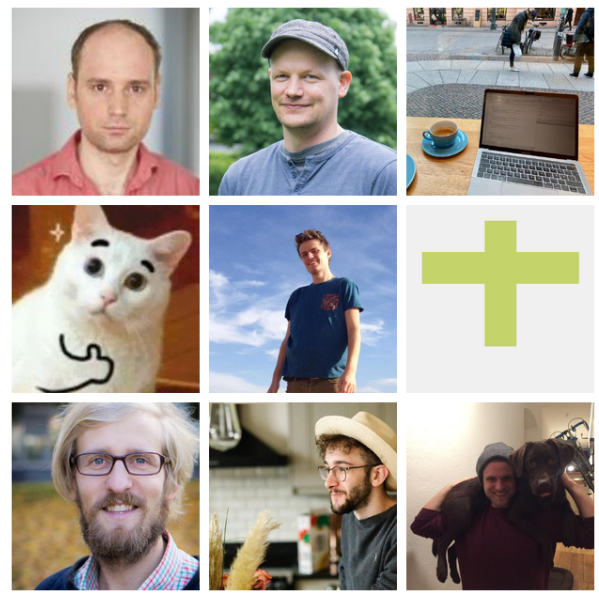
Modern Machine Learning in R

https://mlr-org.com/

https://github.com/mlr-org

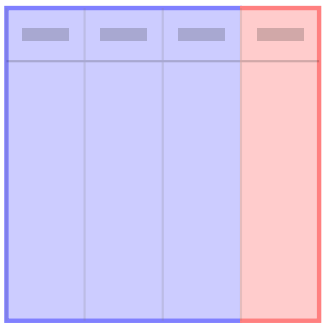


Bernd Bischl, Michel Lang, Martin Binder, Florian Pfisterer, Jakob Richter, Patrick Schratz, Lennart Schneider, Raphael Sonabend, Marc Becker

