Modern Machine Learning in R

mlr3

Department of Statistics – LMU Munich

September 24, 2019

Intro

SO YOU WANT TO DO ML IN R

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

Ingredients:

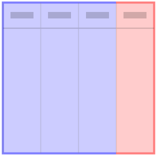
- Data
- Learning Algorithms
- Performance Evaluation
- Performance Comparison

Data

DATA

- Tabular data
- Features
- Target / outcome to predict
  - discrete for classification
  - continuous for regression

  ⇒ data determines the machine learning "Task"



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#>   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
#> 1          5.1         3.5          1.4         0.2  setosa
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task = TaskClassif$new("iris", iris, "Species")
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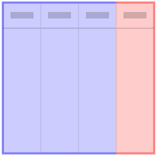

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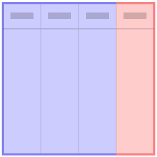

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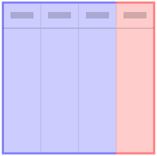

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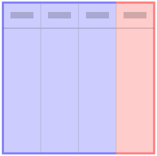

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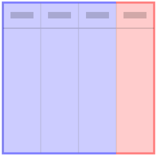

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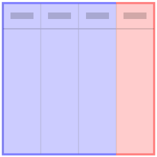

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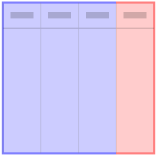

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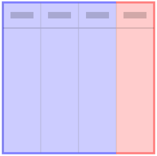

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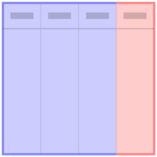

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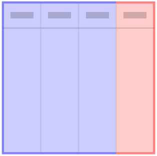

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```

Task ID   data   target name

```
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
```

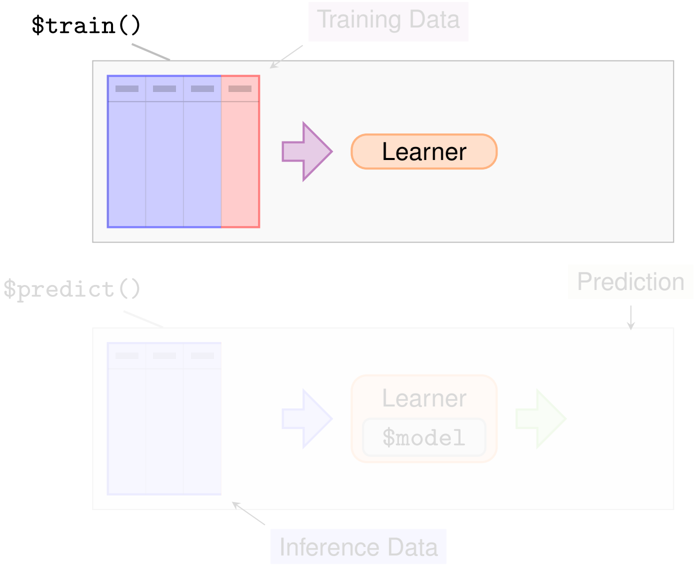
```r
task$ncol
task$nrow
task$feature_names
task$target_names
```

```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 = )
```

Learning Algorithms

LEARNING ALGORITHMS



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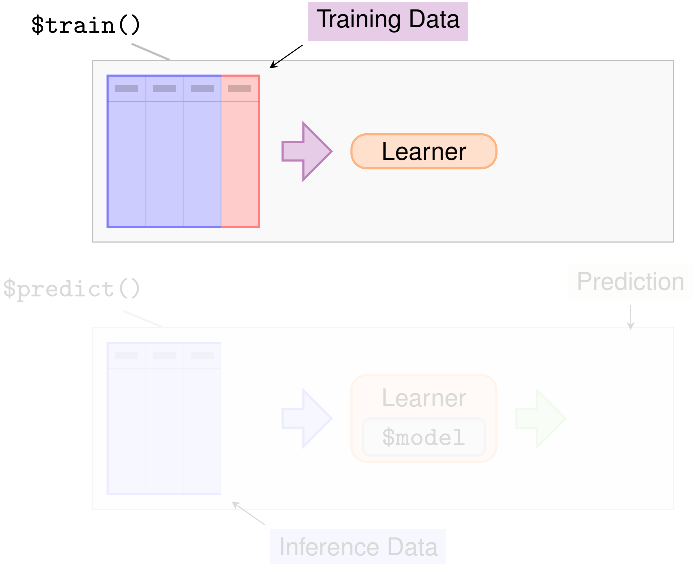

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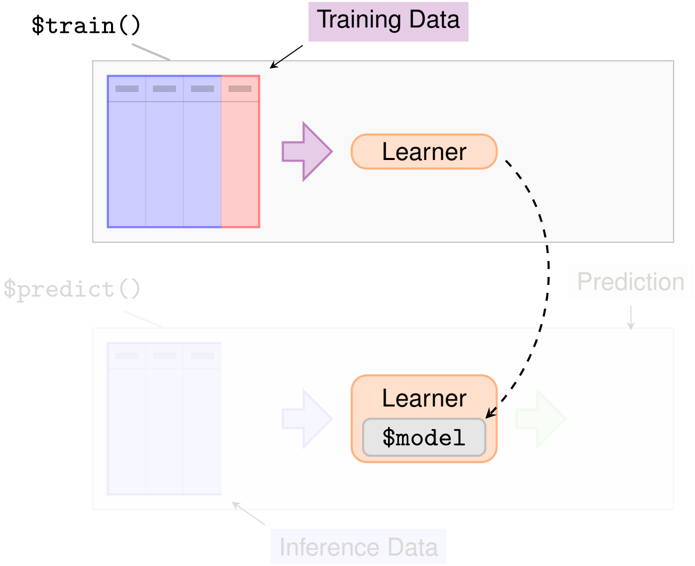

