Modern Machine Learning in R

mlr3

Department of Statistics – LMU Munich

Intro

SO YOU WANT TO DO ML IN R

- R gives you access to many machine learning methods

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Example:

```
# Specify what we want to model in a formula: target ~ features
svm_model = e1071::svm(Species ~ ., data = iris)
```

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- . . . but without a unified interface
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Example:

```
# Specify what we want to model in a formula: target ~ features
svm_model = e1071::svm(Species ~ ., data = iris)
```

vs.

```
# Pass the features as a matrix and the target as a vector
xgb_model = xgboost::xgboost(data = as.matrix(iris[1:4]),
  label = iris$Species, nrounds = 10)
```

SO YOU WANT TO DO ML IN R

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

Ingredients:

- Data / Task
- Learning Algorithms
- Performance Evaluation
- Performance Comparison

R6

R6 – ALL YOU NEED TO KNOW

`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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- Objects have *methods* that are called like functions:

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task$filter(rows = 1:10)
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```
task$nrow
#> [1] 150
```

- Objects have *methods* that are called like functions:

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

- Methods may change (“mutate”) the object (reference semantics)!

```
task$nrow
#> [1] 10
```

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:  Field/Binding is read-only
```

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- Active bindings for read-only fields

```
task$nrow = 11
#> Error:  Field/Binding is read-only
```

- 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

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  - Make use of inheritance
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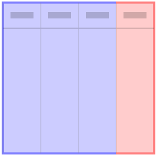
- Embrace **data.table**, both for arguments and internally
  - Fast operations for tabular data
  - List columns to arrange complex objects in tabular structure
- Be **light on dependencies**:
  - `R6`, `data.table`, `lgr`, `uuid`, `mlbench`, `digest`
  - Plus some of our own packages (`backports`, `checkmate`, ...)

Data

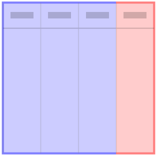
DATA

- Tabular data



DATA

- Tabular data
- Features



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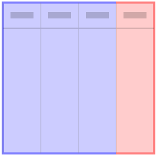

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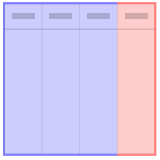
  - continuous for regression



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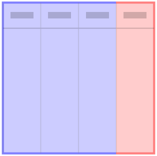

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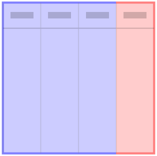

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#> 1          5.1         3.5          1.4         0.2  setosa
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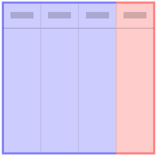

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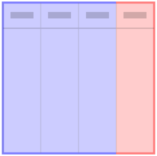

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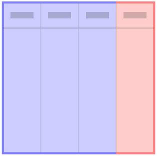

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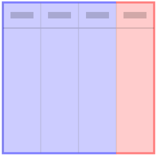

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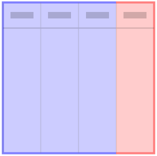

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Task ID ↘ data ↓ target name ↙

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

DATA

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

```r
print(task)
```

```
# <TaskClassif:iris> (150 x 5)
# * Target: Species
# * Properties: multiclass
# * Features (4):
#   - dbl (4): Petal.Length, Petal.Width, Sepal.Length, Sepal.Width
```

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

```r
task$head(n = )
task$truth(row_ids = )
task$data(rows = ,
          cols = )
```

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

Dictionaries

DICTIONARIES

- Ordinary constructors: `TaskClassif$new()` / `LearnerClassifRpart$new()`

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- They access `Dictionary` of objects:

Object	Dictionary	Short Form
`Task`	`mlr_tasks`	`tsk()`
`Learner`	`mlr_learners`	`lrn()`
`Measure`	`mlr_measures`	`msr()`
`Resampling`	`mlr_resamplings`	`rsmp()`

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

DICTIONARIES

```
# list items
tsk()

#> <DictionaryTask> with 15 stored values
#> Keys: boston_housing, breast_cancer, faithful,
#>   german_credit, iris, lung, mtcars, pima, precip, rats,
#>   sonar, spam, unemployment, wine, zoo

# retrieve object
tsk("iris")

#> <TaskClassif:iris> (150 x 5)
#> * Target: Species
#> * Properties: multiclass
#> * Features (4):
#>   - dbl (4): Petal.Length, Petal.Width, Sepal.Length,
#>     Sepal.Width
```

SHORT FORMS AND DICTIONARIES

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

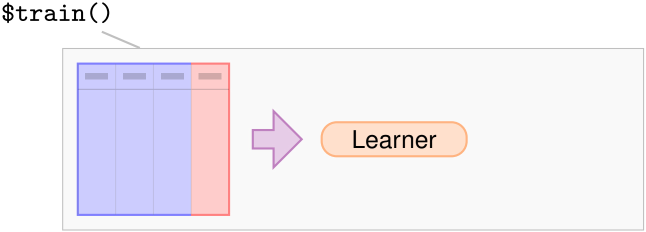
```
mlr_learners_table = as.data.table(mlr_learners)

mlr_learners_table[1:10, c("key", "packages", "predict_types")]

#                    key packages predict_types
#  1:   classif.cv_glmnet   glmnet response,prob
#  2:       classif.debug          response,prob
#  3: classif.featureless          response,prob
#  4:      classif.glmnet   glmnet response,prob
#  5:        classif.kknn     kknn response,prob
#  6:         classif.lda     MASS response,prob
#  7:     classif.log_reg    stats response,prob
#  8:    classif.multinom     nnet response,prob
#  9: classif.naive_bayes    e1071 response,prob
# 10:         classif.qda     MASS response,prob
```

Learning Algorithms

LEARNING ALGORITHMS



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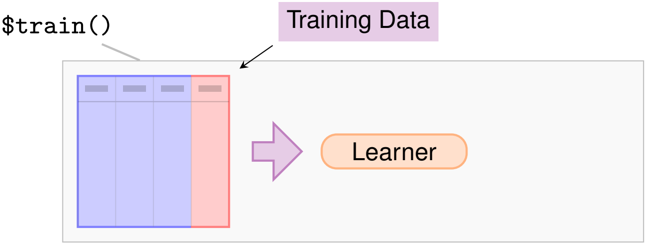