February 11, 2021

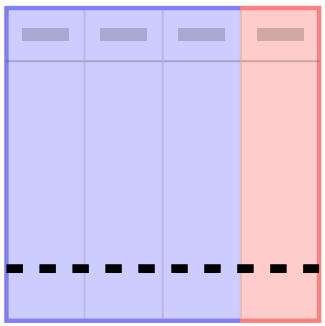
Resampling

RESAMPLING



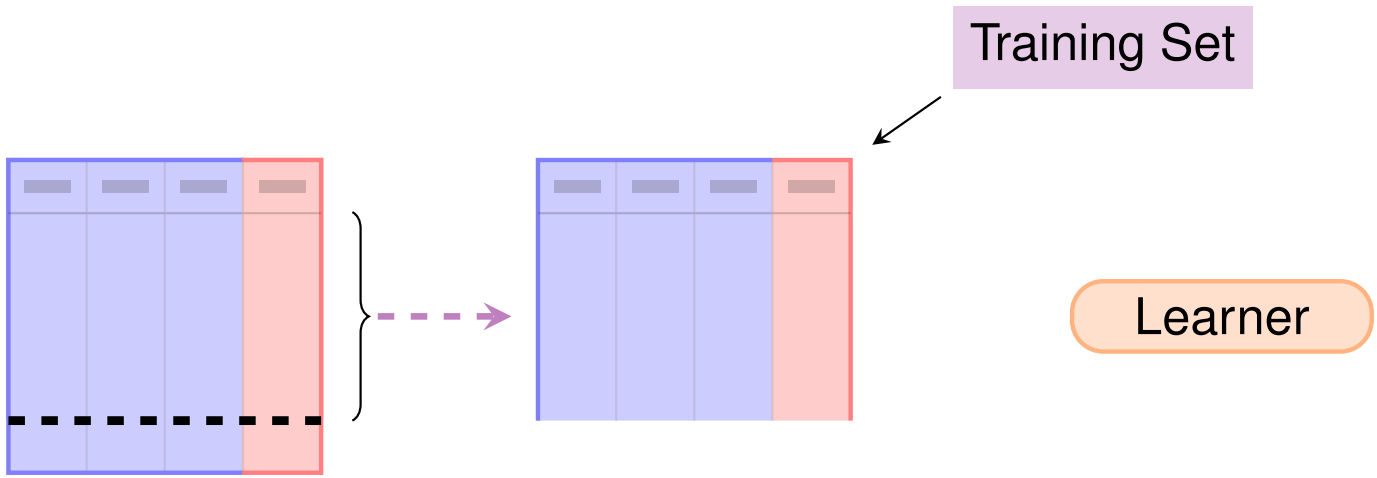
Learner

RESAMPLING



Learner

RESAMPLING



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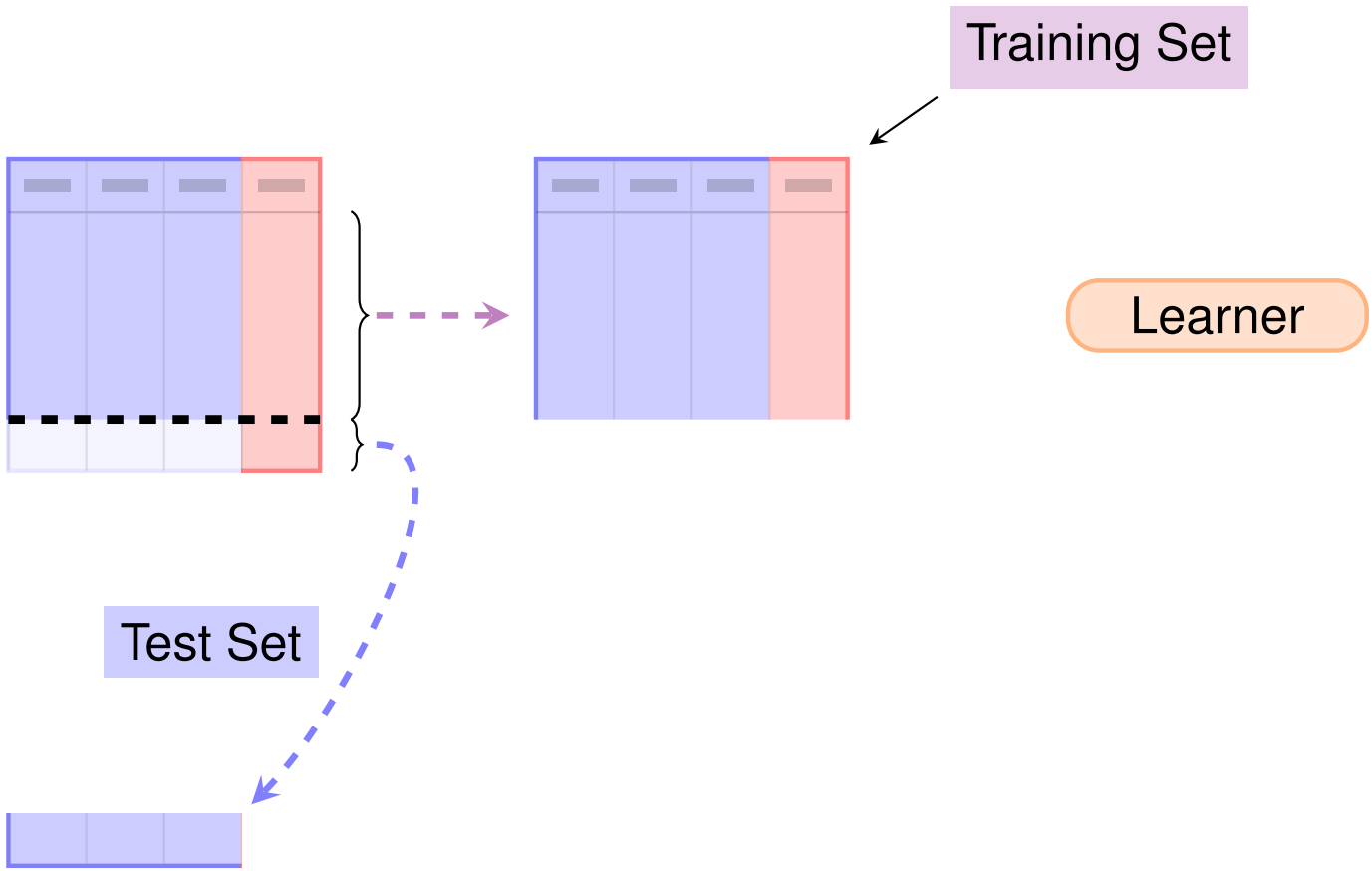