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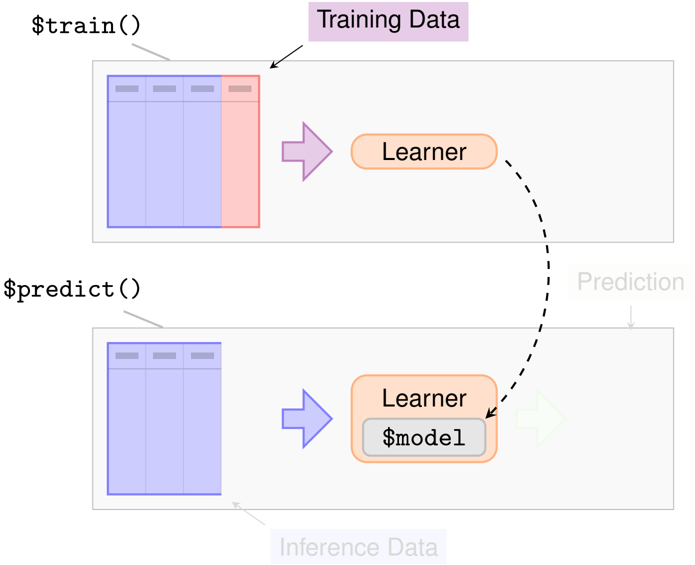

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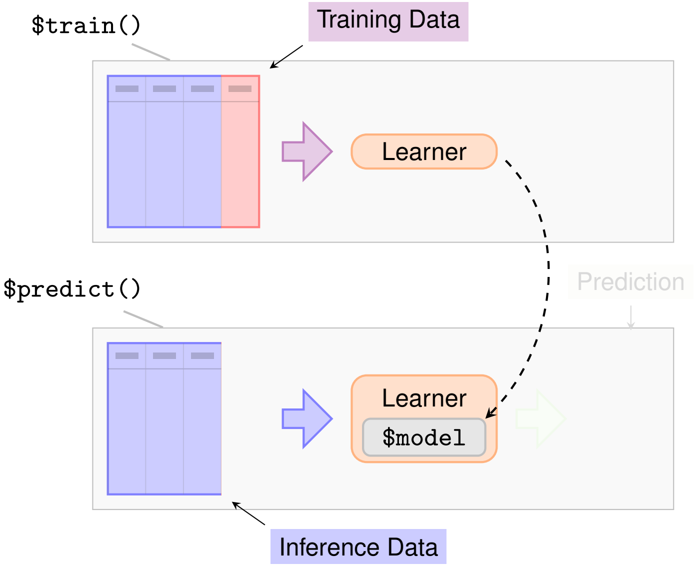

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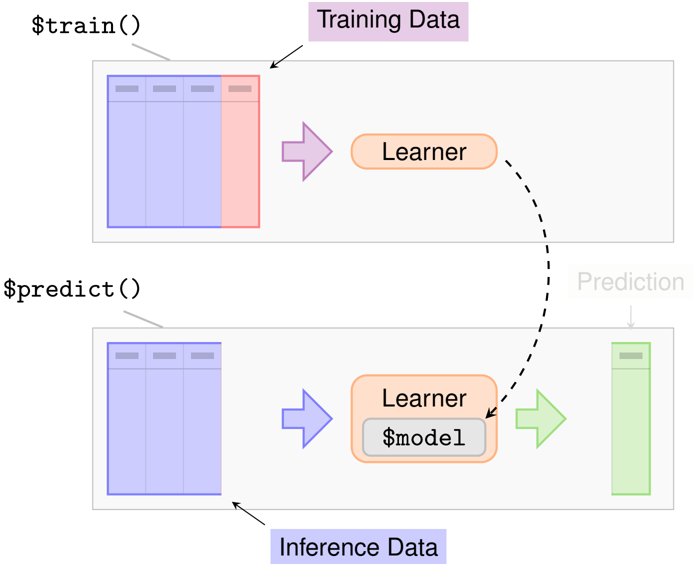

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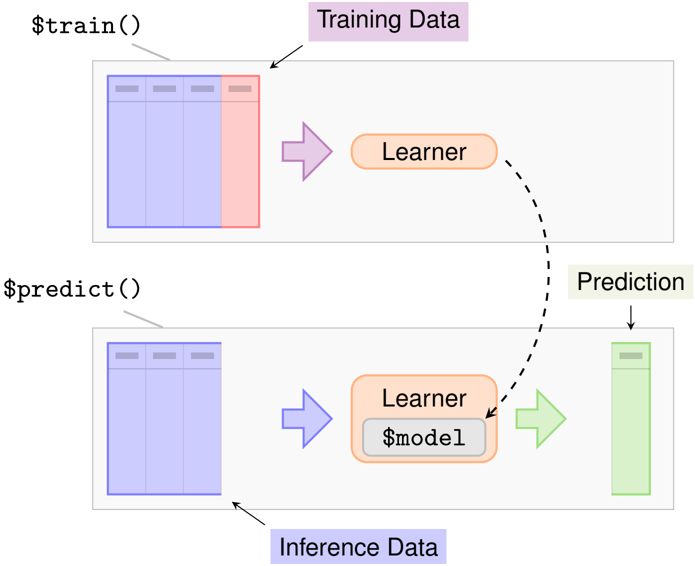

LEARNING ALGORITHMS

- Get a `Learner` provided by `mlr`

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

- 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)
#>   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) *
```

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```

HYPERPARAMETERS

- Learners have *hyperparameters*

```
learner$param_set

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

- Changing them changes the `Learner` behavior

```
learner$param_set$values = list(maxdepth = 1)

learner$train(task)
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HYPERPARAMETERS

- 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
```