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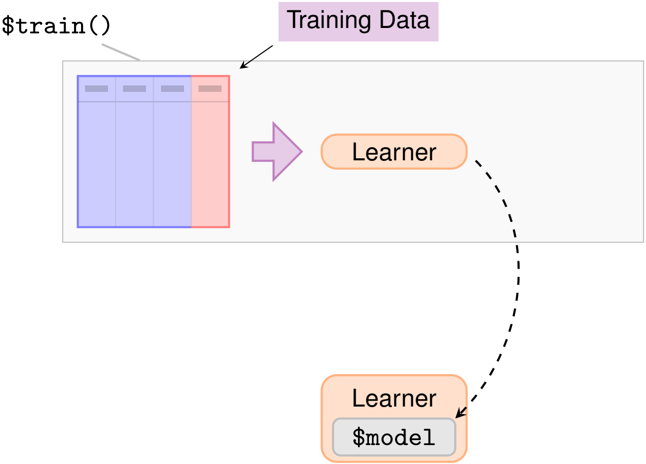

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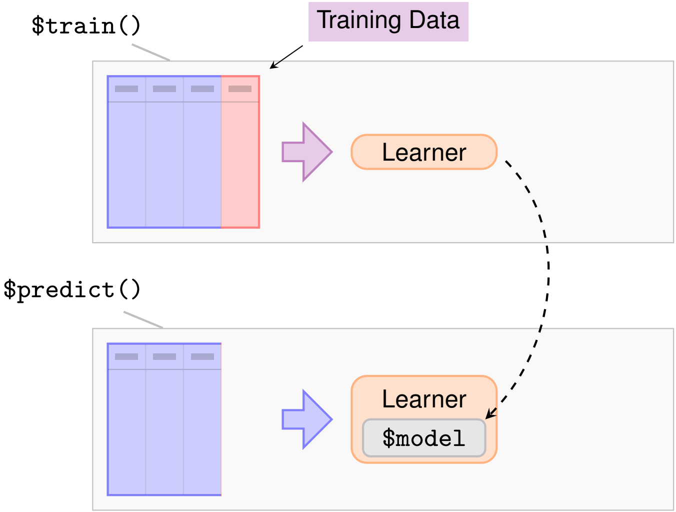

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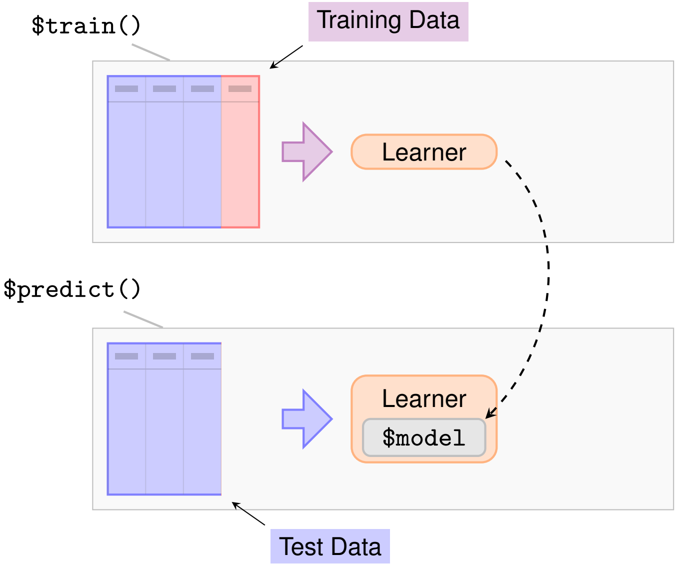

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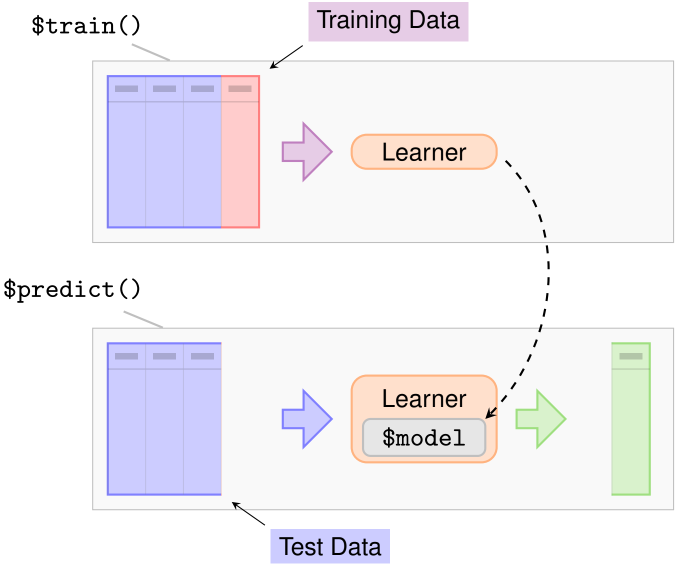

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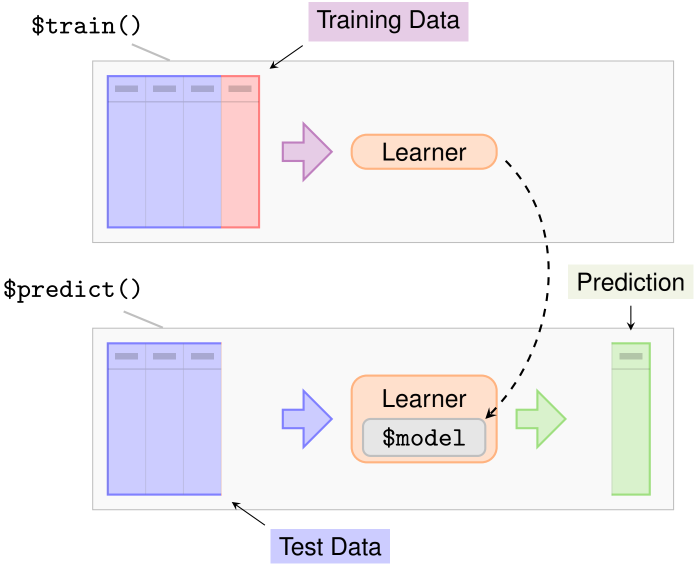

