

Modern Machine Learning in R

mlr3

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Intro

• R gives you access to many machine learning methods

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Example:

```
svm_model = e1071::svm(Species ~ ., data = iris)
```

VS.

```
xgb_model = xgboost::xgboost(as.matrix(iris[1:4]), iris$Species,
    nrounds = 10)
```

```
library("mlr3")
```

Ingredients:

- Data
- Learning Algorithms
- Performance Evaluation
- Performance Comparison

R6

mlr3 uses the *R6* class system. Some things may seem unusual if you see them for the first time.

• Objects are created using <Class>\$new().

```
task = TaskClassif$new("iris", iris, "Species")
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• Objects have *fields* that contain information about the object.

```
task$nrow
#> [1] 150
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task$filter(rows = 1:10)
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Methods may change ("mutate") the object!

R6 AND REFERENCE SEMANTICS

R6 objects have "Reference Semantics": copies have to created explicitly with \$clone() if they should not be changed.

 We conduct an experiment: task_two is not a copy of task but refers to the same object:

```
task = TaskClassif$new("iris", iris, "Species")
task_two = task
task_clone = task$clone(deep = TRUE)
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task_two = task
task_clone = task$clone(deep = TRUE)
```

We mutate task:

```
task$filter(rows = 1:10)
```

• task_two has changed, task_clone has not.

```
task$nrow
#> [1] 10
task_two$nrow
#> [1] 10
task_clone$nrow
#> [1] 150
```

R6 AND ACTIVE BINDINGS

Some fields of R6-objects may be "Active Bindings". Internally they are realized as functions that are called whenever the value is set or retrieved.

Active bindings for read-only fields

```
task$nrow = 11
#> Error in (function () : unused argument (base::quote(11))
```

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Active bindings for read-only fields

```
task$nrow = 11
#> Error in (function () : unused argument (base::quote(11))
```

Active bindings for argument checking

```
task$properties = NULL

#> Error in assert_set(rhs, .var.name = "properties"):
Assertion on 'properties' failed: Must be of type
'character', not 'NULL'.

task$properties = c("property1", "property2") # works
```

MLR3 PHILOSOPHY

- Overcome limitations of S3 with the help of R6
 - Truly object-oriented: data and methods live in the same object
 - Make use of inheritance
 - Reference semantics

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 - Fast operations for tabular data
 - List columns to arrange complex objects in tabular structure

MLR3 PHILOSOPHY

- Overcome limitations of S3 with the help of R6
 - Truly object-oriented: data and methods live in the same object
 - Make use of inheritance
 - Reference semantics
- Embrace data.table, both for arguments and internally
 - Fast operations for tabular data
 - List columns to arrange complex objects in tabular structure
- Be light on dependencies:
 - R6, data.table, Metrics, lgr, uuid, mlbench, digest
 - Plus some of our own packages (backports, checkmate, ...)

Data

Tabular data

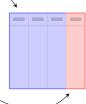


- Tabular data
- Features



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```
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```

- Tabular data
- Features
- Target / outcome to predict ~
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Task ID

```
task = TaskClassif$new("iris", iris, "Species")
```

- Tabular data
- Features
- Target / outcome to predict ~
 - discrete for classification
 - continuous for regression
 - ⇒ data determines the machine learning "Task"

```
Task ID data
\( \sqrt{task} = TaskClassif$new("iris", iris, "Species")
```

- Tabular data
- Features
- Target / outcome to predict -
 - discrete for classification
 - · continuous for regression
 - ⇒ data determines the machine learning "Task"

```
Task ID data target name
\( \sqrt{task} = TaskClassif$new("iris", iris, "Species")
```

```
task = TaskClassif$new("iris", iris, "Species")
```

```
print(task)

# <TaskClassif:iris> (150 x 5)

# * Target: Species

# * Properties: multiclass

# * Features (4):

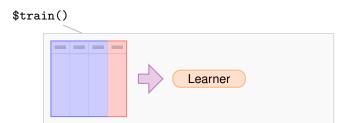
# - dbl (4): Petal.Length, Petal.Width, Sepal.Length, Sepal.Width
```

```
task$ncol
task$nrow
task$feature_names
task$target_names
```

