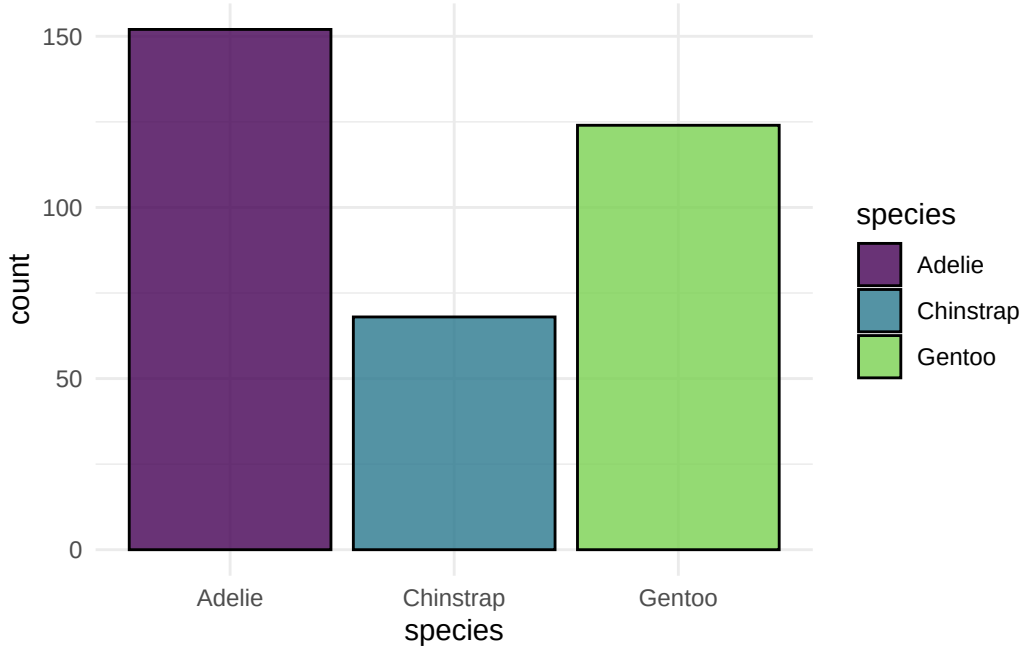
```
<TaskClassif:penguins> (344 x 8): Palmer Penguins
* Target: species
* Properties: multiclass
* Features (7):
  - int (3): body_mass, flipper_length, year
  - dbl (2): bill_depth, bill_length
  - fct (2): island, sex
```

```
tsk("penguins")$head()
```

```
   species bill_depth bill_length body_mass flipper_length    island    sex
1:  Adelie       18.7        39.1      3750            181 Torgersen   male
2:  Adelie       17.4        39.5      3800            186 Torgersen female
3:  Adelie       18.0        40.3      3250            195 Torgersen female
4:  Adelie         NA          NA        NA             NA Torgersen   <NA>
```

```
5:  Adelie       19.3        36.7      3450           193 Torgersen female
6:  Adelie       20.6        39.3      3650           190 Torgersen   male
1 variable not shown: [year]
```

```
autoplot(tsk("penguins"))
```



See more at `?mlr_tasks_penguins`.

