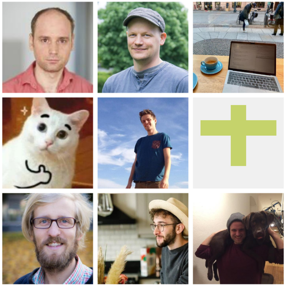
Modern Machine Learning in R

https://mlr-org.com/

https://github.com/mlr-org



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March 2, 2022

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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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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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 in assert_ro_binding(rhs):  Field/Binding is
read-only
```

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```
task$nrow = 11
#> Error in assert_ro_binding(rhs):  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
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  - List columns to arrange complex objects in tabular structure

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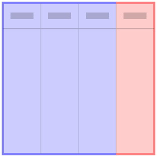
- Embrace **data.table**, both for arguments and internally
  - Fast operations for tabular data
  - List columns to arrange complex objects in tabular structure
- Be **light on dependencies**:
  - `R6`, `data.table`, `lgr`, `uuid`, `mlbench`, `digest`
  - Plus some of our own packages (`backports`,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

Data

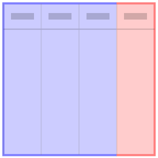
DATA

- Tabular data



DATA

- Tabular data
- Features



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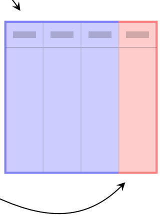
- Target / outcome to predict



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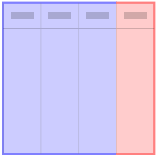
  - discrete for classification
  - continuous for regression



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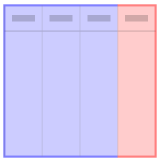

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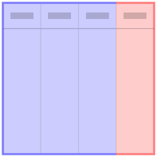

```
print(iris)  # included in R

#>   Sepal.Length Sepal.Width Petal.Length Petal.Width Species
#> 1          5.1         3.5          1.4         0.2  setosa
#> 2          4.9         3.0          1.4         0.2  setosa
#> ...
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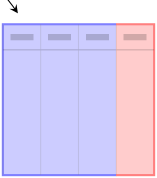

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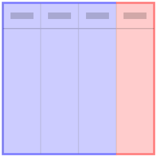

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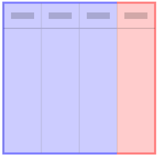

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Task ID

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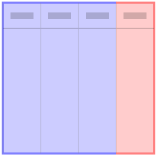

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Task ID data

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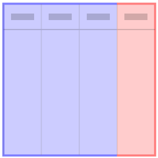

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#> ...
```

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 = )
```

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 11 stored values
#> Keys: boston_housing, breast_cancer, german_credit, iris,
#>   mtcars, penguins, pima, sonar, spam, 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:

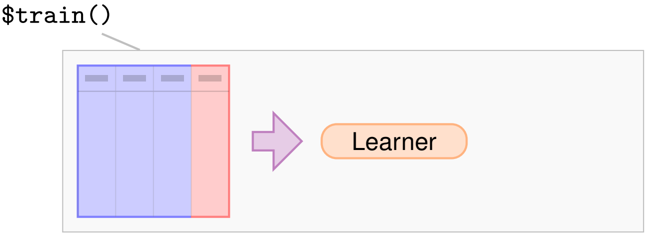
```
mlr_learners_table = as.data.table(mlr_learners)

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

#                    key                    packages
#  1:   classif.cv_glmnet mlr3,mlr3learners,glmnet
#  2:       classif.debug                       mlr3
#  3: classif.featureless                       mlr3
#  4:      classif.glmnet mlr3,mlr3learners,glmnet
#  5:        classif.kknn   mlr3,mlr3learners,kknn
#  6:         classif.lda   mlr3,mlr3learners,MASS
#  7:     classif.log_reg  mlr3,mlr3learners,stats
#  8:    classif.multinom   mlr3,mlr3learners,nnet
#  9: classif.naive_bayes  mlr3,mlr3learners,e1071
# 10:        classif.nnet   mlr3,mlr3learners,nnet
#      predict_types
#  1: response,prob
#  2: response,prob
#  3: response,prob
#  4: response,prob
#  5: response,prob
```

Learning Algorithms

LEARNING ALGORITHMS



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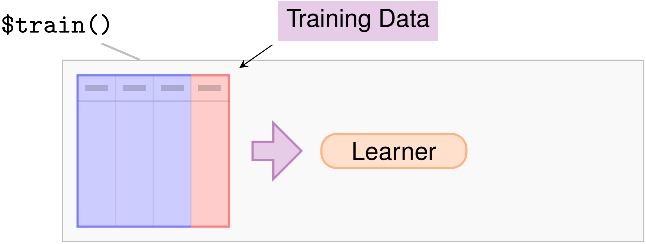