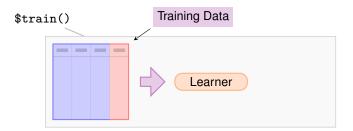
```
task$select(cols = )
task$filter(rows = )
task$cbind(data = )
task$rbind(data = )
```

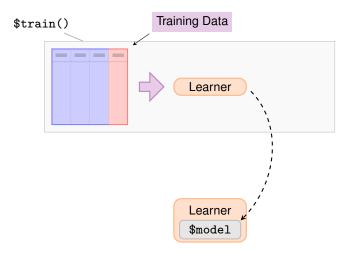
Learning Algorithms

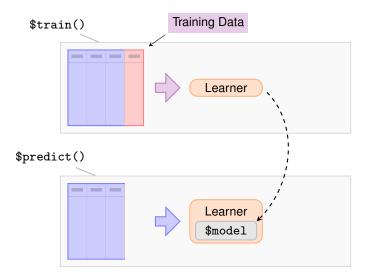
LEARNING ALGORITHMS

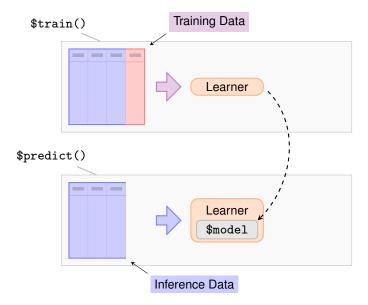


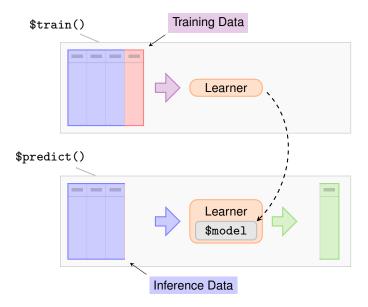
LEARNING ALGORITHMS

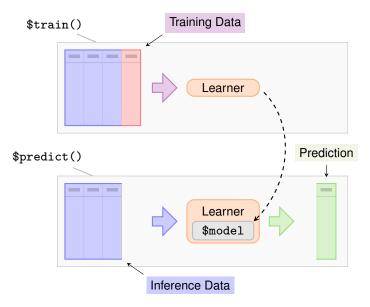












• Get a Learner provided by mlr

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

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• Train the Learner

learner\$train(task)

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• Train the Learner

```
learner$train(task)
```

The \$model is the rpart model: a decision tree

```
print(learner$model)
\#> n= 150
#>
  node), split, n, loss, yval, (yprob)
       * denotes terminal node
#>
#>
  1) root 150 100 setosa (0.333 0.333 0.333)
    #>
    3) Petal.Length>=2.5 100 50 versicolor (0.000 0.500 0.500)
#>
      6) Petal.Width< 1.8 54 5 versicolor (0.000 0.907 0.093) *
#>
      7) Petal.Width>=1.8 46
                           1 virginica (0.000 0.022 0.978) *
#>
```

Learners have hyperparameters

```
learner$param_set
#> ParamSet:
                  class lower upper levels default value
#>
              id
#> 1: minsplit ParamInt
                               Inf
                                             20
             cp ParamDbl
                           0 1
                                           0.01
#> 2:
#> 3:
      maxcompete ParamInt
                           0 Inf
#> 4: maxsurrogate ParamInt
                           0 Inf
        maxdepth ParamInt
                           1 30
                                             30
#> 5:
#> 6:
           xval ParamInt
                           0 Inf
                                             10
```