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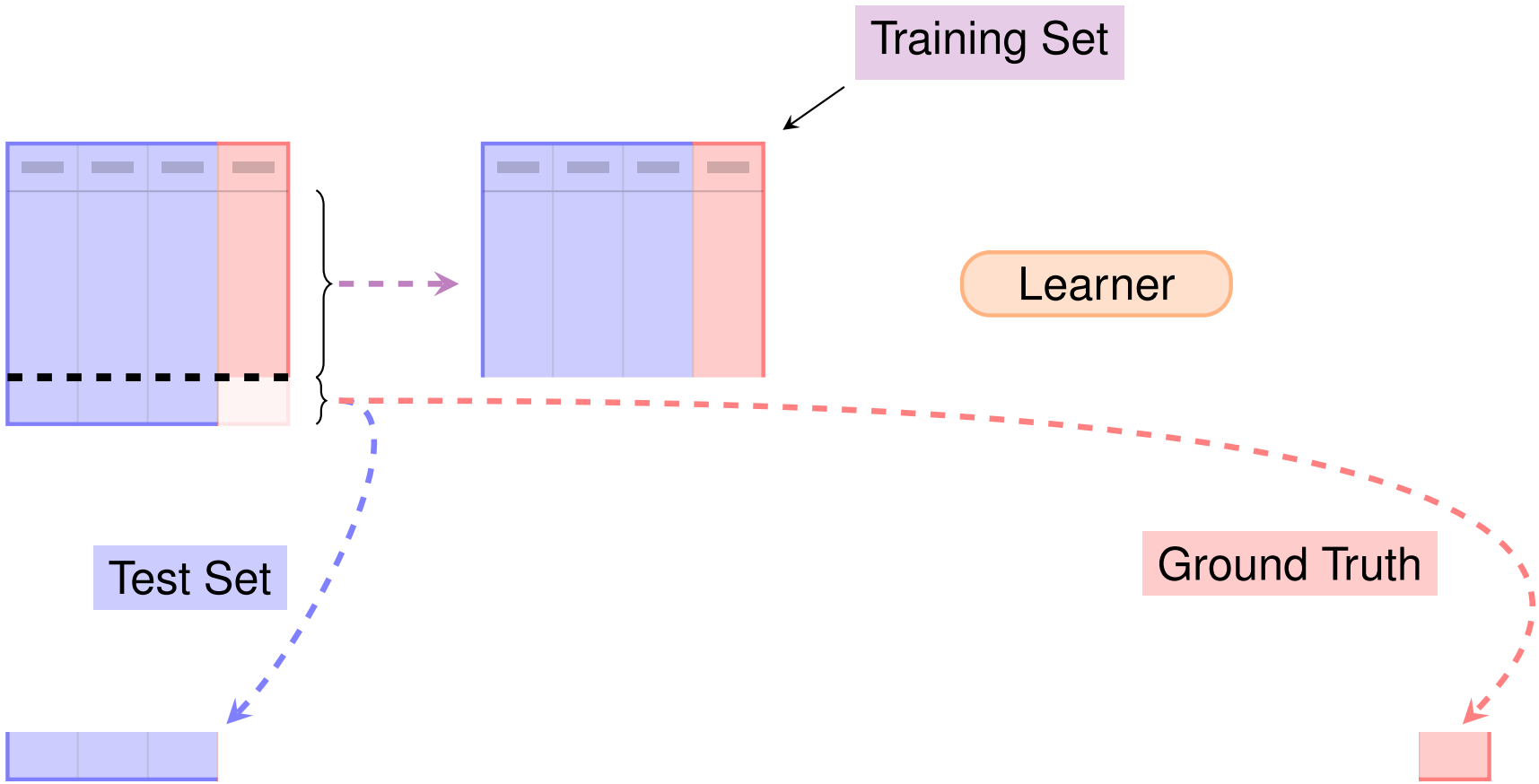