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PREDICTION

- Lets 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 and the old **Task**

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

- We get a `Prediction` object:

```
prediction

#> <PredictionClassif> for 2 observations:
#>  row_id truth   response
#>     151  <NA>     setosa
#>     152  <NA> versicolor
```

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PREDICTION

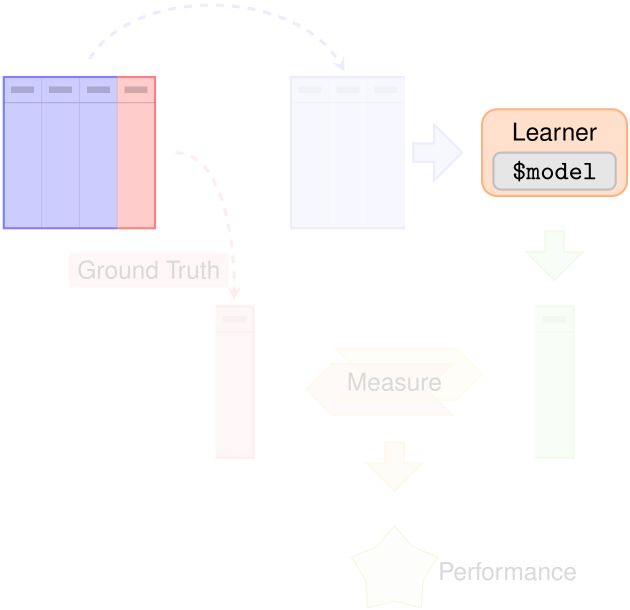
- We can make the `Learner` predict *probabilities* when we set `predict_type`:

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

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

Performance

PERFORMANCE EVALUATION



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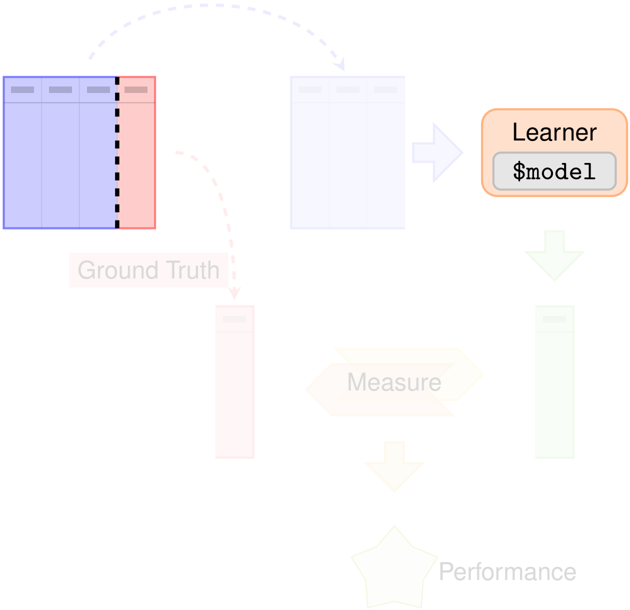

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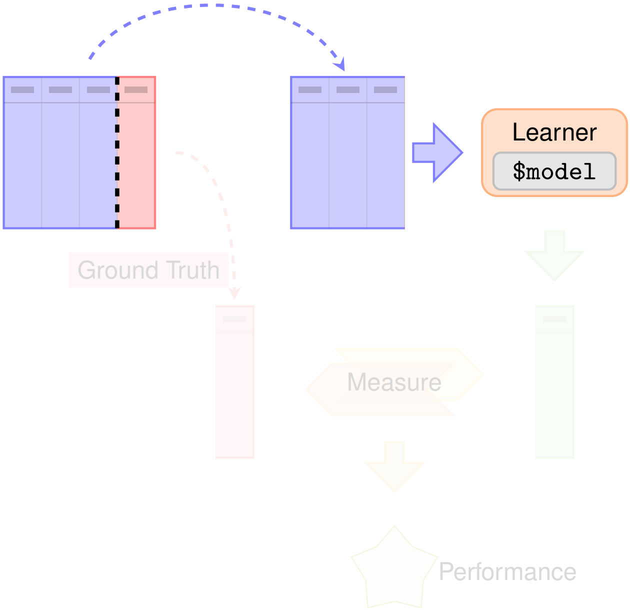

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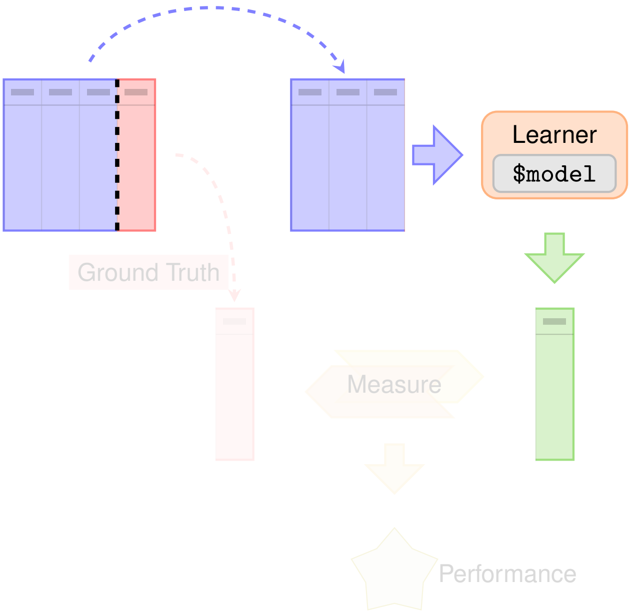