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```
learner$param_set
#> ParamSet:
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                          0 Inf
        maxdepth ParamInt 1 30
                                           30
#> 5:
           xval ParamInt
                          0 Inf
                                           10
#> 6:
```

• Changing them changes the Learner behavior

```
learner$param_set$values = list(maxdepth = 1, xval = 0)
learner$train(task)
```

This gives a smaller decision tree

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 Instead of assigning \$values a list(), we can change individual parameters

```
learner$param_set$values$maxdepth = 10
```

• Let's make a prediction

```
new_data

# Sepal.Length Sepal.Width Petal.Length Petal.Width

# 1 4 3 2 1

# 2 2 2 3 2
```

Let's make a prediction

```
new_data
# Sepal.Length Sepal.Width Petal.Length Petal.Width
# 1     4     3     2     1
# 2     2     2     3     2
```

• Call \$predict_newdata() with the data

```
prediction = learner$predict_newdata(new_data)
```

Let's make a prediction

```
new_data
# Sepal.Length Sepal.Width Petal.Length Petal.Width
# 1     4     3     2     1
# 2     2     2     3     2
```

• Call \$predict_newdata() with the data

```
prediction = learner$predict_newdata(new_data)
```

We get a Prediction object:

```
prediction
#> <PredictionClassif> for 2 observations:
#> row_id truth response
#> 1 <NA> setosa
#> 2 <NA> versicolor
```

Let's make a prediction

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     row_id truth
                    response
              <NA>
                       setosa
              <NA> versicolor
```

 We can make the Learner predict probabilities when we set predict_type:

```
learner$predict_type = "prob"
learner$predict_newdata(new_data)

# <PredictionClassif> for 2 observations:
# row_id truth response prob.setosa prob.versicolor
# 1 <NA> setosa 1 0.0
# 2 <NA> versicolor 0 0.5
# prob.virginica
# 0.0
# 0.5
```

What exactly is a Prediction object?

• Contains predictions and offers useful access fields / methods

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- Contains predictions and offers useful access fields / methods
- ⇒ Raw data in \$data

```
prediction$data

#> $tab

#> row_id truth response

#> 1: 1 <NA> setosa

#> 2: 2 <NA> versicolor
```

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- Contains predictions and offers useful access fields / methods
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prediction$data

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```

⇒ Active bindings and functions that give further information: \$response, \$truth,...

```
prediction$response

#> [1] setosa versicolor

#> Levels: setosa versicolor virginica
```

What exactly is a Prediction object?

- Contains predictions and offers useful access fields / methods
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```
prediction$data
#> $tab
#> row_id truth response
#> 1: 1 <NA> setosa
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```

⇒ Active bindings and functions that give further information: \$response, \$truth,...

```
prediction$response

#> [1] setosa versicolor

#> Levels: setosa versicolor virginica
```

⇒ Use as.data.table() to get a data.table for analysis

```
as.data.table(prediction)

#> row_id truth response

#> 1: 1 <NA> setosa

#> 2: 2 <NA> versicolor
```