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- Get a `Learner` provided by `mlr`

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learner = lrn("classif.rpart")
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learner$train(task)
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learner$train(task)
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- 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)
#>   2) Petal.Length< 2.5 50   0 setosa (1.000 0.000 0.000) *
#>   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) *
```

HYPERPARAMETERS

- Learners have *hyperparameters*

```
as.data.table(learner$param_set)[, 1:6]

#>                  id    class lower upper      levels nlevels
#>  1:        minsplit ParamInt     1   Inf                 Inf
#>  2:       minbucket ParamInt     1   Inf                 Inf
#>  3:              cp ParamDbl     0     1                 Inf
#>  4:      maxcompete ParamInt     0   Inf                 Inf
#>  5:    maxsurrogate ParamInt     0   Inf                 Inf
#>  6:        maxdepth ParamInt     1    30                  30
#>  7:    usesurrogate ParamInt     0     2                   3
#>  8: surrogatestyle ParamInt     0     1                   2
#>  9:            xval ParamInt     0   Inf                 Inf
#> 10:      keep_model ParamLgl    NA    NA  TRUE,FALSE       2
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```

- Changing them changes the `Learner` behavior

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

learner$train(task)
```

HYPERPARAMETERS

- This gives a smaller decision tree

```
print(learner$model)

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#>
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#>   2) Petal.Length< 2.5 50   0 setosa (1.00 0.00 0.00) *
#>   3) Petal.Length>=2.5 100  50 versicolor (0.00 0.50 0.50) *
```

PREDICTION

- Let's make a prediction for some new data, e.g.:

```
new_data

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

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- To do so, we call the `$predict_newdata()` method using the new data:

```
prediction = learner$predict_newdata(new_data)
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- We get a `Prediction` object:

```
prediction

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

PREDICTION

- 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
```

PREDICTION

What exactly is a `Prediction` object?

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⇒ Use `as.data.table()` to extract data

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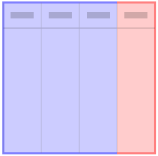
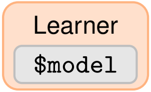
⇒ Active bindings and functions that give further information: `$response`, `$truth`, ...

```
prediction$response
#> [1] setosa     versicolor
#> Levels: setosa versicolor virginica
```

Performance

PERFORMANCE EVALUATION





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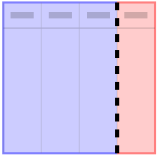

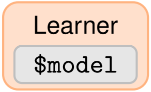

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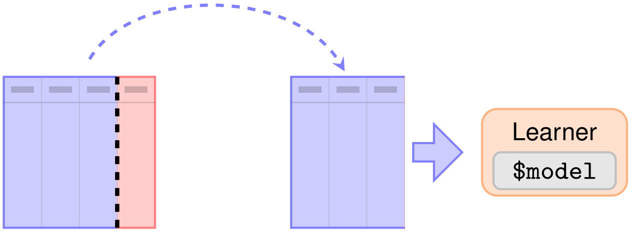

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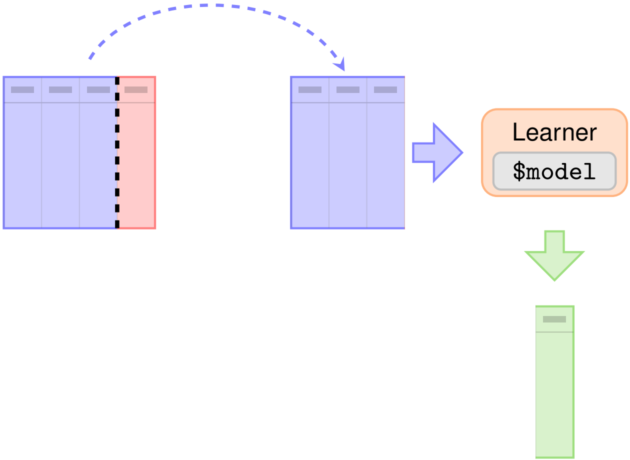
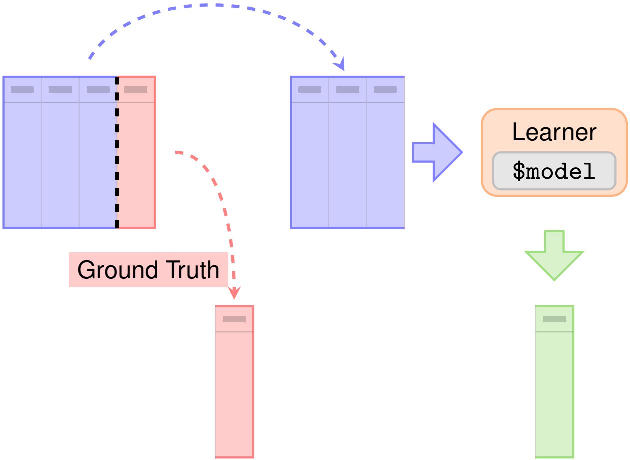
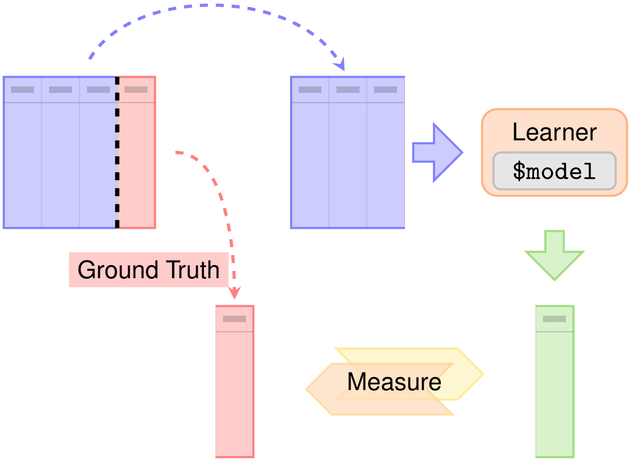


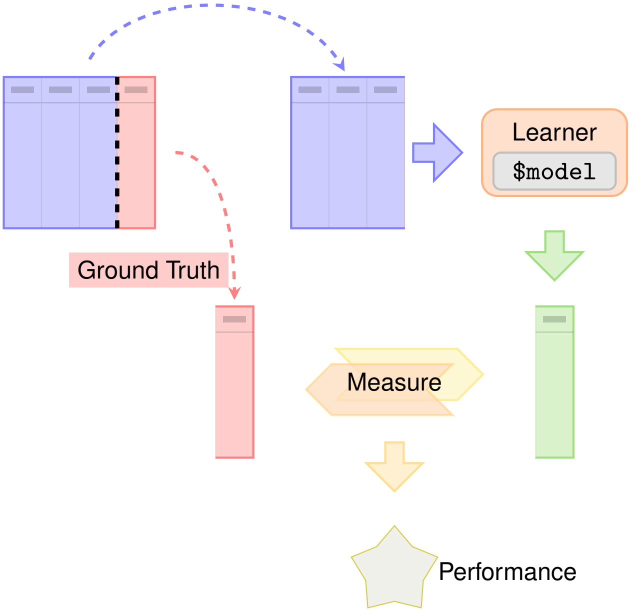
PERFORMANCE EVALUATION



PERFORMANCE EVALUATION



PERFORMANCE EVALUATION



PERFORMANCE EVALUATION

- Prediction ‘Task‘ with known data