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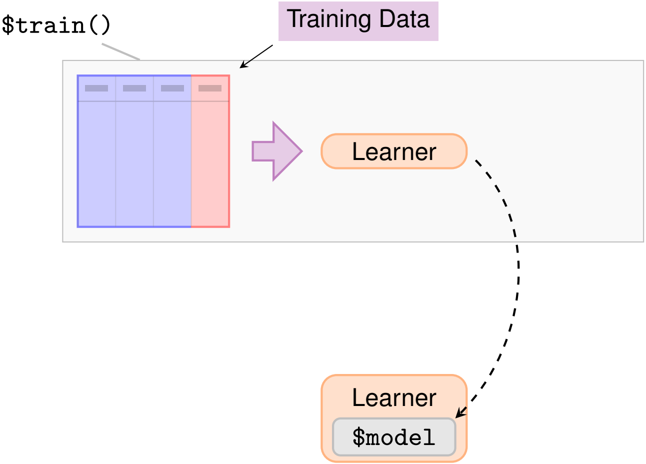

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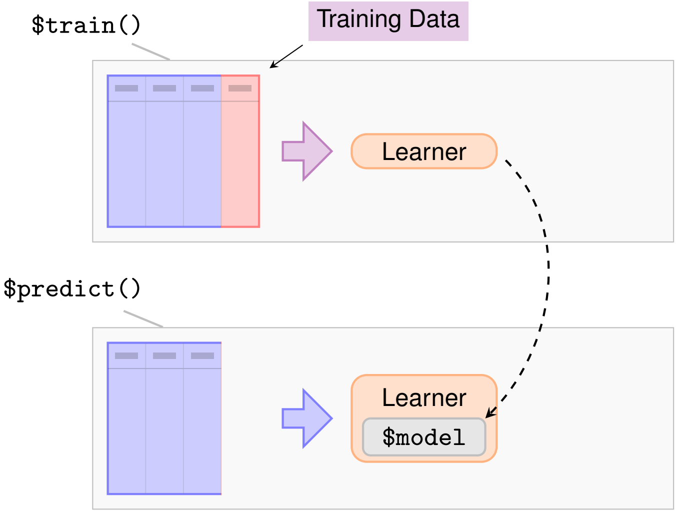

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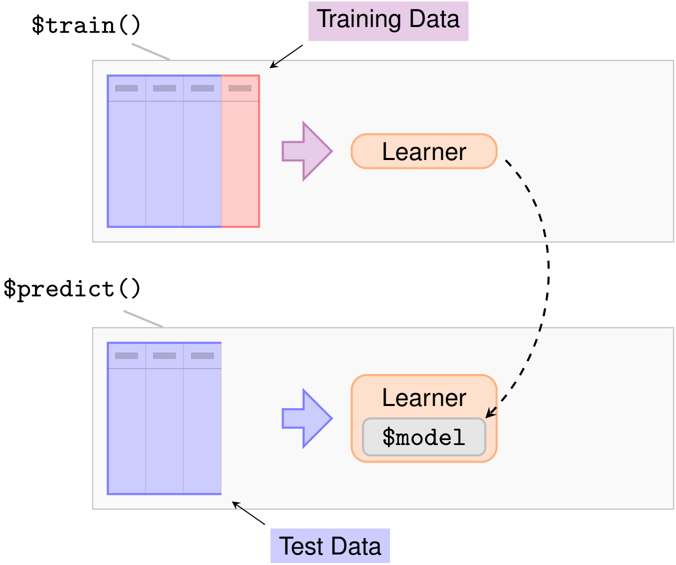

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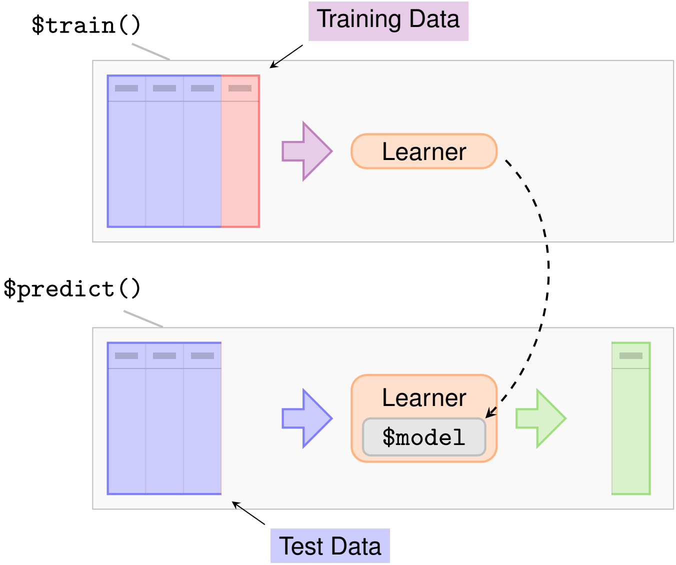