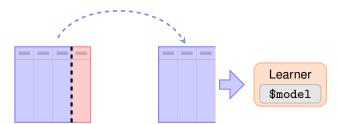
Performance

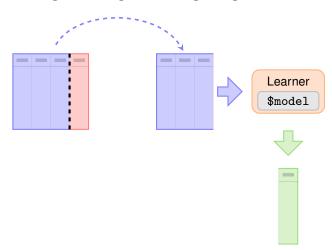


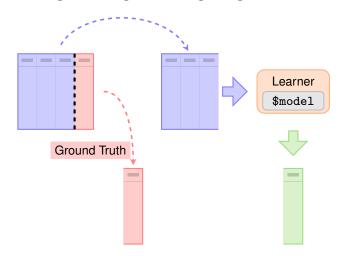


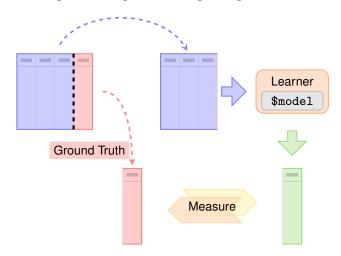


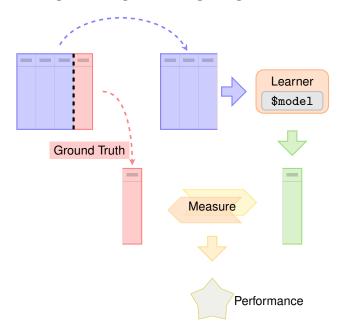












Prediction 'Task' with known data

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Predict again

```
pred = learner$predict(known_truth_task)
pred

#> <PredictionClassif> for 2 observations:
#> row_id truth response
#> 1 setosa setosa
#> 2 setosa virginica
```

Prediction 'Task' with known data

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#> <PredictionClassif> for 2 observations:
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```

Score the prediction

```
pred$score(msr("classif.ce"))
#> classif.ce
#> 0.5
```

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```

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#> classif.ce
#> 0.5
```

Confusion Matrix

```
pred
#> <PredictionClassif> for 2 observations:
#>