```
known_truth_task$data()
```

```
#    Species Petal.Length Petal.Width Sepal.Length Sepal.Width
# 1:  setosa            2           1            4           3
# 2:  setosa            3           2            2           2
```

PERFORMANCE EVALUATION

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# 1:   setosa            2           1            4           3
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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
```

PERFORMANCE EVALUATION

- Prediction ‘Task‘ with known data

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```

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- Score the prediction

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

```
#> classif.ce
#>        0.5
```

PERFORMANCE EVALUATION

- Prediction ‘Task‘ with known data

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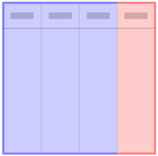
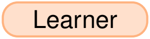
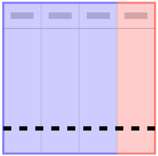
Resampling

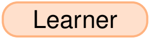
RESAMPLING





RESAMPLING





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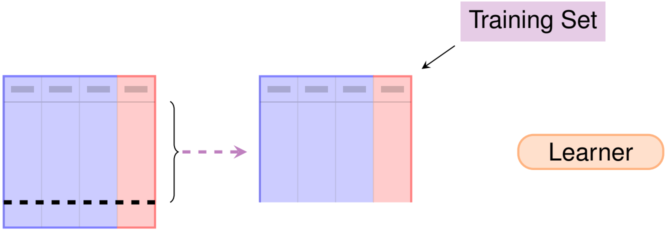

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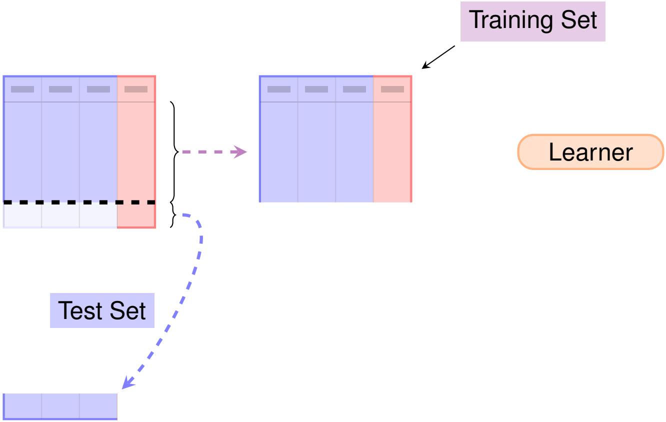

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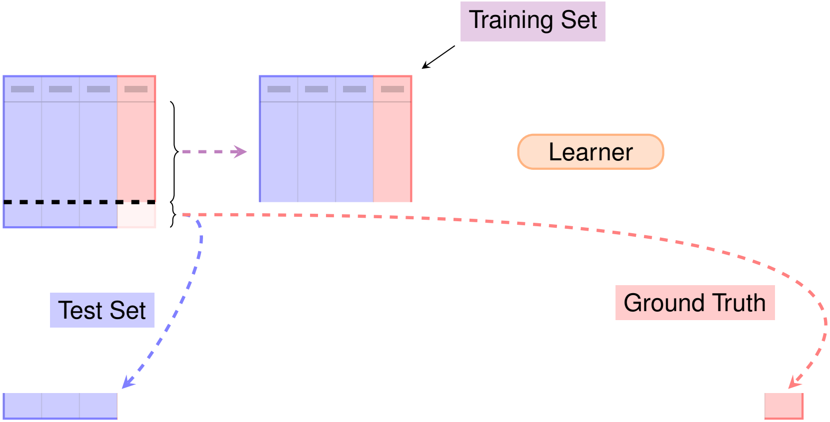