C.2.2. penguins_simple

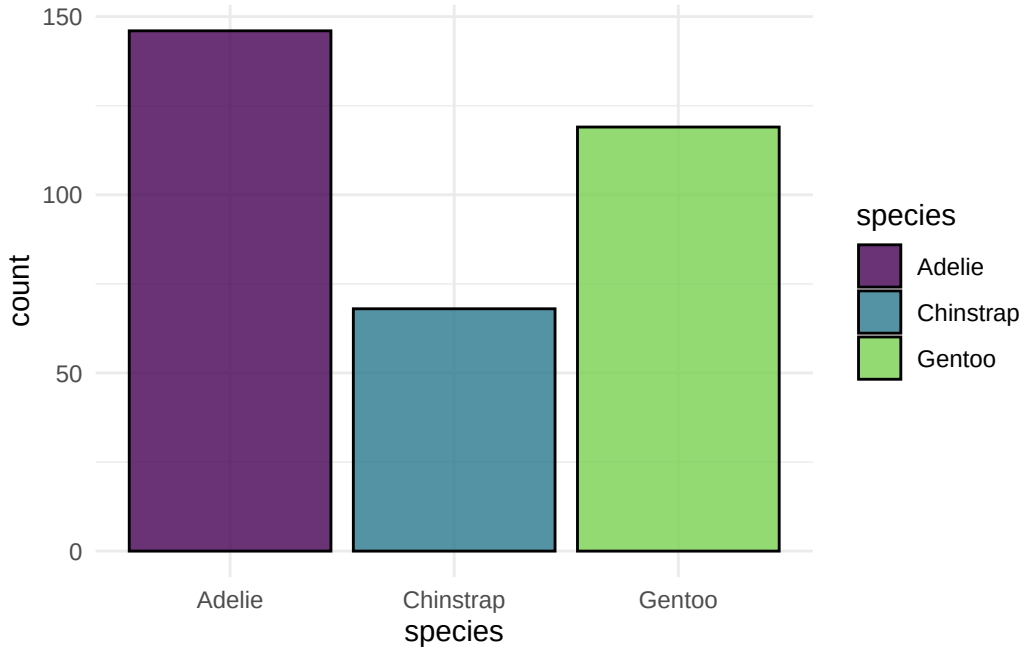
```
tsk("penguins_simple")
```

```
<TaskClassif:penguins> (333 x 11): Simplified Palmer Penguins
* Target: species
* Properties: multiclass
* Features (10):
  - dbl (7): bill_depth, bill_length, island.Biscoe, island.Dream,
    island.Torgersen, sex.female, sex.male
  - int (3): body_mass, flipper_length, year
```

```
tsk("penguins_simple")$head()
```

```
   species bill_depth bill_length body_mass flipper_length island.Biscoe
1:  Adelie       18.7        39.1      3750            181             0
2:  Adelie       17.4        39.5      3800            186             0
3:  Adelie       18.0        40.3      3250            195             0
4:  Adelie       19.3        36.7      3450            193             0
5:  Adelie       20.6        39.3      3650            190             0
6:  Adelie       17.8        38.9      3625            181             0
5 variables not shown: [island.Dream, island.Torgersen, sex.female, sex.male, year]
```

```
autoplot(tsk("penguins_simple"))
```



See more at `?mlr3data::mlr_tasks_penguins_simple`.

C.2.3. sonar

```
tsk("sonar")
```

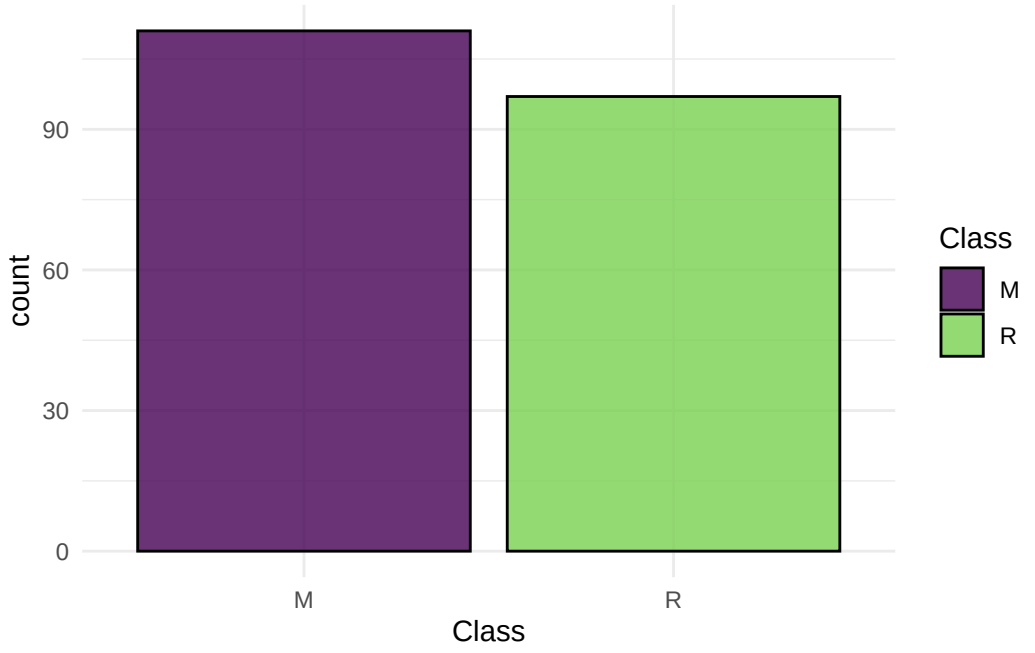
```
<TaskClassif:sonar> (208 x 61): Sonar: Mines vs. Rocks
* Target: Class
* Properties: twoclass
* Features (60):
  - dbl (60): V1, V10, V11, V12, V13, V14, V15, V16, V17, V18, V19, V2,
    V20, V21, V22, V23, V24, V25, V26, V27, V28, V29, V3, V30, V31,
    V32, V33, V34, V35, V36, V37, V38, V39, V4, V40, V41, V42, V43,
    V44, V45, V46, V47, V48, V49, V5, V50, V51, V52, V53, V54, V55,
```

```
    V56, V57, V58, V59, V6, V60, V7, V8, V9
```

```
tsk("sonar")$head()
```

```
   Class     V1    V10    V11    V12    V13    V14    V15    V16    V17    V18
1:     R 0.0200 0.2111 0.1609 0.1582 0.2238 0.0645 0.0660 0.2273 0.3100 0.2999
2:     R 0.0453 0.2872 0.4918 0.6552 0.6919 0.7797 0.7464 0.9444 1.0000 0.8874
3:     R 0.0262 0.6194 0.6333 0.7060 0.5544 0.5320 0.6479 0.6931 0.6759 0.7551
4:     R 0.0100 0.1264 0.0881 0.1992 0.0184 0.2261 0.1729 0.2131 0.0693 0.2281
5:     R 0.0762 0.4459 0.4152 0.3952 0.4256 0.4135 0.4528 0.5326 0.7306 0.6193
6:     R 0.0286 0.3039 0.2988 0.4250 0.6343 0.8198 1.0000 0.9988 0.9508 0.9025
50 variables not shown: [V19, V2, V20, V21, V22, V23, V24, V25, V26, V27, ...]
```

```
autoplot(tsk("sonar"))
```