   row_id truth response
#>
      1 setosa
                setosa
       2 setosa virginica
#>
pred$confusion
#>
         truth
setosa
#>
#> versicolor
#> virginica
```

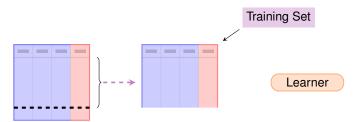
Resampling

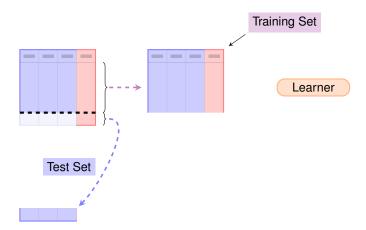


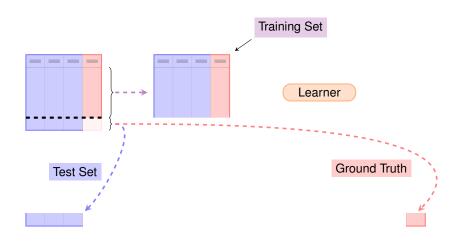
Learner

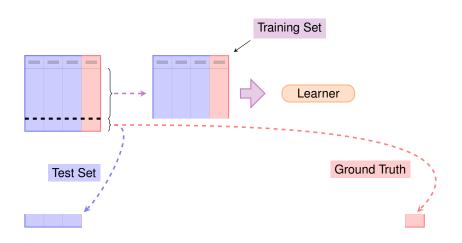


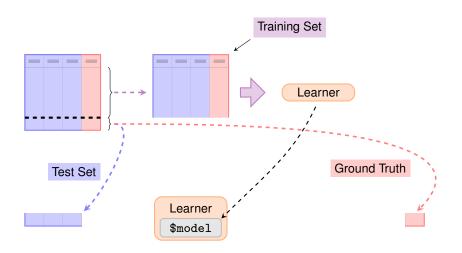
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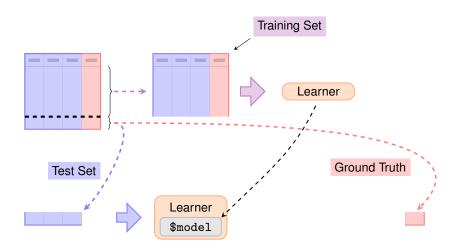


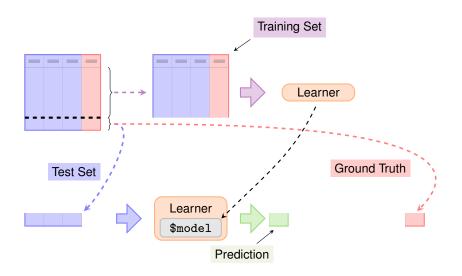


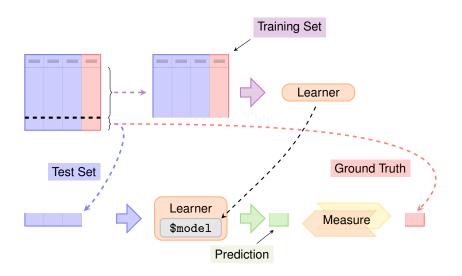


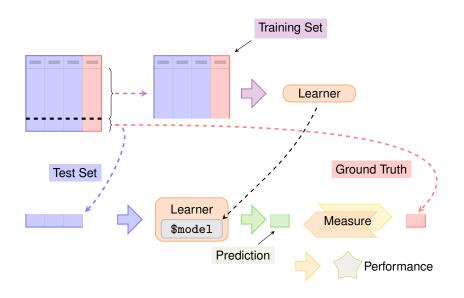


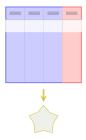


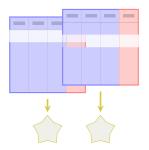


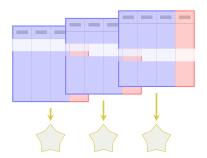


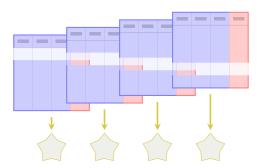


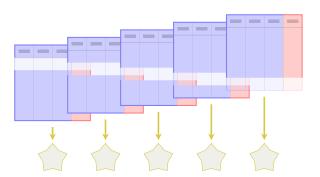


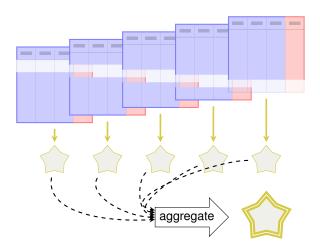


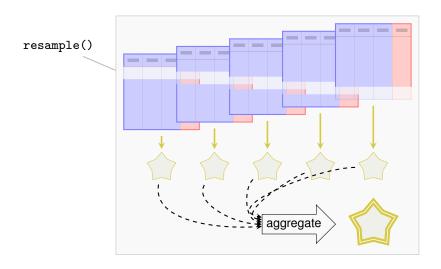












• Resample description: How to split the data