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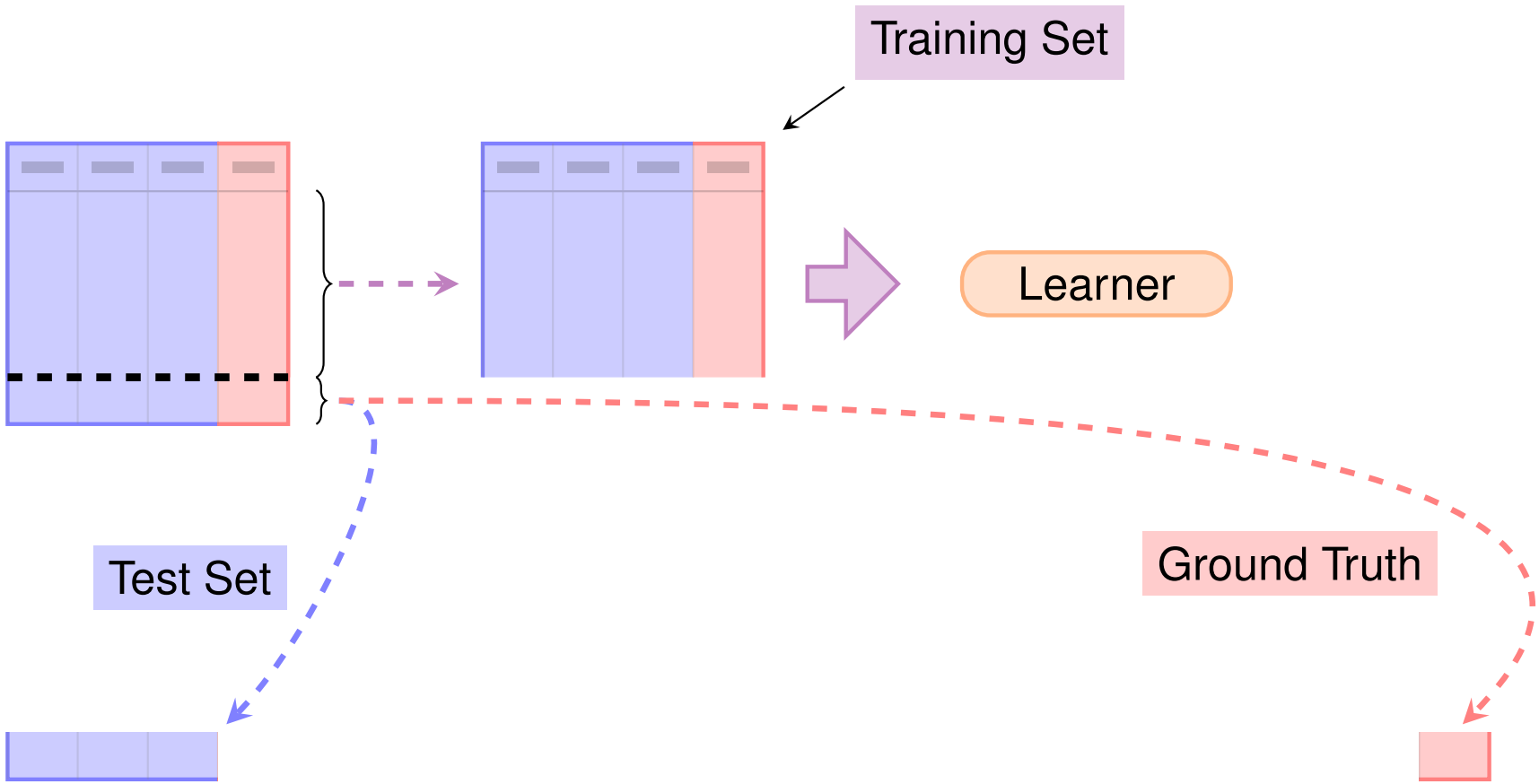

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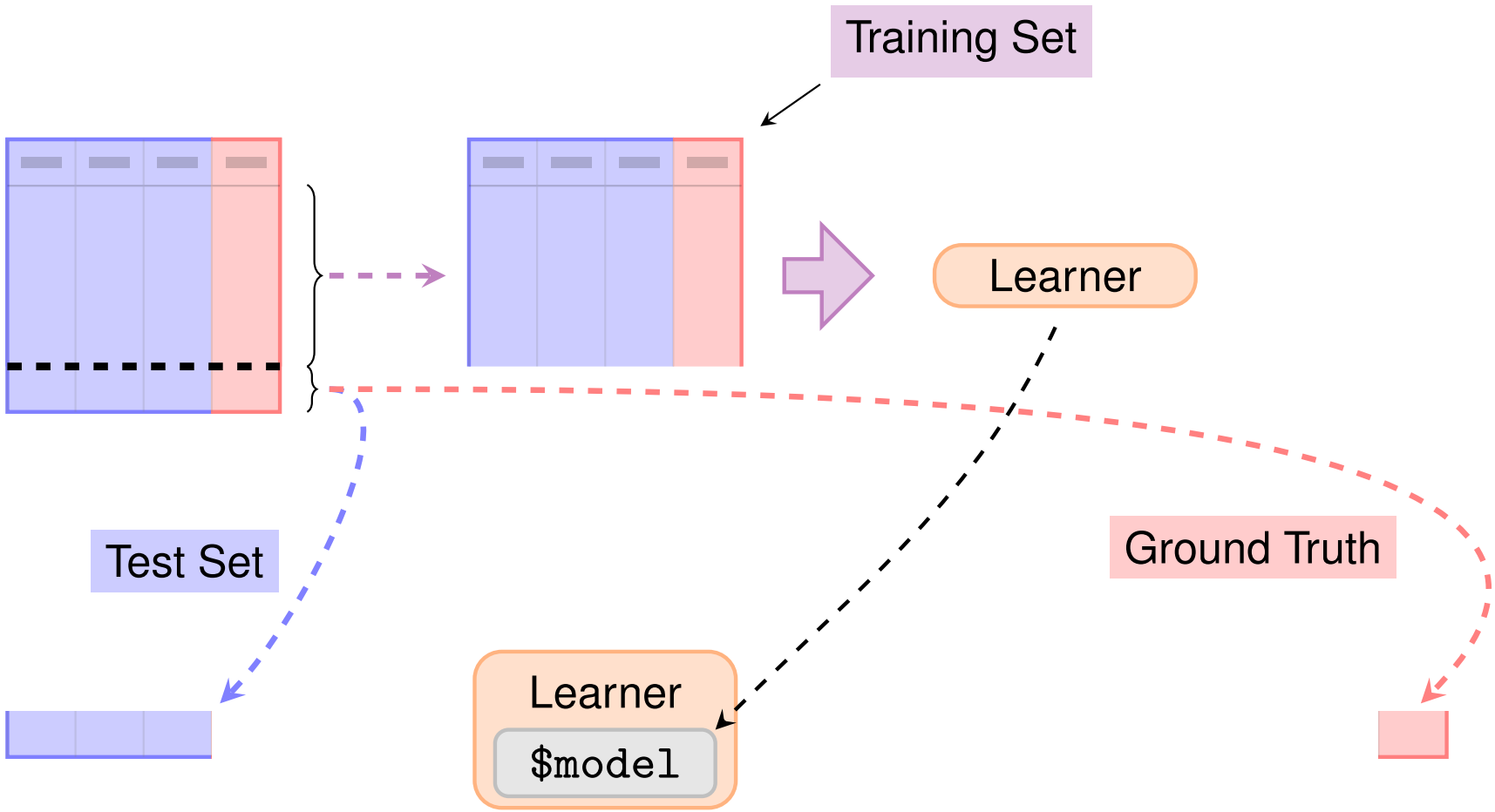