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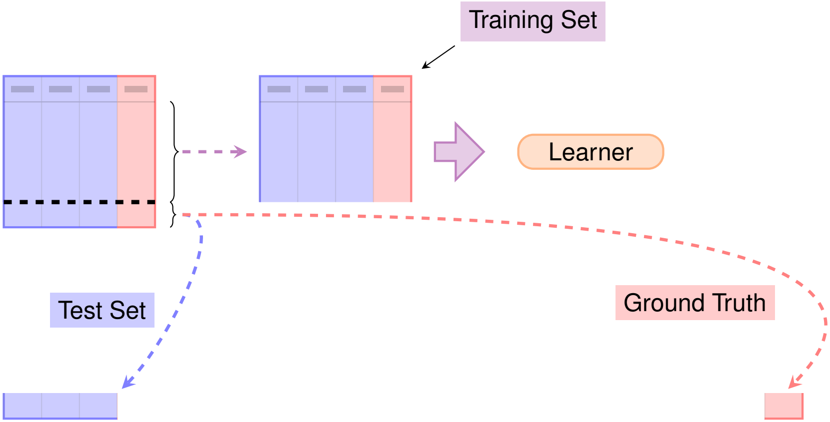
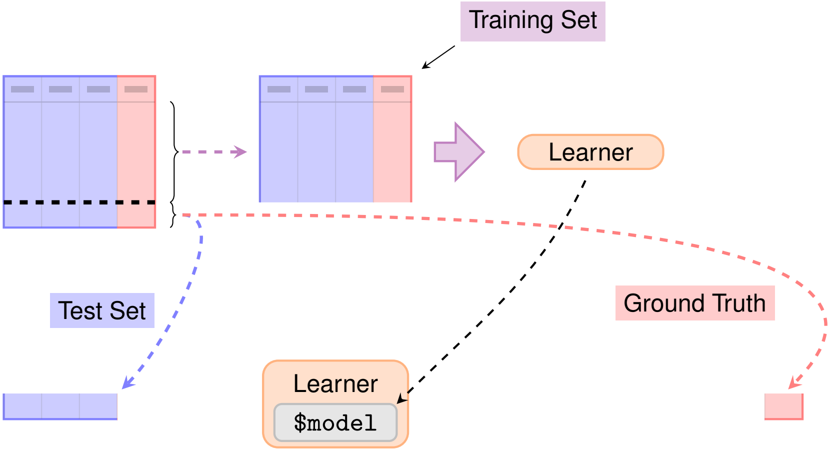


RESAMPLING



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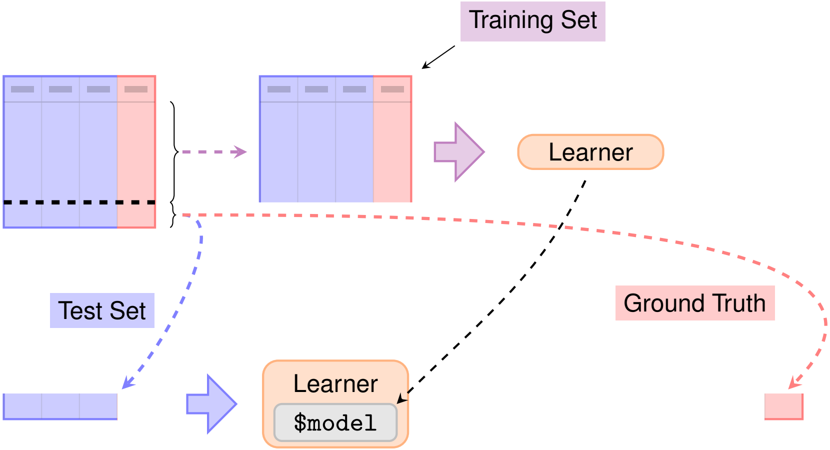

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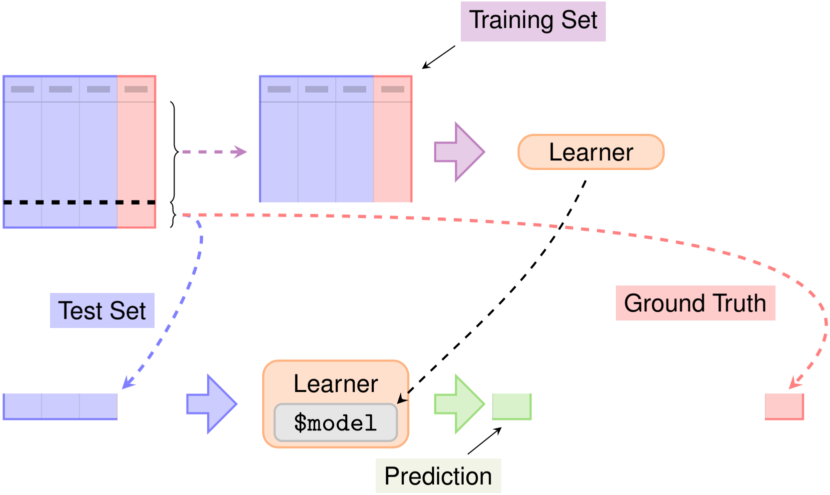
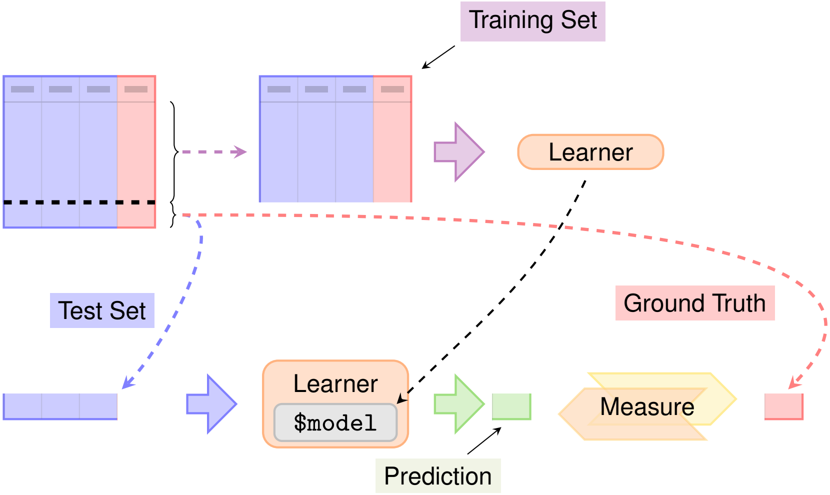
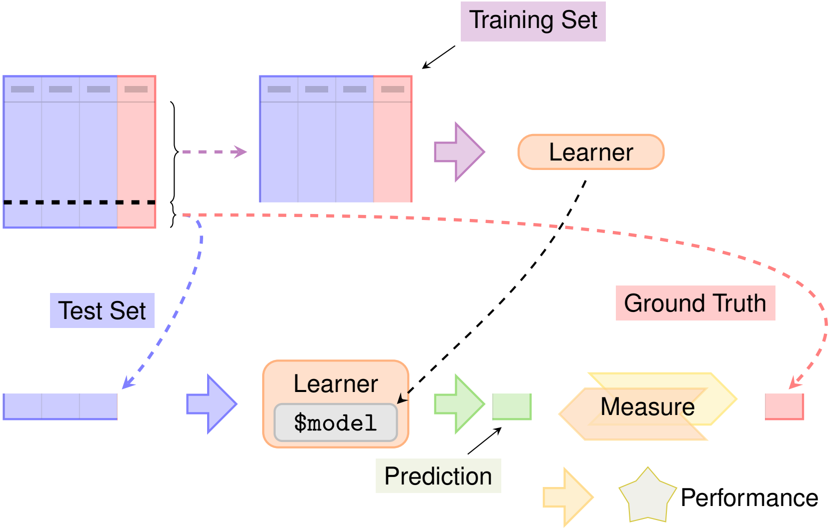