See more at `?mlr_tasks_sonar`.

C.2.4. spam

```
tsk("spam")
```

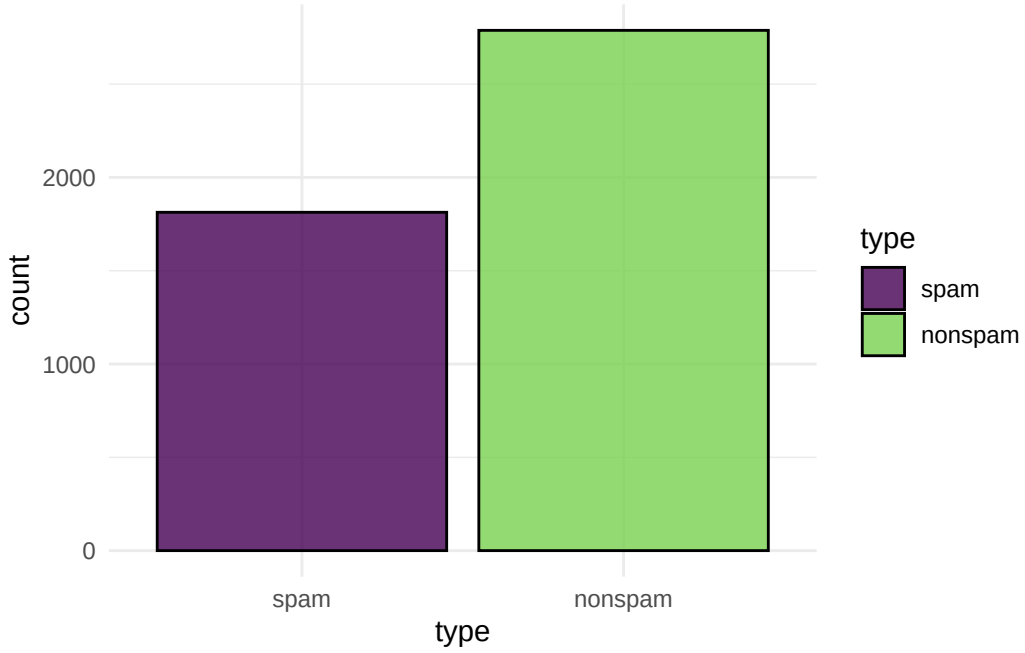
```
<TaskClassif:spam> (4601 x 58): HP Spam Detection
* Target: type
```

```
* Properties: twoclass
* Features (57):
  - dbl (57): address, addresses, all, business, capitalAve,
    capitalLong, capitalTotal, charDollar, charExclamation, charHash,
    charRoundbracket, charSemicolon, charSquarebracket, conference,
    credit, cs, data, direct, edu, email, font, free, george, hp, hpl,
    internet, lab, labs, mail, make, meeting, money, num000, num1999,
    num3d, num415, num650, num85, num857, order, original, our, over,
    parts, people, pm, project, re, receive, remove, report, table,
    technology, telnet, will, you, your
```

```
tsk("spam")$head()
```

```
   type address addresses  all business capitalAve capitalLong capitalTotal
1: spam    0.64      0.00 0.64     0.00      3.756          61          278
2: spam    0.28      0.14 0.50     0.07      5.114         101         1028
3: spam    0.00      1.75 0.71     0.06      9.821         485         2259
4: spam    0.00      0.00 0.00     0.00      3.537          40          191
5: spam    0.00      0.00 0.00     0.00      3.537          40          191
6: spam    0.00      0.00 0.00     0.00      3.000          15           54
50 variables not shown: [charDollar, charExclamation, charHash, charRoundbracket, charSemicolon
```

```
autoplot(tsk("spam"))
```



See more at `?mlr_tasks_spam`.