```
cv5 = rsmp("cv", folds = 5)
```

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• Use the resample() function for resampling:

```
rr = resample(task, learner, cv5)
```

Resample description: How to split the data

```
cv5 = rsmp("cv", folds = 5)
```

• Use the resample() function for resampling:

```
rr = resample(task, learner, cv5)
```

• We get a ResamplingResult object:

```
print(rr)
#> <ResampleResult> of 5 iterations
#> * Task: iris
#> * Learner: classif.rpart
#> * Warnings: 0 in 0 iterations
#> * Errors: 0 in 0 iterations
```

What exactly is a ResamplingResult object?

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Raw data in \$data field

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- Raw data in \$data field
- Get a table representation using as.data.table()

What exactly is a ResamplingResult object? Remember Prediction:

- Baw data in \$data field
- Get a table representation using as.data.table()

• Active bindings and functions that make information easily accessible

• Get performance:

```
rr$aggregate(msr("classif.ce"))
#> classif.ce
#> 0.067
```

Get performance:

```
rr$aggregate(msr("classif.ce"))
#> classif.ce
#> 0.067
```

Get predictions

```
rr$prediction()
#> <PredictionClassif> for 150 observations:
      row_id
#>
                truth
                       response
          16 setosa
#>
                         setosa
#>
          20 setosa setosa
#>
          21
               setosa
                         setosa
#>
         136 virginica virginica
         139 virginica virginica
#>
         148 virginica virginica
#>
```

Predictions of individual folds

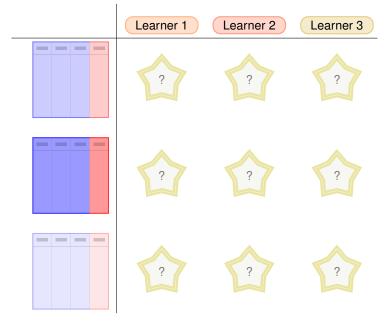
```
predictions = rr$predictions()
predictions[[1]]
#> <PredictionClassif> for 30 observations:
#>
      row_id truth response
          16 setosa
#>
                         setosa
#>
          20 setosa setosa
#>
          21
                setosa setosa
#>
#>
         147 virginica virginica
#>
         149 virginica virginica
#>
         150 virginica virginica
```

Predictions of individual folds

```
predictions = rr$predictions()
predictions[[1]]
#> <PredictionClassif> for 30 observations:
#>
      row_id truth response
          16 setosa setosa
#>
#>
          20 setosa setosa
#>
          21 setosa setosa
#> ---
#>
         147 virginica virginica
#>
         149 virginica virginica
#>
         150 virginica virginica
```

Score of individual folds.

Benchmark



Multiple Learners, multiple Tasks:

```
library("mlr3learners")
learners = list(lrn("classif.rpart"), lrn("classif.kknn"))
tasks = list(tsk("iris"), tsk("sonar"), tsk("wine"))
```

Multiple Learners, multiple Tasks:

```
library("mlr3learners")
learners = list(lrn("classif.rpart"), lrn("classif.kknn"))
tasks = list(tsk("iris"), tsk("sonar"), tsk("wine"))
```

• Set up the *design* and execute benchmark:

```
design = benchmark_grid(tasks, learners, cv5)
bmr = benchmark(design)
```

Multiple Learners, multiple Tasks:

```
library("mlr3learners")
learners = list(lrn("classif.rpart"), lrn("classif.kknn"))
tasks = list(tsk("iris"), tsk("sonar"), tsk("wine"))
```

• Set up the *design* and execute benchmark:

```
design = benchmark_grid(tasks, learners, cv5)
bmr = benchmark(design)
```

 We get a BenchmarkResult object which shows that kknn outperforms rpart:

```
bmr_ag = bmr$aggregate()
bmr_ag[, c("task_id", "learner_id", "classif.ce")]

#> task_id learner_id classif.ce

#> 1: iris classif.rpart 0.067

#> 2: iris classif.kknn 0.047

#> 3: sonar classif.rpart 0.308

#> 4: sonar classif.kknn 0.125

#> 5: wine classif.rpart 0.112

#> 6: wine classif.kknn 0.050
```

BENCHMARK RESULT

What exactly is a BenchmarkResult object?

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Just like Prediction and ResamplingResult!

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- Table representation using as.data.table()

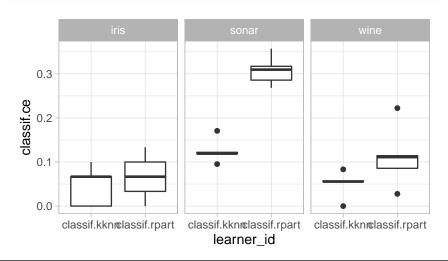
What exactly is a BenchmarkResult object?

Just like Prediction and ResamplingResult!

- Raw data in \$data field
- Table representation using as.data.table()
- Active bindings and functions that make information easily accessible

The mlr3viz package contains autoplot() functions for some mlr3 objects

```
library(mlr3viz)
autoplot(bmr)
```



Short Forms and Dictionaries

• Ordinary constructors: LearnerClassifRpart\$new()

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Object	Dictionary	Short Form
Task	mlr_tasks	tsk()
Learner	mlr_learners	lrn()
Measure	mlr_measures	msr()
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-orm
)

• Use Dictionary\$keys() method to list available items