Training Set
Learner
Test Set
Ground Truth
Learner
$model
Prediction

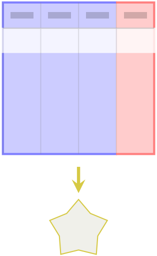
RESAMPLING


Training Set
Learner
Test Set
Ground Truth
Learner
$model
Measure
Prediction

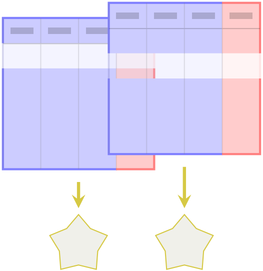
RESAMPLING


Training Set
Learner
Test Set
Ground Truth
Learner
$model
Measure
Prediction
Performance

RESAMPLING



RESAMPLING



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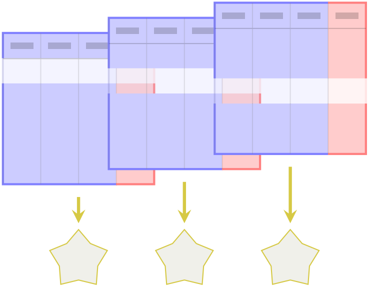

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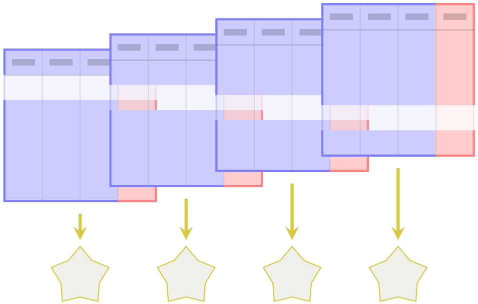

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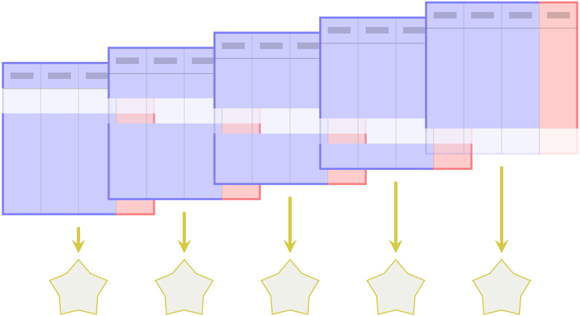
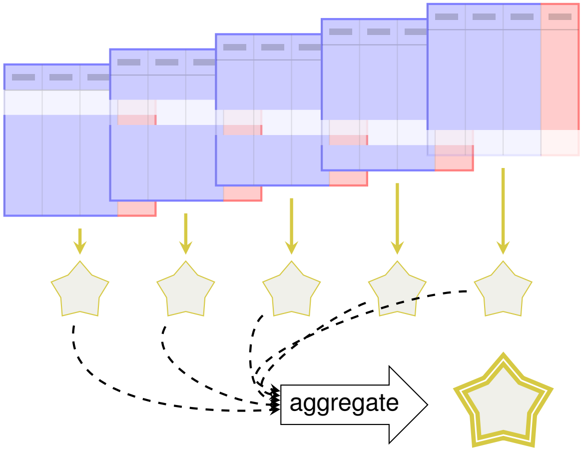
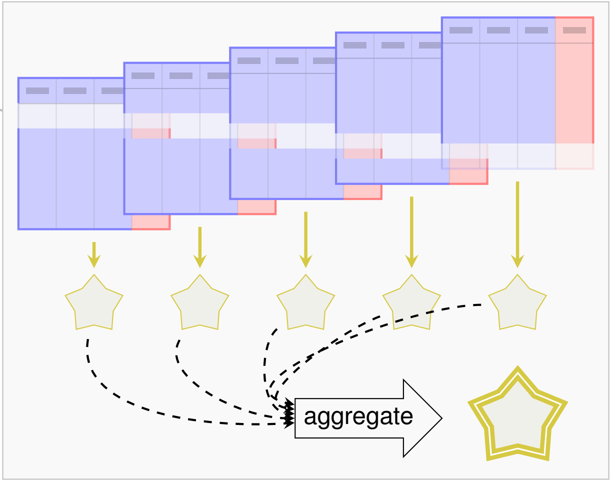


RESAMPLING



RESAMPLING

`resample()`



RESAMPLING

- Resample description: How to split the data

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

RESAMPLING

- Resample description: How to split the data

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

- Use the `resample()` function for resampling:

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

RESAMPLING

- 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
```

RESAMPLING RESULTS

What exactly is a `ResamplingResult` object?

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What exactly is a `ResamplingResult` object?
Remember `Prediction`:

RESAMPLING RESULTS

What exactly is a `ResamplingResult` object?

Remember `Prediction`:

- Get a table representation using `as.data.table()`

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

print(rr_table)
```

```
#                  task                learner          resampling i...
# 1: <TaskClassif[44]> <LearnerClassifRpart[32]> <ResamplingCV[19]>  ...
# 2: <TaskClassif[44]> <LearnerClassifRpart[32]> <ResamplingCV[19]>  ...
# 3: <TaskClassif[44]> <LearnerClassifRpart[32]> <ResamplingCV[19]>  ...
# 4: <TaskClassif[44]> <LearnerClassifRpart[32]> <ResamplingCV[19]>  ...
# 5: <TaskClassif[44]> <LearnerClassifRpart[32]> <ResamplingCV[19]>  ...
```

RESAMPLING RESULTS

What exactly is a `ResamplingResult` object?
Remember `Prediction`:

- Get a table representation using `as.data.table()`

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

print(rr_table)
```

```
#                    task                     learner         resampling i...
# 1: <TaskClassif[44]> <LearnerClassifRpart[32]> <ResamplingCV[19]>  ...
# 2: <TaskClassif[44]> <LearnerClassifRpart[32]> <ResamplingCV[19]>  ...
# 3: <TaskClassif[44]> <LearnerClassifRpart[32]> <ResamplingCV[19]>  ...
# 4: <TaskClassif[44]> <LearnerClassifRpart[32]> <ResamplingCV[19]>  ...
# 5: <TaskClassif[44]> <LearnerClassifRpart[32]> <ResamplingCV[19]>  ...
```

- Active bindings and functions that make information easily accessible

RESAMPLING RESULTS

- Calculate performance:

```r
rr$aggregate(msr("classif.ce"))
#> classif.ce
#>      0.073
```

RESAMPLING RESULTS

- Calculate performance:

```
rr$aggregate(msr("classif.ce"))
#> classif.ce
#>      0.073
```

- Get predictions

```
rr$prediction()
#> <PredictionClassif> for 150 observations:
#>     row_id     truth   response
#>          5    setosa     setosa
#>         14    setosa     setosa
#>         18    setosa     setosa
#> ---
#>        139 virginica virginica
#>        145 virginica virginica
#>        146 virginica virginica
```

RESAMPLING

- Predictions of individual folds

```
predictions = rr$predictions()
predictions[[1]]
```

```
#> <PredictionClassif> for 30 observations:
#>     row_id     truth  response
#>          5    setosa    setosa
#>         14    setosa    setosa
#>         18    setosa    setosa
#> ---
#>        132 virginica virginica
#>        137 virginica virginica
#>        147 virginica virginica
```

RESAMPLING

- Predictions of individual folds

```
predictions = rr$predictions()
predictions[[1]]
```

```
#> <PredictionClassif> for 30 observations:
#>     row_id     truth  response
#>          5    setosa    setosa
#>         14    setosa    setosa
#>         18    setosa    setosa
#> ---
#>        132 virginica virginica
#>        137 virginica virginica
#>        147 virginica virginica
```

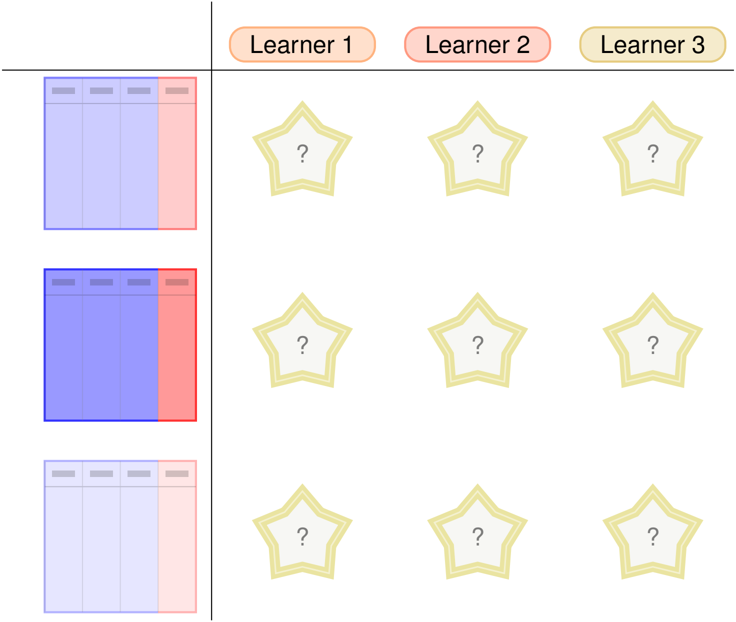
- Score of individual folds

```
scores = rr$score()
scores[1:3, c("iteration", "classif.ce")]
```

```
#>    iteration classif.ce
#> 1:         1      0.033
#> 2:         2      0.033
#> 3:         3      0.100
```

Benchmark

PERFORMANCE COMPARISON



PERFORMANCE COMPARISON

- Multiple Learners, multiple Tasks:

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

PERFORMANCE COMPARISON

- Multiple Learners, multiple Tasks:

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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)
```

PERFORMANCE COMPARISON

- Multiple Learners, multiple Tasks:

```
library("mlr3learners")
learners = list(lrn("classif.rpart"), lrn("classif.kknn"))
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```

- 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      0.060
#> 2:    iris  classif.kknn      0.060
#> 3:   sonar classif.rpart      0.279
#> 4:   sonar  classif.kknn      0.168
#> 5:    wine classif.rpart      0.101
#> 6:    wine  classif.kknn      0.051
```