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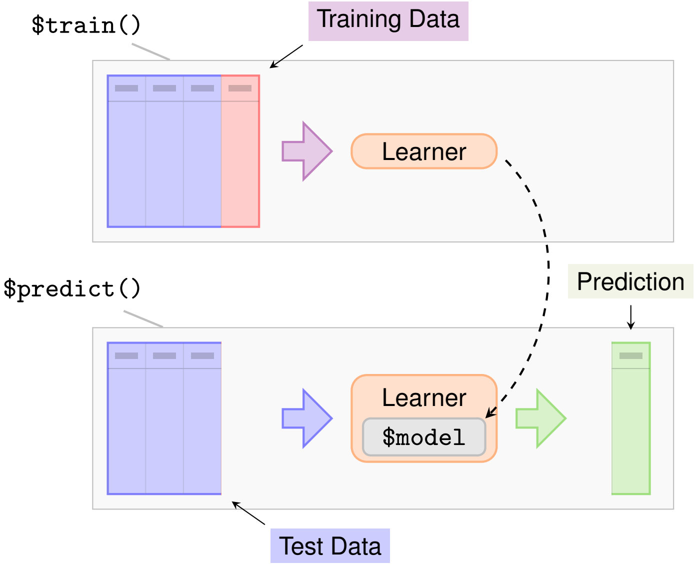

LEARNING ALGORITHMS

- Get a `Learner` provided by `mlr`

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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< 2.4 50   0 setosa (1.000 0.000 0.000) *
#>   3) Petal.Length>=2.4 100  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:             cp ParamDbl     0     1                 Inf
#>  2:     keep_model ParamLgl    NA    NA  TRUE,FALSE       2
#>  3:     maxcompete ParamInt     0   Inf                 Inf
#>  4:       maxdepth ParamInt     1    30                  30
#>  5:   maxsurrogate ParamInt     0   Inf                 Inf
#>  6:      minbucket ParamInt     1   Inf                 Inf
#>  7:       minsplit ParamInt     1   Inf                 Inf
#>  8: surrogatestyle ParamInt     0     1                   2
#>  9:   usesurrogate ParamInt     0     2                   3
#> 10:           xval ParamInt     0   Inf                 Inf
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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

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#>   3) Petal.Length>=2.4 100  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_ids truth   response
#>        1  <NA>     setosa
#>        2  <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(new_data)
```

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

- Contains predictions and offers useful access fields / methods

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

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#>    row_ids truth   response
#> 1:       1  <NA>     setosa
#> 2:       2  <NA> versicolor
```
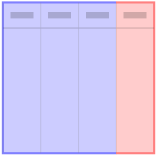
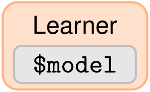

⇒ Active bindings and functions that give further information: `$response`, `$truth`, ...