C.3. Survival Tasks

C.3.1. rats

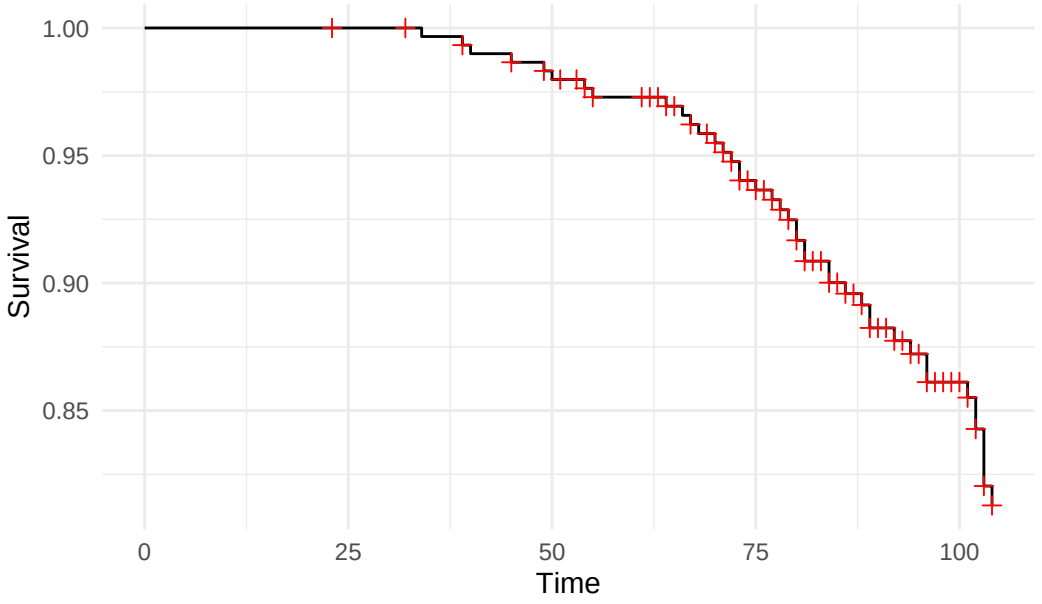
```
tsk("rats")
```

```
<TaskSurv:rats> (300 x 5): Rats
* Target: time, status
* Properties: -
* Features (3):
  - int (2): litter, rx
  - fct (1): sex
```

```
tsk("rats")$head()
```

```
   time status litter rx sex
1:  101      0      1  1   f
2:   49      1      1  0   f
3:  104      0      1  0   f
4:   91      0      2  1   m
5:  104      0      2  0   m
6:  102      0      2  0   m
```

```
autoplot(tsk("rats"))
```



See more at `?mlr3proba::mlr_tasks_rats`.

C.4. Density Tasks

C.4.1. precip

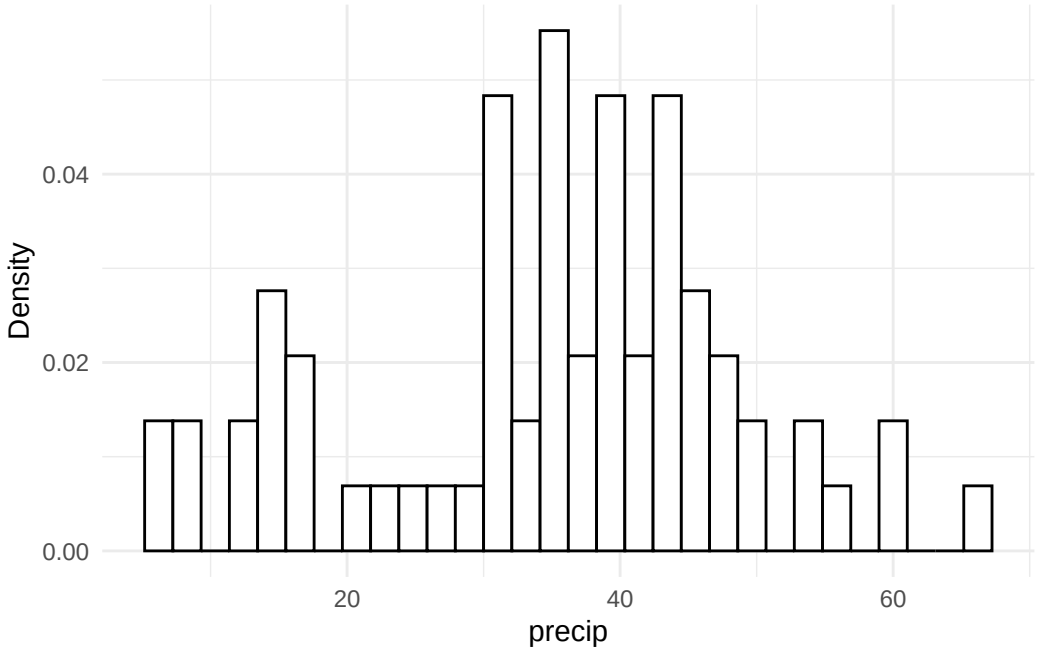
```
tsk("precip")
```

```
<TaskDens:precip> (70 x 1): Annual Precipitation
* Target: -
* Properties: -
* Features (1):
  - dbl (1): precip
```

```
tsk("precip")$head()
```

```
   precip
1:   67.0
2:   54.7
3:    7.0
4:   48.5
5:   14.0
6:   17.2
```

```
autoplot(tsk("precip"))
```



See more at `?mlr3proba::mlr_tasks_precip`.