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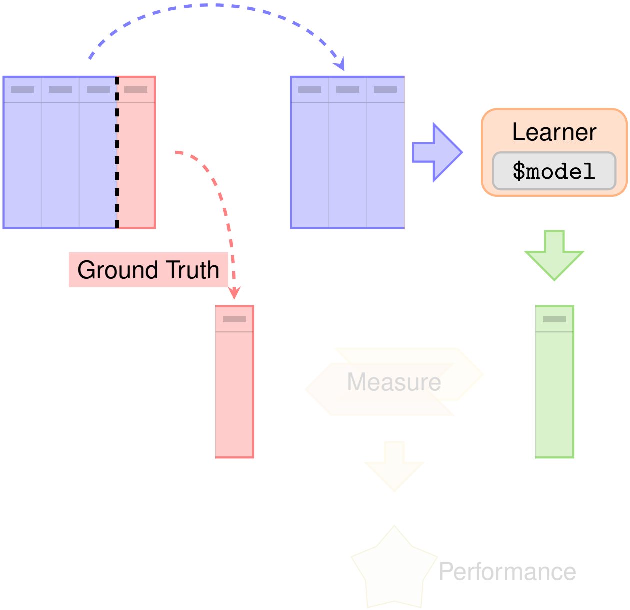

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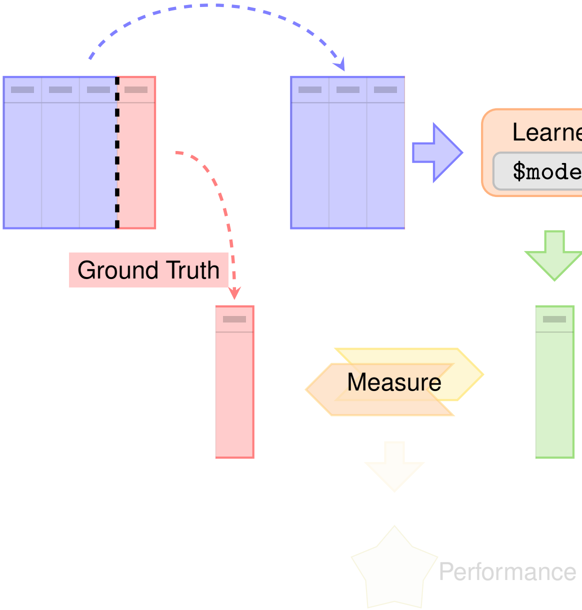

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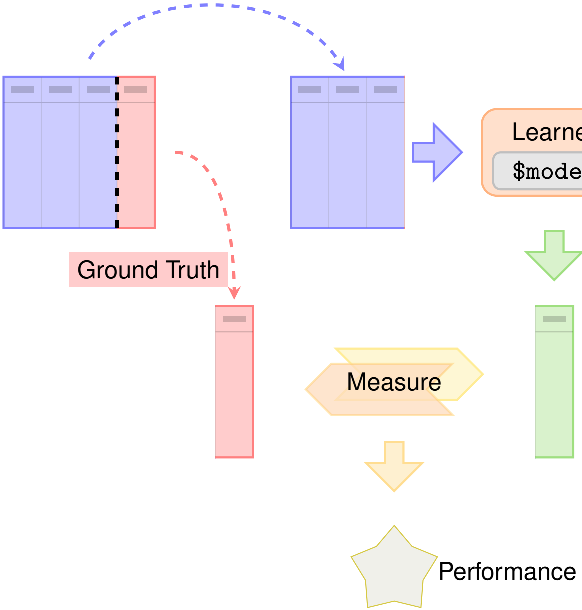

PERFORMANCE EVALUATION

- 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
```

- Predict again

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

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

- Score the prediction

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

#> classif.ce
#>        0.5
```

PERFORMANCE EVALUATION

- Prediction 'Task' with known data

```
known_truth_task$data()

#    Species Petal.Length Petal.Width Sepal.Length Sepal.Width
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- 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
```