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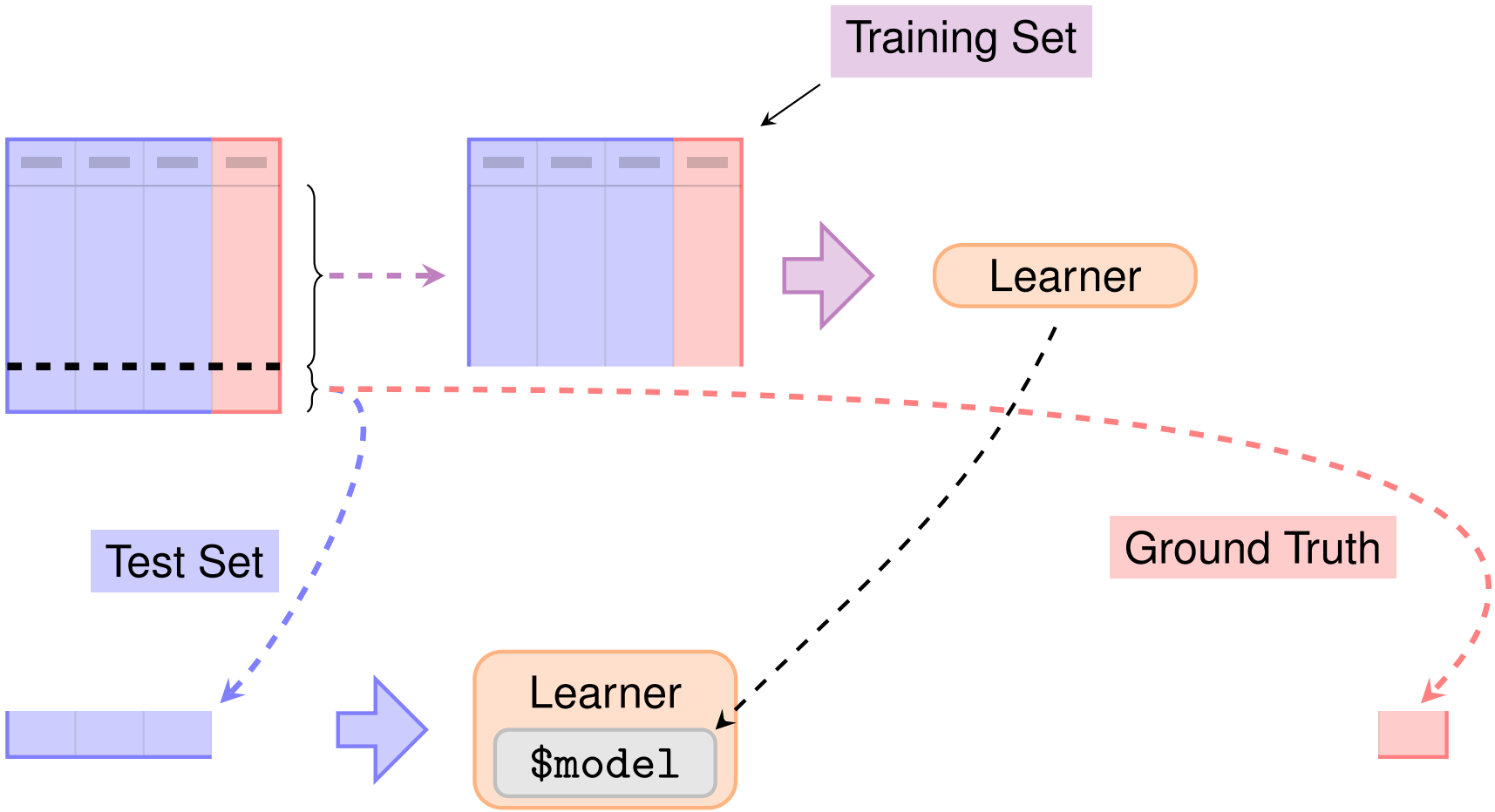