```
mlr_resamplings$keys()
#> [1] "bootstrap" "custom" "cv" "holdout"
#> [5] "repeated_cv" "subsampling"
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mlr_resamplings$keys()
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```

• Dictionaries can get populated by add-on packages (e.g. mlr3learners)

as.data.table(<DICTIONARY>) creates a data.table with metadata about objects in dictionaries:

```
mlr_learners_table = as.data.table(mlr_learners)
mlr_learners_table[1:10, c("key", "packages", "predict_types")]
#
                       kev
                             packages predict_types
   1:
            classif.debug
                                       response, prob
   2: classif.featureless
                                       response, prob
   3:
           classif.glmnet
                               glmnet response, prob
   4:
             classif.kknn withr,kknn response,prob
                                 MASS response, prob
   5:
               classif.lda
#
   6:
                                 stats response, prob
          classif.log_reg
      classif.naive_bayes
                                e1071 response, prob
  8:
               classif.qda
                                 MASS response, prob
   9:
           classif.ranger
                               ranger response, prob
# 10:
            classif.rpart
                                rpart response, prob
```

How to get Help

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```
class(bmr)
#> [1] "BenchmarkResult" "R6"
```

② Go to the corresponding help page:

?BenchmarkResult

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- Why does this not work?
 - Ask at stackoverflow https://stackoverflow.com/questions/tagged/mlr3
 - Write a GitHub issue (in the according project)

Advanced Topics

CONTROL OF EXECUTION

Parallelization

```
future::plan("multicore")
```

- runs each resampling iteration as a job
- also allows nested resampling (although not needed here)

Encapsulation

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

- Spawns a separate R process to train the learner
- Learner may segfault without tearing down the session
- · Logs are captured
- Possibilty to have a fallback to create predictions

OUT-OF-MEMORY DATA

- Task stores data in a DataBackend:
 - DataBackendDataTable: Default backend for dense data (in-memory)
 - DataBackendMatrix: Backend for sparse numerical data (in-memory)
 - DataBackendDplyr: Backend for many DBMS (out-of-memory)
 - DataBackendCbind: Combine backends in a cbind() fashion (virtual)
 - DataBackendRbind: Combine backends in a rbind() fashion (virtual)
- Backends are immutable
 - Filtering rows or selecting columns just modifies the "view" on the data
 - Multiple tasks can share the same backend
- Example: Interface a read-only MariaDB with DataBackendDplyr, add generated features via DataBackendDataTable

Outro

OVERVIEW

Main things remember about mlr3:

Short forms & Data / Control Objects

```
\begin{array}{ll} \texttt{tsk()} & \mapsto \texttt{Task} \\ \texttt{lrn()} & \mapsto \texttt{Learner} \\ \texttt{rsmp()} & \mapsto \texttt{Resampling} \\ \texttt{msr()} & \mapsto \texttt{Measure} \end{array}
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- Result Objects
 - ResampleResult, BenchmarkResult
 - Have \$data slot and provide as.data.table()

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```

- Result Objects
 - ResampleResult, BenchmarkResult
 - Have \$data slot and provide as.data.table()
- Functions
 - $\bullet \ \ \, \text{resample():} \\ \hspace{0.5cm} (\text{Task, Learner, Resampling}) \mapsto \text{ResampleResult}$
 - benchmark_grid(), benchmark():
 (Task, Learner, Resampling) → BenchmarkResult

SO YOU WANT TO DO ML IN R

Ingredients:



TaskClassif,
TaskRegr,
tsk()

Learning Algorithms



lrn() ⇒ Learner,
\$train(),
\$predict() ⇒ Prediction

Performance Evaluation



 $rsmp() \Rightarrow Resampling,$ $msr() \Rightarrow Measure,$ $resample() \Rightarrow ResamplingResult,$ aggregate()

Performance Comparison



benchmark_grid(),
benchmark() ⇒ BenchmarkResult