- Predict again

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

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

- Score the prediction

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

#> classif.ce
#>        0.5
```

PERFORMANCE EVALUATION

- Confusion Matrix

```
pred

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

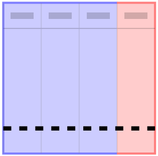
pred$confusion

#>             truth
#> response     setosa versicolor virginica
#>   setosa          1          0         0
#>   versicolor      0          0         0
#>   virginica       1          0         0
```

Resampling

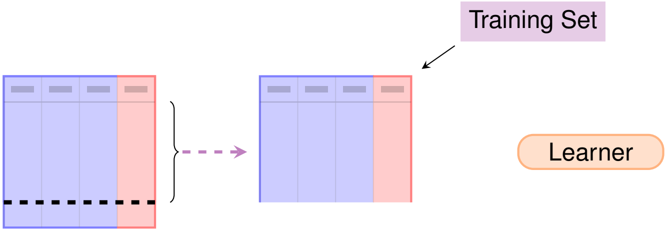
RESAMPLING

RESAMPLING

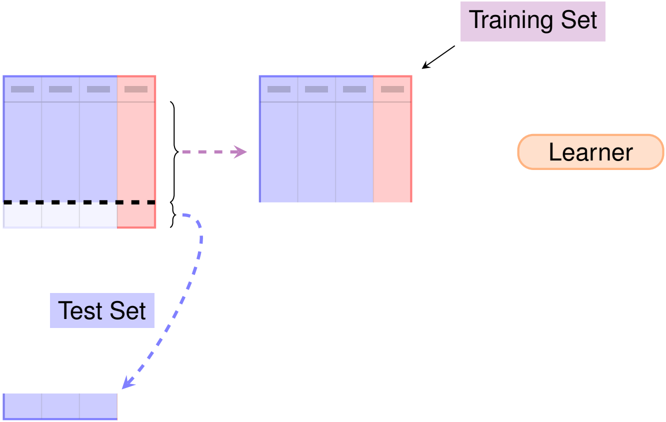


Learner

RESAMPLING



RESAMPLING



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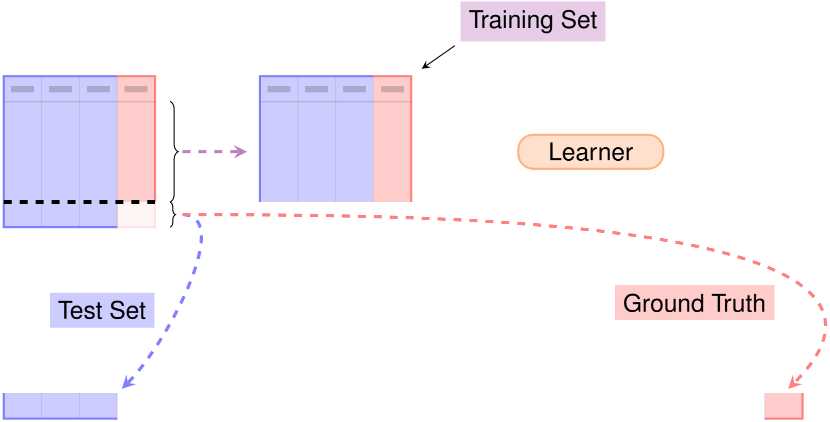

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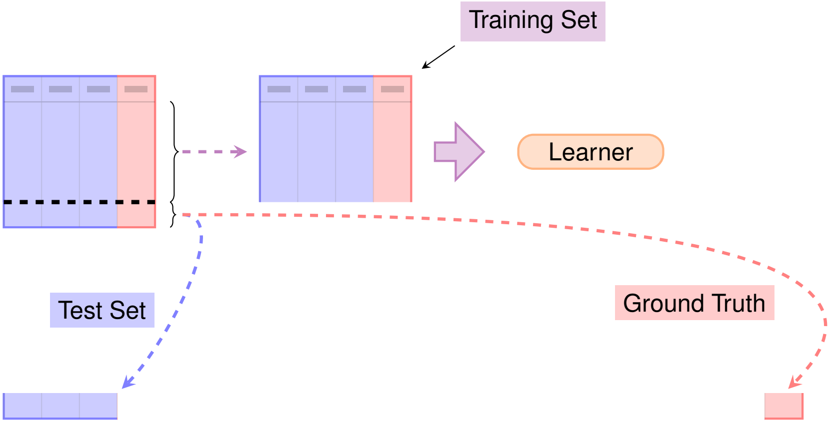
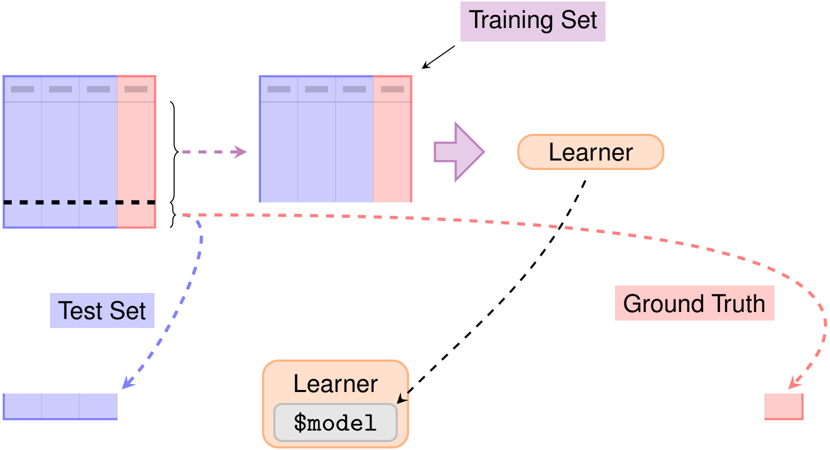
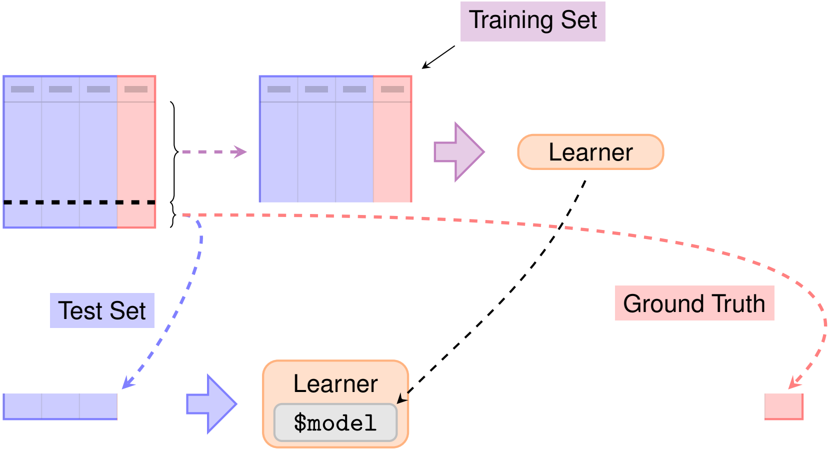