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()`

BENCHMARK RESULT

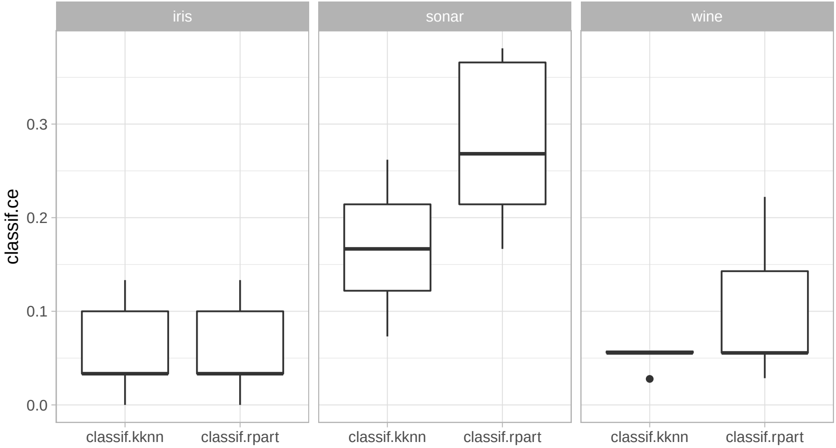
What exactly is a `BenchmarkResult` object?
Just like `Prediction` and `ResamplingResult`!

- Table representation using `as.data.table()`
- Active bindings and functions that make information easily accessible

BENCHMARK RESULT

The `mlr3viz` package contains `autoplot()` functions for many mlr3 objects

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



Control of Execution

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

How to get Help

HOW TO GET HELP

- Where to start?
  - Check these slides
  - **Check the mlr3book https://mlr3book.mlr-org.com**

HOW TO GET HELP

- Where to start?
  - Check these slides
  - **Check the mlr3book https://mlr3book.mlr-org.com**
- Get help for R6 objects?
  1. Find out what kind of R6 object you have:

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

  2. Go to the corresponding help page:

     ```
     ?BenchmarkResult
     ```

  New: open the corresponding man page with

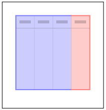
```
learner$help()
```

Outro

OVERVIEW

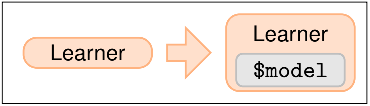
Ingredients:

Data



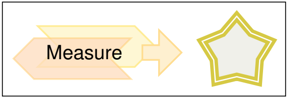
`TaskClassif`,
`TaskRegr`,
`tsk()`

Learning Algorithms



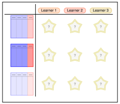
`lrn()` ⇒ `Learner`,
`$train()`,
`$predict()` ⇒ `Prediction`

Performance Evaluation

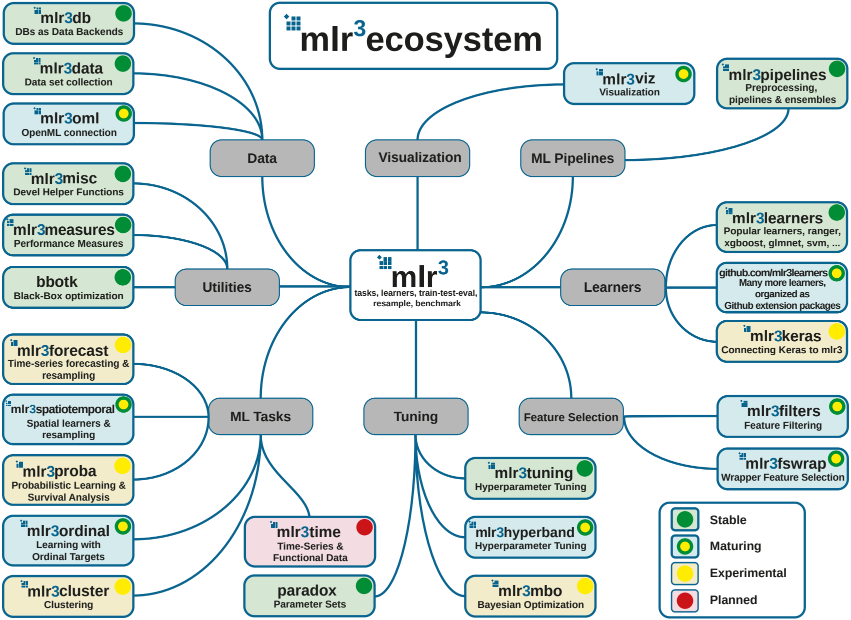


`rsmp()` ⇒ `Resampling`,
`msr()` ⇒ `Measure`,
`resample()` ⇒ `ResamplingResult`,
`$aggregate()`

Performance Comparison



`benchmark_grid()`,
`benchmark()` ⇒ `BenchmarkResult`


mlr3 ecosystem
mlr3db
DBs as Data Backends
mlr3data
Data set collection
mlr3oml
OpenML connection
Data
Visualization
mlr3viz
Visualization
ML Pipelines
mlr3pipelines
Preprocessing, pipelines & ensembles
mlr3misc
Devel Helper Functions
mlr3measures
Performance Measures
bbotk
Black-Box optimization
Utilities
mlr3
tasks, learners, train-test-eval, resample, benchmark
Learners
mlr3learners
Popular learners, ranger, xgboost, glmnet, svm, ...
github.com/mlr3learners
Many more learners, organized as Github extension packages
mlr3keras
Connecting Keras to mlr3
mlr3forecast
Time-series forecasting & resampling
mlr3spatiotemporal
Spatial learners & resampling
mlr3proba
Probabilistic Learning & Survival Analysis
mlr3ordinal
Learning with Ordinal Targets
mlr3cluster
Clustering
ML Tasks
Tuning
Feature Selection
mlr3filters
Feature Filtering
mlr3fswrap
Wrapper Feature Selection
mlr3time
Time-Series & Functional Data
paradox
Parameter Sets
mlr3tuning
Hyperparameter Tuning
mlr3hyperband
Hyperparameter Tuning
mlr3mbo
Bayesian Optimization
Stable
Maturing
Experimental
Planned