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

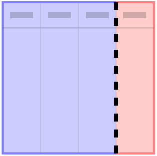
Performance

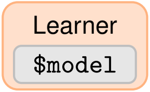
PERFORMANCE EVALUATION



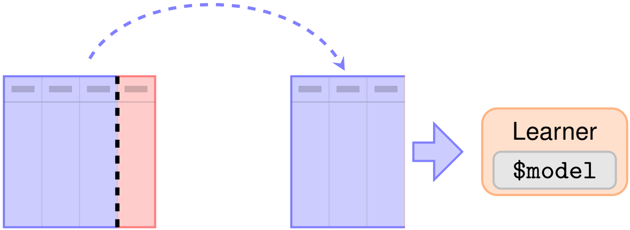


PERFORMANCE EVALUATION

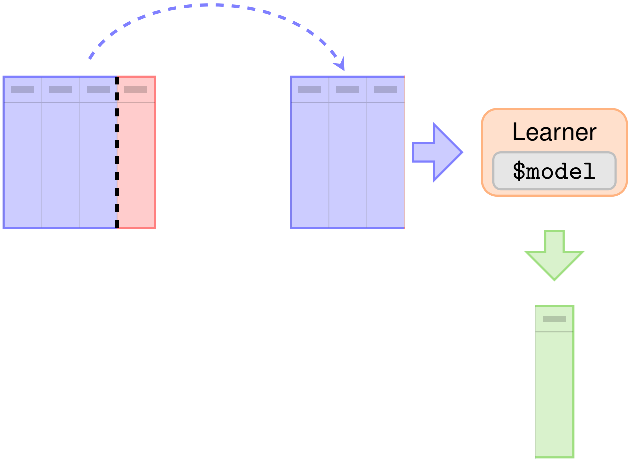




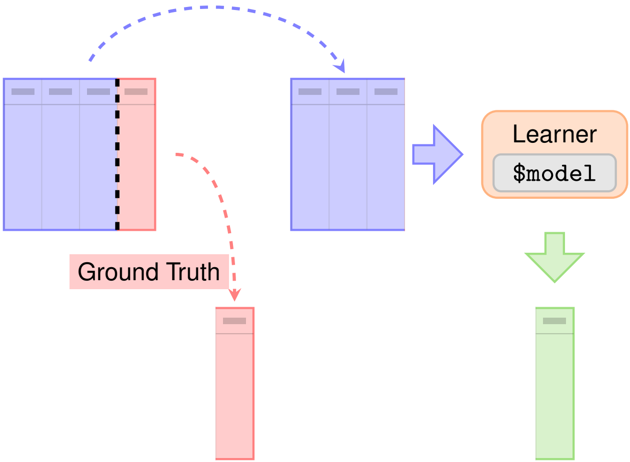
PERFORMANCE EVALUATION



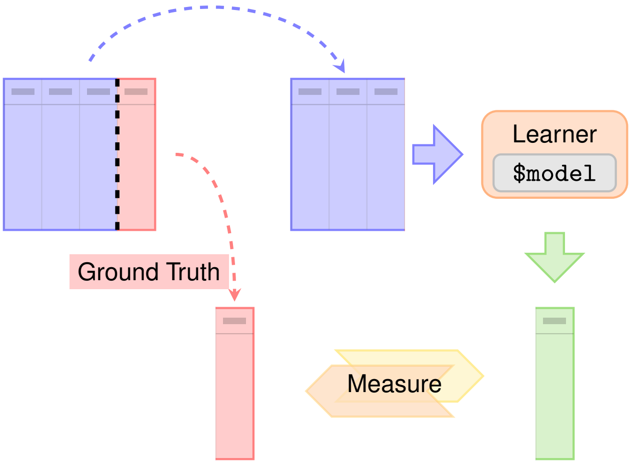
PERFORMANCE EVALUATION



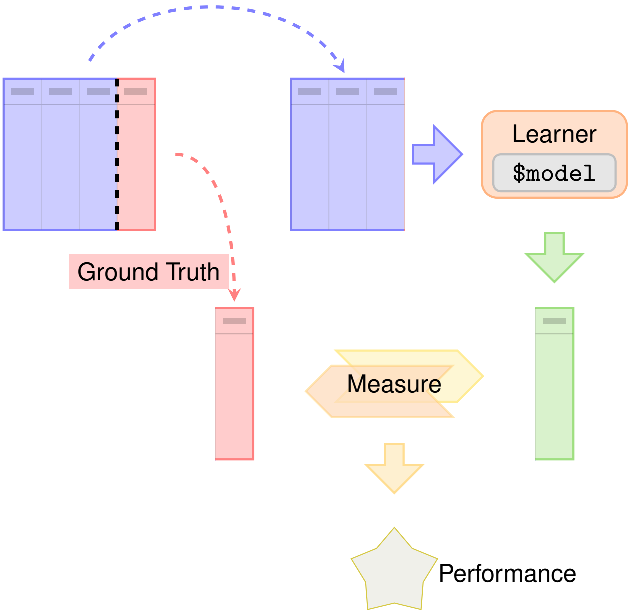
PERFORMANCE EVALUATION



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

- 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_ids  truth  response
#>        1 setosa    setosa
#>        2 setosa virginica
```

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_ids  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
# 1:  setosa            2           1            4           3
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```

- Predict again

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

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

- Score the prediction

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

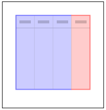
```
#> classif.ce
#>        0.5
```

Outro

OVERVIEW

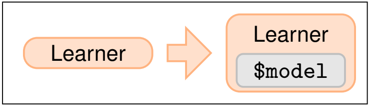
Ingredients:

Data



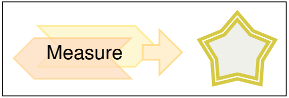
`TaskClassif`,
`TaskRegr`,
`tsk()`

Learning Algorithms



`lrn()` $\Rightarrow$ `Learner`,
$\hookrightarrow$ `Learner$train()`,
$\hookrightarrow$ `Learner$predict()` $\Rightarrow$ `Prediction`

Measure Performance



`Prediction$score()`,
`msr()` $\Rightarrow$ `Measure`