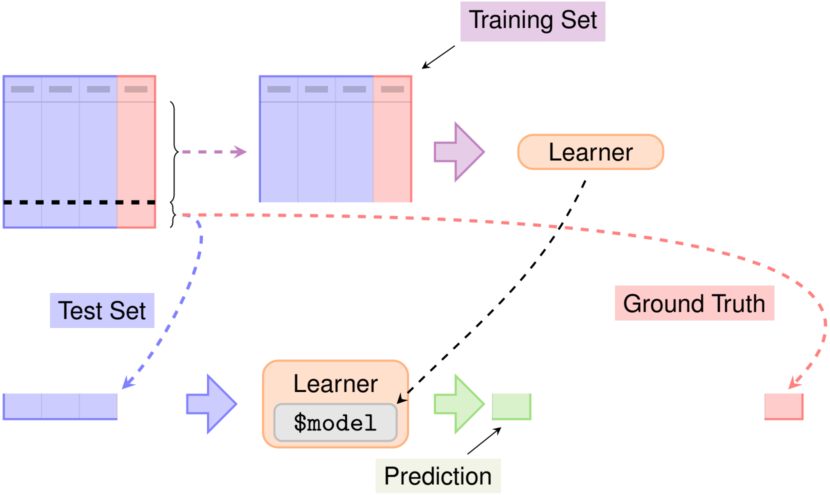
RESAMPLING



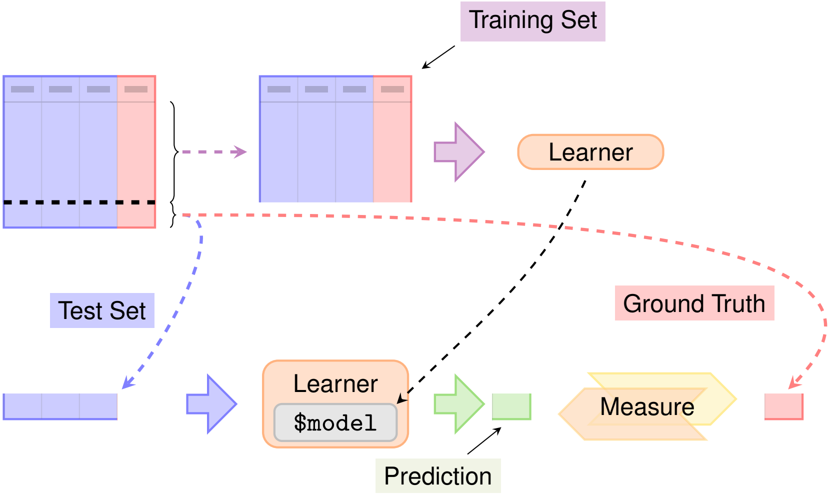
RESAMPLING



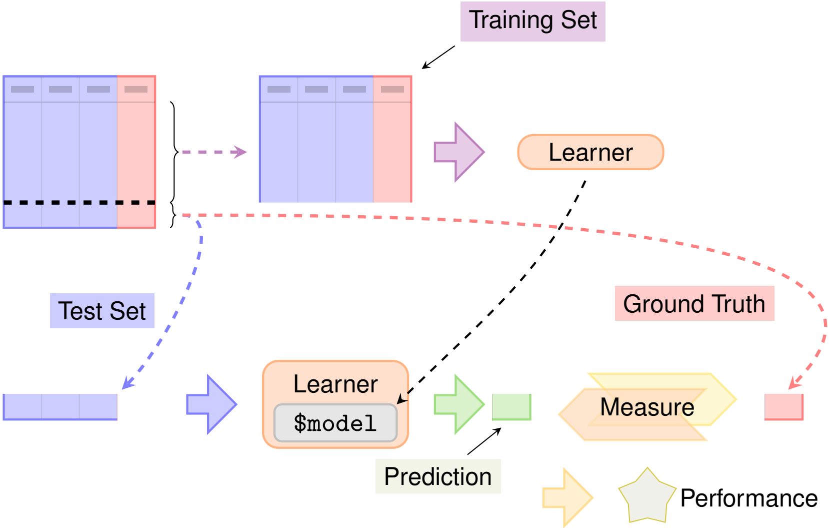
RESAMPLING


Training Set
Learner
Test Set
Ground Truth
Learner
$model
Prediction

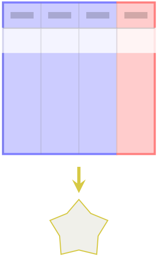
RESAMPLING


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

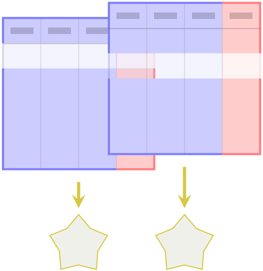
RESAMPLING


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

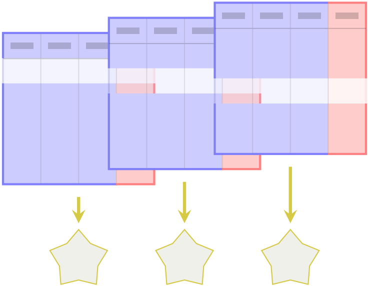
RESAMPLING



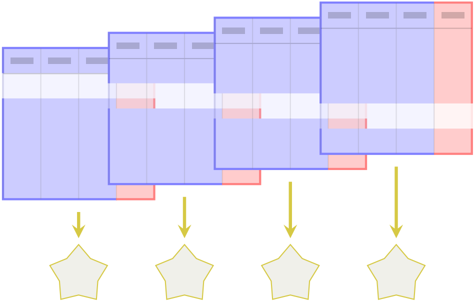
RESAMPLING



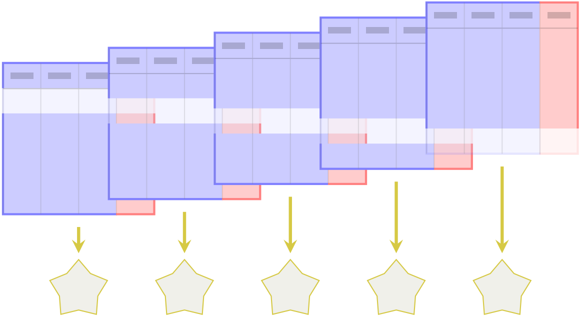
RESAMPLING



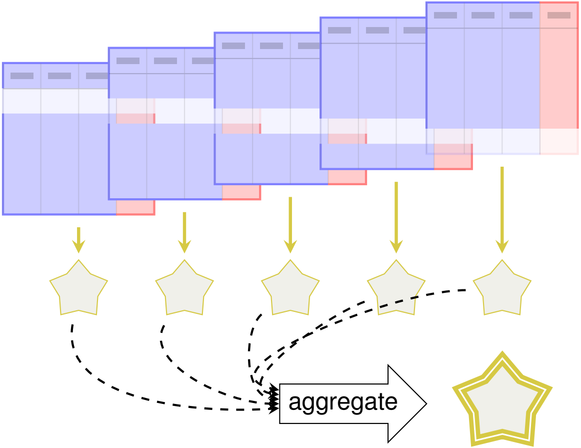
RESAMPLING



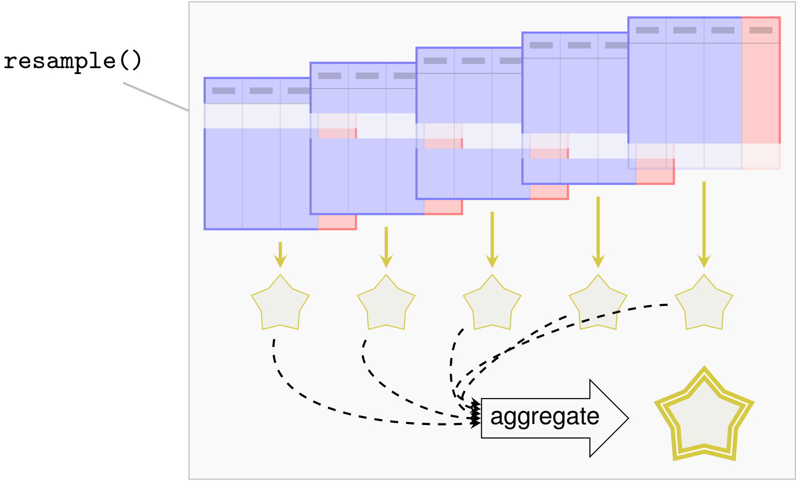
RESAMPLING



RESAMPLING



RESAMPLING



RESAMPLING

- Resample description: How to split the data

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

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

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

- The resampling result:

```r
print(result)

#> <ResampleResult> of 5 iterations
#> * Task: iris
#> * Learner: classif.rpart
#> * Performance: 0.067 [classif.ce]
#> * Warnings: 0 in 0 iterations
#> * Errors: 0 in 0 iterations
```

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#> * Learner: classif.rpart
#> * Performance: 0.067 [classif.ce]
#> * Warnings: 0 in 0 iterations
#> * Errors: 0 in 0 iterations
```

RESAMPLING

- Get performance:

```
result$aggregate(msr("classif.ce"))
```

```
#> classif.ce
#>      0.067
```

- Get predictions

```
result$prediction()
```

```
#> <PredictionClassif> for 150 observations:
#>     row_id     truth  response
#>          1    setosa    setosa
#>          4    setosa    setosa
#>          9    setosa    setosa
#> ---
#>        140 virginica virginica
#>        147 virginica virginica
#>        148 virginica virginica
```

RESAMPLING

- Get performance:

```
result$aggregate(msr("classif.ce"))

#> classif.ce
#>      0.067
```

- Get predictions

```
result$prediction()

#> <PredictionClassif> for 150 observations:
#>     row_id     truth  response
#>          1    setosa    setosa
#>          4    setosa    setosa
#>          9    setosa    setosa
#> ---
#>        140 virginica virginica
#>        147 virginica virginica
#>        148 virginica virginica
```

RESAMPLING

- Predictions of individual folds

```
result$predictions()[[1]]
```

```
#> <PredictionClassif> for 30 observations:
#>     row_id     truth  response
#>          1    setosa    setosa
#>          4    setosa    setosa
#>          9    setosa    setosa
#> ---
#>        134 virginica virginica
#>        136 virginica virginica
#>        146 virginica virginica
```

- Score of individual folds

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

```
#>    iteration classif.ce
#> 1:         1      0.067
#> 2:         2      0.033
#> 3:         3      0.100
#> 4:         4      0.067
#> 5:         5      0.067
```

RESAMPLING

- Predictions of individual folds

```
result$predictions()[[1]]

#> <PredictionClassif> for 30 observations:
#>     row_id     truth  response
#>          1    setosa    setosa
#>          4    setosa    setosa
#>          9    setosa    setosa
#> ---
#>        134 virginica virginica
#>        136 virginica virginica
#>        146 virginica virginica
```

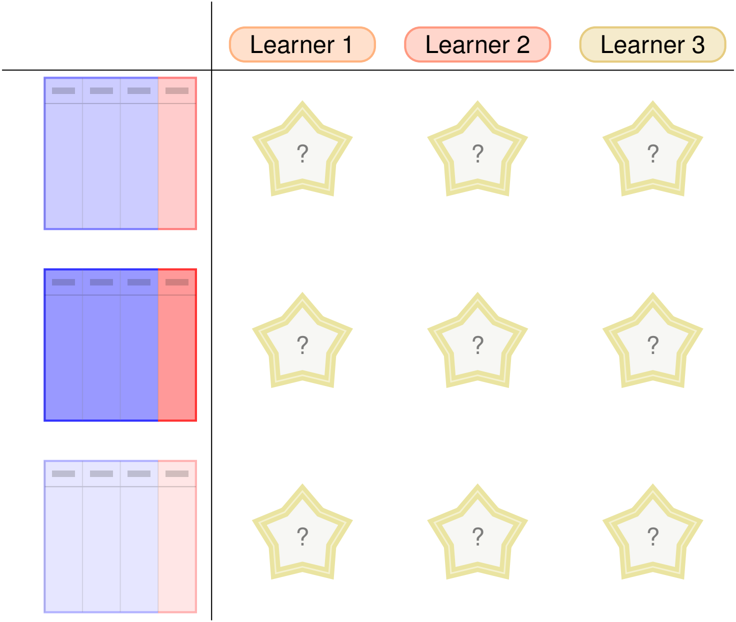
- Score of individual folds

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

#>    iteration classif.ce
#> 1:         1      0.067
#> 2:         2      0.033
#> 3:         3      0.100
#> 4:         4      0.067
#> 5:         5      0.067
```

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"))
```