C.5. Spatiotemporal Tasks

C.5.1. ecuador

```
tsk("ecuador")
```

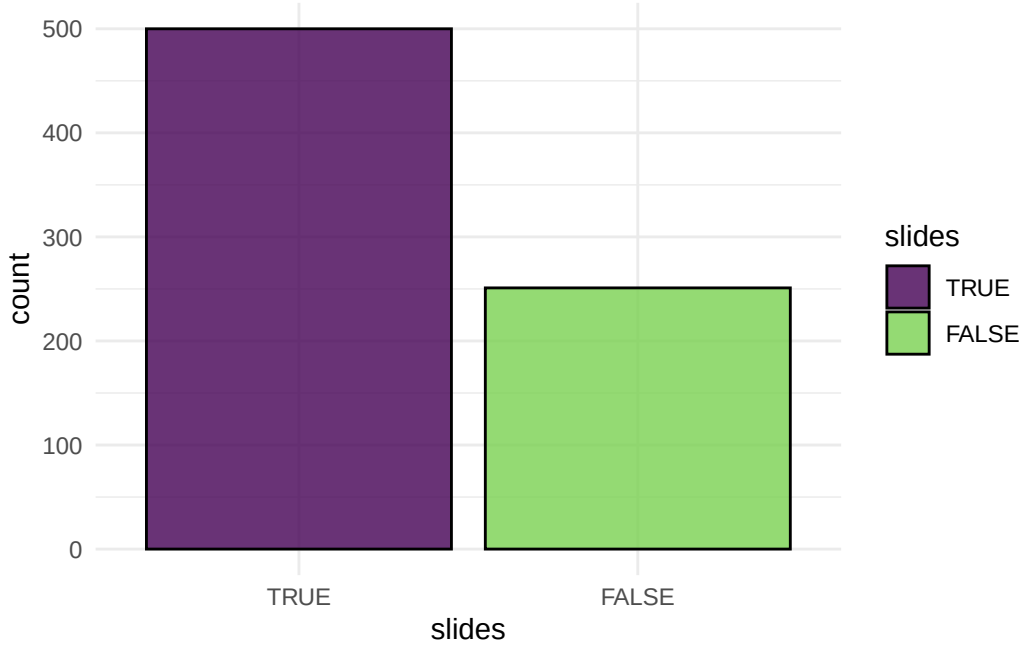
```
<TaskClassifST:ecuador> (751 x 11): Ecuador landslides
* Target: slides
* Properties: twoclass
* Features (10):
  - dbl (10): carea, cslope, dem, distdeforest, distroad,
    distslidespast, hcurv, log.carea, slope, vcurv
* Coordinates:
           x       y
  1: 712882.5 9560002
  2: 715232.5 9559582
  3: 715392.5 9560172
  4: 715042.5 9559312
  5: 715382.5 9560142
 ---
747: 714472.5 9558482
748: 713142.5 9560992
749: 713322.5 9560562
```

```
750: 715392.5 9557932
751: 713802.5 9560862
```

```
tsk("ecuador")$head()
```

```
   slides       carea   cslope     dem distdeforest distroad distslidespast
1:   TRUE   5577.3916 34.42789 1911.52        15.00      300              9
2:   TRUE   1399.2329 30.71569 2198.66       300.00      300             21
3:   TRUE 351155.1250 32.81444 1988.71       300.00      300             40
4:   TRUE    500.5027 33.90592 2320.49       300.00      300            100
5:   TRUE    671.1807 41.60017 2021.07       300.00      300             21
6:   TRUE    634.3320 30.29457 1838.40         9.15      300              2
4 variables not shown: [hcurv, log.carea, slope, vcurv]
```

```
autoplot(tsk("ecuador"))
```



See more at `?mlr3spatiotempcv::mlr_tasks_ecuador`.