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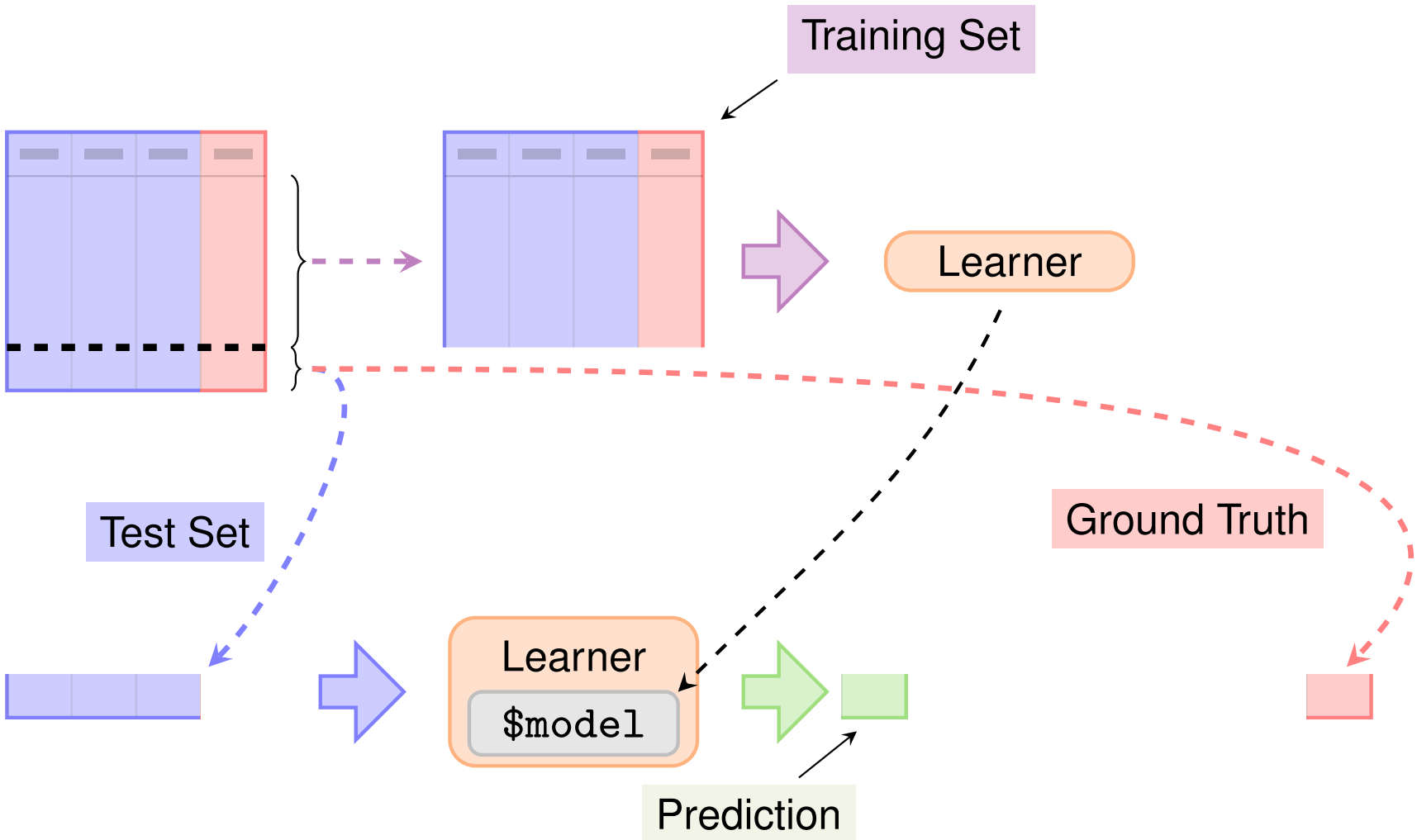