- Set up the *design* and execute benchmark:

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

- The benchmark result shows that `kknn` outperforms `rpart`:

```
bmr$aggregate()[, .(task_id, learner_id, classif.ce)]

#>    task_id    learner_id classif.ce
#> 1:    iris classif.rpart      0.053
#> 2:    iris  classif.kknn      0.053
#> 3:   sonar classif.rpart      0.303
#> 4:   sonar  classif.kknn      0.178
#> 5:    wine classif.rpart      0.136
#> 6:    wine  classif.kknn      0.051
```

PERFORMANCE COMPARISON

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library("mlr3learners")
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```
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#>    task_id    learner_id classif.ce
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```

PERFORMANCE COMPARISON

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```

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

- The benchmark result shows that `kknn` outperforms `rpart`:

```r
bmr$aggregate()[, .(task_id, learner_id, classif.ce)]

#>    task_id    learner_id classif.ce
#> 1:    iris classif.rpart      0.053
#> 2:    iris  classif.kknn      0.053
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#> 5:    wine classif.rpart      0.136
#> 6:    wine  classif.kknn      0.051
```

Short Forms

SHORT FORMS

- Ordinary constructors: `LearnerClassifRpart$new()`

⇒ Short form constructors

- 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()`

```
mlr_measures
```

```
#> <DictionaryMeasure> with 30 stored values
#> Keys: classif.acc, classif.auc, classif.ce, classif.costs,
#>   classif.f1, classif.fdr, classif.fn, classif.fnr,
#>   classif.for, classif.fp, classif.fpr, classif.npv,
#>   classif.ppv, classif.precision, classif.recall,
#>   classif.sensitivity, classif.specificity, classif.tn,
#>   classif.tnr, classif.tp, classif.tpr, debug, oob_error,
#>   regr.mae, regr.mse, regr.rmse, selected_features,
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`Resampling`	`mlr_resamplings`	`rsmp()`

```
mlr_measures

#> <DictionaryMeasure> with 30 stored values
#> Keys: classif.acc, classif.auc, classif.ce, classif.costs,
#>   classif.f1, classif.fdr, classif.fn, classif.fnr,
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⇒ Short form constructors

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

```
mlr_measures
```

```
#> <DictionaryMeasure> with 30 stored values
#> Keys: classif.acc, classif.auc, classif.ce, classif.costs,
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#>   classif.ppv, classif.precision, classif.recall,
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`Measure`	`mlr_measures`	`msr()`
`Resampling`	`mlr_resamplings`	`rsmp()`

```
mlr_measures


#> <DictionaryMeasure> with 30 stored values
#> Keys: classif.acc, classif.auc, classif.ce, classif.costs,
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Object	Dictionary	Short Form
Task	mlr_tasks	tsk()
Learner	mlr_learners	lrn()
Measure	mlr_measures	msr()
Resampling	mlr_resamplings	rsmp()

```
mlr_measures

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#>   classif.ppv, classif.precision, classif.recall,
#>   classif.sensitivity, classif.specificity, classif.tn,
#>   classif.tnr, classif.tp, classif.tpr, debug, oob_error,
#>   regr.mae, regr.mse, regr.rmse, selected_features,
#>   time_both, time_predict, time_train
```

Details for Nerds

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`, ...)

INTERNAL DATA STRUCTURE

Results objects (`resample()`, `benchmark()`, `...`) share the same structure

```
print(as.data.table(result))

#>                task                 learner     resampling iterati...
#> 1: <TaskClassif> <LearnerClassifRpart> <ResamplingCV>          ...
#> 2: <TaskClassif> <LearnerClassifRpart> <ResamplingCV>          ...
#> 3: <TaskClassif> <LearnerClassifRpart> <ResamplingCV>          ...
#> 4: <TaskClassif> <LearnerClassifRpart> <ResamplingCV>          ...
#> 5: <TaskClassif> <LearnerClassifRpart> <ResamplingCV>          ...
```

Combining R6 and data.table

- Not the objects are stored, but pointers to them
- Inexpensive to work on:
  - `rbind()`: copying R6 objects $\leftrightarrow$ copying pointers
  - `cbind()`: `data.table()` over-allocates columns, no copies
  - `[i, ]`: lookup row (possibly hashed), create a list of pointers
  - `[, j]`: direct access to list elements

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

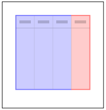
- Task stores data in a `DataBackend`:
  - `DataBackendDataTable`: Default backend for dense data (in-memory)
  - `DataBackendMatrix`: Backend for sparse numerical data (in-memory)
  - `DataBackendDplyr`: Backend for many DBMS (out-of-memory)
  - `DataBackendCbind`: Combine backends in a `cbind()` fashion (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

SO YOU WANT TO DO ML IN R

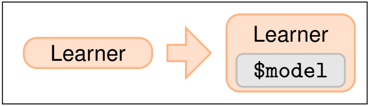
Ingredients:

Data



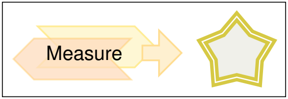
```
TaskClassif,
TaskRegr,
tsk()
```

Learning Algorithms



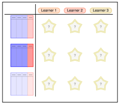

```
lrn(),
$train(),
$predict()
```

Performance Evaluation




```
msr(),
resample()
$aggregate()
```

Performance Comparison




```
benchmark_grid(),
benchmark()
```