C.6. Clustering Tasks

C.6.1. usarrests

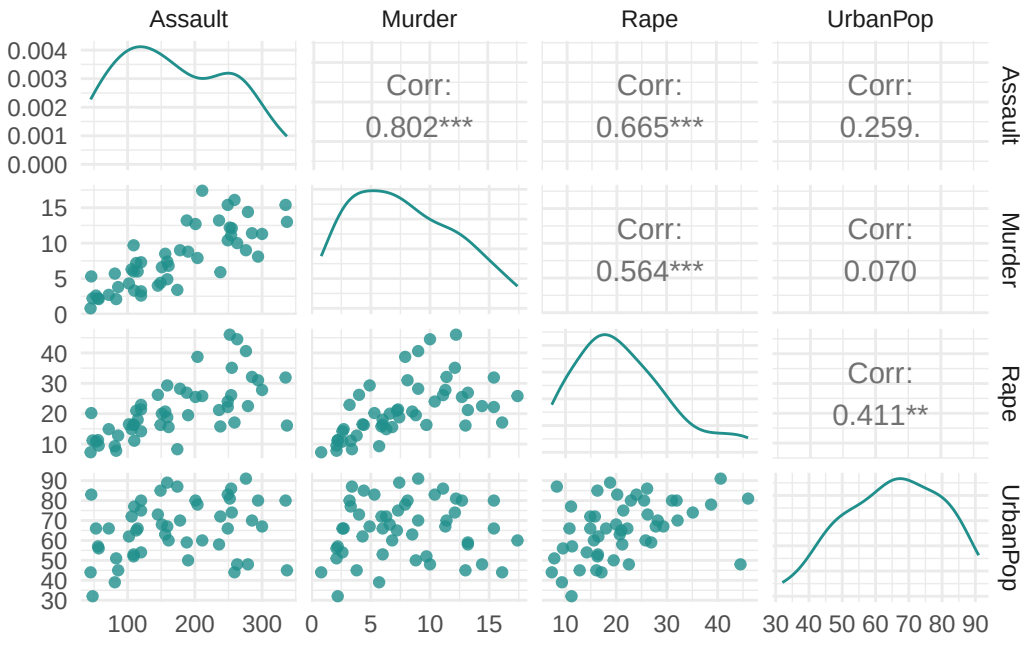
```
tsk("usarrests")
```

```
<TaskClust:usarrests> (50 x 4): US Arrests
* Target: -
* Properties: -
* Features (4):
  - int (2): Assault, UrbanPop
  - dbl (2): Murder, Rape
```

```
tsk("usarrests")$head()
```

```
   Assault Murder Rape UrbanPop
1:     236   13.2 21.2       58
2:     263   10.0 44.5       48
3:     294    8.1 31.0       80
4:     190    8.8 19.5       50
5:     276    9.0 40.6       91
6:     204    7.9 38.7       78
```

```
autoplot(tsk("usarrests"))
```



See more at `?mlr3cluster::mlr_tasks_usarrests`.

D. Overview Tables

Our homepage provides overviews and tables of the following objects:

Description	Link
Packages overview	https://mlr-org.com/packages.html
Task overview	https://mlr-org.com/tasks.html
Learner overview	https://mlr-org.com/learners.html
Resampling overview	https://mlr-org.com/resamplings.html
Measure overview	https://mlr-org.com/measures.html
PipeOp overview	https://mlr-org.com/pipeops.html
Graph overview	https://mlr-org.com/graphs.html
Tuner overview	https://mlr-org.com/tuners.html
Terminator overview	https://mlr-org.com/terminators.html
Tuning space overview	https://mlr-org.com/tuning_spaces.html
Filter overview	https://mlr-org.com/filters.html
FSelector overview	https://mlr-org.com/fselectors.html

```
library(mlr3verse)
library(mlr3proba)
library(mlr3spatiotempcv)
library(mlr3spatial)
library(mlr3extralearners)
library(mlr3hyperband)
library(mlr3mbo)
```

```
mlr_tasks
```

```
<DictionaryTask> with 32 stored values
Keys: actg, bike_sharing, boston_housing, breast_cancer, cookfarm_mlr3,
  diplodia, ecuador, faithful, gbcs, german_credit, grace, ilpd, iris,
  kc_housing, leipzig, lung, moneyball, mtcars, optdigits, penguins,
  penguins_simple, pima, precip, rats, sonar, spam, titanic,
  unemployment, usarrests, whas, wine, zoo
```

```
mlr_learners
```

```
<DictionaryLearner> with 145 stored values
Keys: classif.abess, classif.AdaBoostM1, classif.bart, classif.C50,
  classif.catboost, classif.cforest, classif.ctree, classif.cv_glmnet,
  classif.debug, classif.earth, classif.featureless, classif.fnn,
  classif.gam, classif.gamboost, classif.gausspr, classif.gbm,
  classif.glmboost, classif.glmer, classif.glmnet, classif.IBk,
  classif.imbalanced_rfsrc, classif.J48, classif.JRip, classif.kknn,
  classif.ksvm, classif.lda, classif.liblinear, classif.lightgbm,
  classif.LMT, classif.log_reg, classif.lssvm, classif.mob,
  classif.multinom, classif.naive_bayes, classif.nnet, classif.OneR,
  classif.PART, classif.priority_lasso, classif.qda,
  classif.randomForest, classif.ranger, classif.rfsrc, classif.rpart,
  classif.svm, classif.xgboost, clust.agnes, clust.ap, clust.cmeans,
  clust.cobweb, clust.dbscan, clust.diana, clust.em, clust.fanny,
  clust.featureless, clust.ff, clust.hclust, clust.kkmeans,
  clust.kmeans, clust.MBatchKMeans, clust.mclust, clust.meanshift,
  clust.pam, clust.SimpleKMeans, clust.xmeans, dens.hist, dens.kde,
  dens.kde_ks, dens.locfit, dens.logspline, dens.mixed, dens.nonpar,
  dens.pen, dens.plug, dens.spline, regr.abess, regr.bart,
  regr.catboost, regr.cforest, regr.ctree, regr.cubist, regr.cv_glmnet,
  regr.debug, regr.earth, regr.featureless, regr.fnn, regr.gam,
  regr.gamboost, regr.gausspr, regr.gbm, regr.glm, regr.glmboost,
  regr.glmnet, regr.IBk, regr.kknn, regr.km, regr.ksvm, regr.liblinear,
  regr.lightgbm, regr.lm, regr.lmer, regr.M5Rules, regr.mars, regr.mob,
  regr.nnet, regr.priority_lasso, regr.randomForest, regr.ranger,
  regr.rfsrc, regr.rpart, regr.rsm, regr.rvm, regr.svm, regr.xgboost,
  surv.akritas, surv.aorsf, surv.blackboost, surv.cforest,
  surv.coxboost, surv.coxph, surv.coxtime, surv.ctree,
  surv.cv_coxboost, surv.cv_glmnet, surv.deephit, surv.deepsurv,
  surv.dnnsurv, surv.flexible, surv.gamboost, surv.gbm, surv.glmboost,
  surv.glmnet, surv.kaplan, surv.loghaz, surv.mboost, surv.nelson,
  surv.obliqueRSF, surv.parametric, surv.pchazard, surv.penalized,
  surv.priority_lasso, surv.ranger, surv.rfsrc, surv.rpart, surv.svm,
  surv.xgboost
```

```
1 mlr_resamplings
```

```
<DictionaryResampling> with 24 stored values
Keys: bootstrap, custom, custom_cv, cv, holdout, insample, loo,
  repeated_cv, repeated_spcv_block, repeated_spcv_coords,
  repeated_spcv_disc, repeated_spcv_env, repeated_spcv_tiles,
  repeated_sptcv_cluto, repeated_sptcv_cstf, spcv_block, spcv_buffer,
  spcv_coords, spcv_disc, spcv_env, spcv_tiles, sptcv_cluto,
  sptcv_cstf, subsampling
```

```
mlr_measures
```

```
<DictionaryMeasure> with 93 stored values
Keys: aic, bic, classif.acc, classif.auc, classif.bacc, classif.bbrier,
  classif.ce, classif.costs, classif.dor, classif.fbeta, classif.fdr,
  classif.fn, classif.fnr, classif.fomr, classif.fp, classif.fpr,
  classif.logloss, classif.mauc_au1p, classif.mauc_au1u,
  classif.mauc_aunp, classif.mauc_aunu, classif.mbrier, classif.mcc,
  classif.npv, classif.ppv, classif.prauc, classif.precision,
  classif.recall, classif.sensitivity, classif.specificity, classif.tn,
  classif.tnr, classif.tp, classif.tpr, clust.ch, clust.db, clust.dunn,
  clust.silhouette, clust.wss, debug, dens.logloss, oob_error,
  regr.bias, regr.ktau, regr.logloss, regr.mae, regr.mape, regr.maxae,
  regr.medae, regr.medse, regr.mse, regr.msle, regr.pbias, regr.rae,
  regr.rmse, regr.rmsle, regr.rrse, regr.rse, regr.rsq, regr.sae,
  regr.smape, regr.srho, regr.sse, selected_features, sim.jaccard,
  sim.phi, surv.brier, surv.calib_alpha, surv.calib_beta,
  surv.chambless_auc, surv.cindex, surv.dcalib, surv.graf,
  surv.hung_auc, surv.intlogloss, surv.logloss, surv.mae, surv.mse,
  surv.nagelk_r2, surv.oquigley_r2, surv.rcll, surv.rmse, surv.schmid,
  surv.song_auc, surv.song_tnr, surv.song_tpr, surv.uno_auc,
  surv.uno_tnr, surv.uno_tpr, surv.xu_r2, time_both, time_predict,
  time_train
```

```
mlr_pipeops
```

```
<DictionaryPipeOp> with 74 stored values
Keys: boxcox, branch, chunk, classbalancing, classifavg, classweights,
  colapply, collapsefactors, colroles, compose_crank, compose_distr,
  compose_probregr, copy, crankcompose, datefeatures, distrcompose,
  encode, encodeimpact, encodelmer, featureunion, filter, fixfactors,
  histbin, ica, imputeconstant, imputehist, imputelearner, imputemean,
  imputemedian, imputemode, imputeoor, imputesample, kernelpca,
  learner, learner_cv, missind, modelmatrix, multiplicityexply,
  multiplicityimply, mutate, nmf, nop, ovrsplit, ovrunite, pca, proxy,
  quantilebin, randomprojection, randomresponse, regravg,
  removeconstants, renamecolumns, replicate, scale, scalemaxabs,
  scalerange, select, smote, spatialsign, subsample, survavg,
  targetinvert, targetmutate, targettrafoscalerange, textvectorizer,
  threshold, trafopred_regrsurv, trafopred_survregr,
  trafotask_regrsurv, trafotask_survregr, tunethreshold, unbranch,
  vtreat, yeojohnson
```

```
mlr_graphs
```

```
<DictionaryGraph> with 13 stored values
Keys: bagging, branch, crankcompositor, distrcompositor, greplicate,
  ovr, probregr, robustify, stacking, survaverager, survbagging,
  survtoregr, targettrafo
```

```
mlr_tuners
```

```
<DictionaryTuner> with 10 stored values
Keys: cmaes, design_points, gensa, grid_search, hyperband, irace, mbo,
  nloptr, random_search, successive_halving
```

```
mlr_terminators
```

```
<DictionaryTerminator> with 8 stored values
Keys: clock_time, combo, evals, none, perf_reached, run_time,
  stagnation, stagnation_batch
```

```
mlr_tuning_spaces
```

```
<DictionaryTuningSpaces> with 24 stored values
Keys: classif.glmnet.default, classif.glmnet.rbv2,
  classif.kknn.default, classif.kknn.rbv2, classif.ranger.default,
  classif.ranger.rbv2, classif.rpart.default, classif.rpart.rbv2,
  classif.svm.default, classif.svm.rbv2, classif.xgboost.default,
  classif.xgboost.rbv2, regr.glmnet.default, regr.glmnet.rbv2,
  regr.kknn.default, regr.kknn.rbv2, regr.ranger.default,
  regr.ranger.rbv2, regr.rpart.default, regr.rpart.rbv2,
  regr.svm.default, regr.svm.rbv2, regr.xgboost.default,
  regr.xgboost.rbv2
```

```
mlr_filters
```

```
<DictionaryFilter> with 21 stored values
Keys: anova, auc, carscore, carsurvscore, cmim, correlation, disr,
  find_correlation, importance, information_gain, jmi, jmim,
  kruskal_test, mim, mrmr, njmim, performance, permutation, relief,
  selected_features, variance
```

```
mlr_fselectors
```

```
<DictionaryFSelector> with 8 stored values
Keys: design_points, exhaustive_search, genetic_search, random_search,
  rfe, rfecv, sequential, shadow_variable_search
```