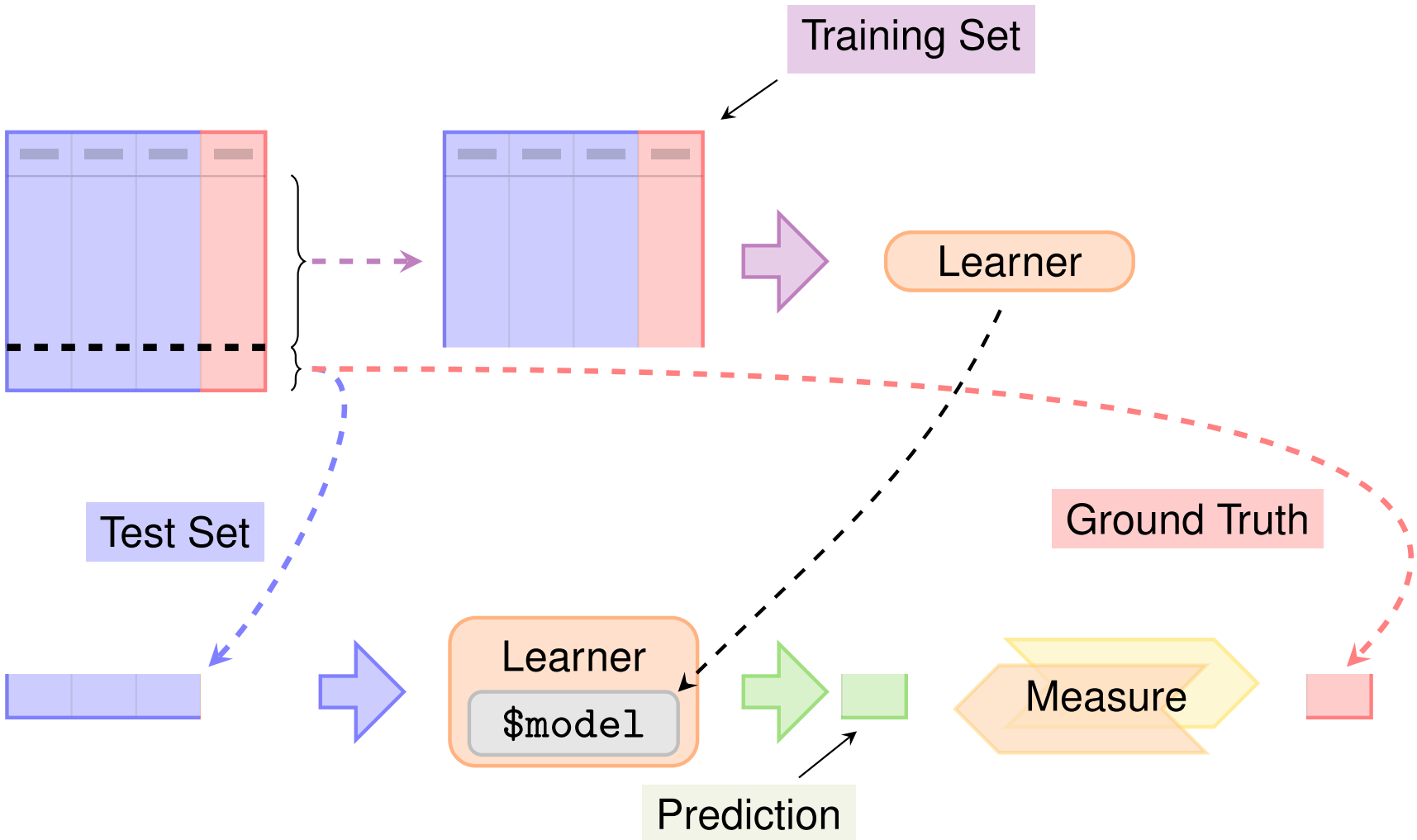
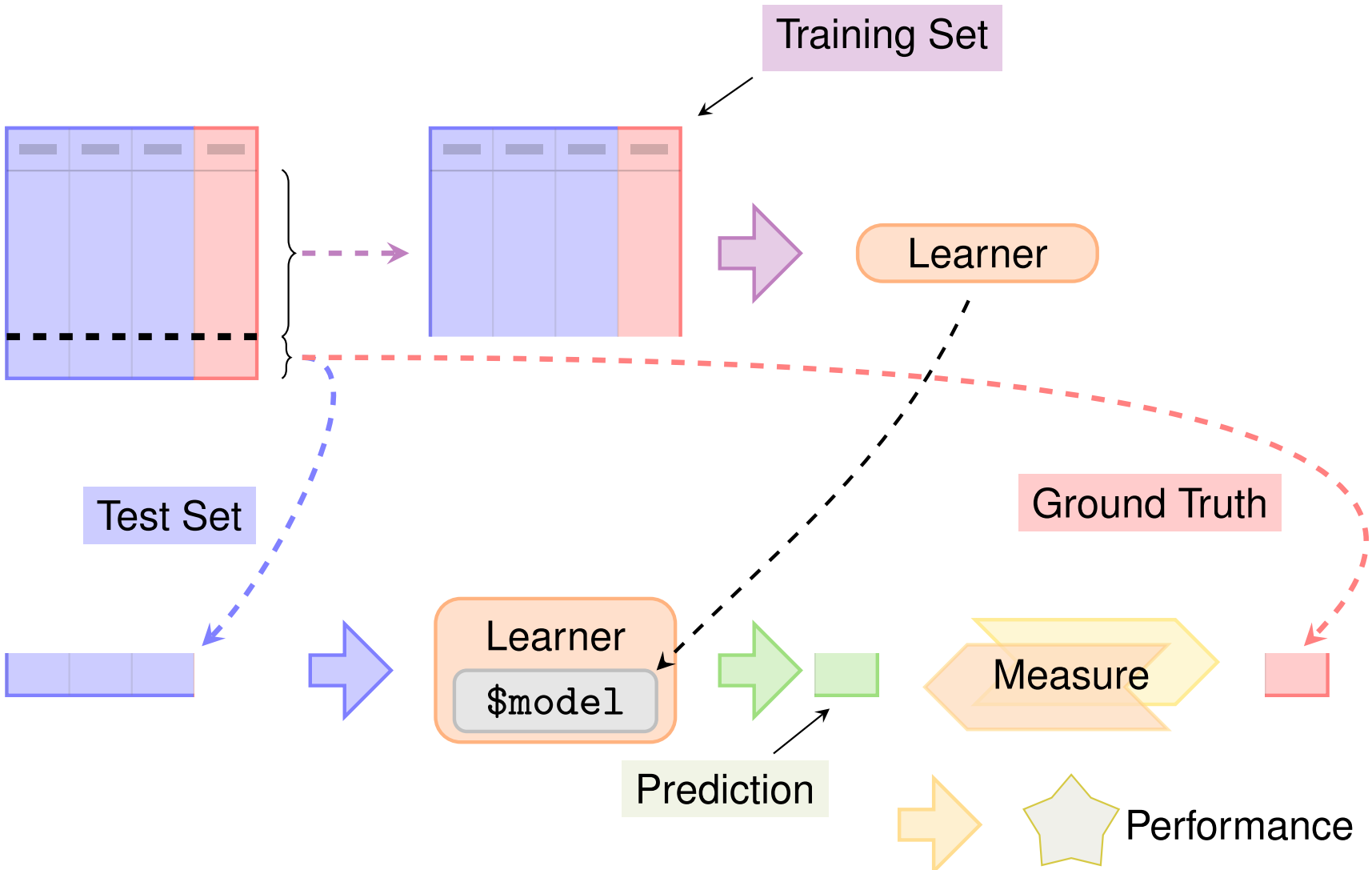