E. Session Info

If you would like to reproduce the results in this book, note the seed set at the top of each chapter (which is the same as the chapter number) and the `sessionInfo` at the time of publication:

```
R version 4.2.2 (2022-10-31)
Platform: x86_64-pc-linux-gnu (64-bit)
Running under: Ubuntu 22.04.2 LTS

Matrix products: default
BLAS:   /usr/lib/x86_64-linux-gnu/openblas-pthread/libblas.so.3
LAPACK: /usr/lib/x86_64-linux-gnu/openblas-pthread/libopenblasp-r0.3.20.so

locale:
 [1] LC_CTYPE=C.UTF-8       LC_NUMERIC=C           LC_TIME=C.UTF-8
 [4] LC_COLLATE=C.UTF-8     LC_MONETARY=C.UTF-8    LC_MESSAGES=C.UTF-8
 [7] LC_PAPER=C.UTF-8       LC_NAME=C              LC_ADDRESS=C
[10] LC_TELEPHONE=C         LC_MEASUREMENT=C.UTF-8 LC_IDENTIFICATION=C

attached base packages:
[1] stats     graphics  grDevices utils     datasets  methods   base

loaded via a namespace (and not attached):
 [1] digest_0.6.30   lifecycle_1.0.3 jsonlite_1.8.4  magrittr_2.0.3
 [5] evaluate_0.18   rlang_1.0.6     stringi_1.7.8   cli_3.4.1
 [9] vctrs_0.5.1     rmarkdown_2.18  tools_4.2.2     stringr_1.5.0
[13] glue_1.6.2      xfun_0.35       fastmap_1.1.0   compiler_4.2.2
[17] htmltools_0.5.3 knitr_1.41
```

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