Training Set
Learner
Test Set
Ground Truth
Learner
$model
Prediction

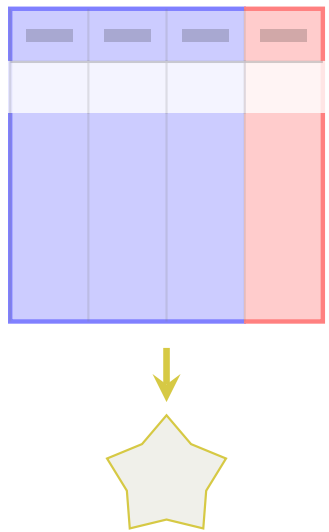
RESAMPLING


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



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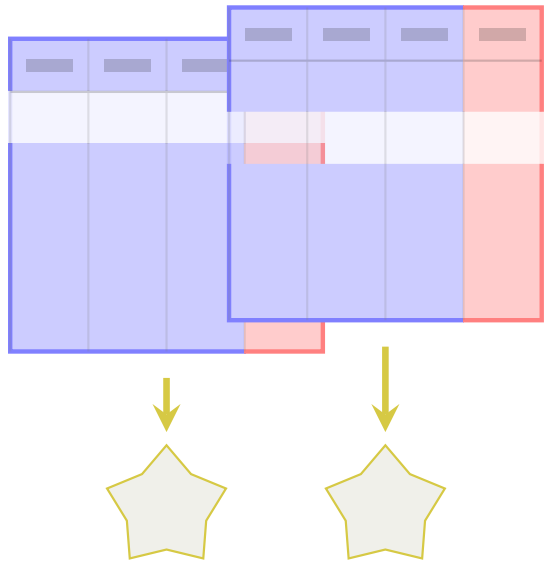

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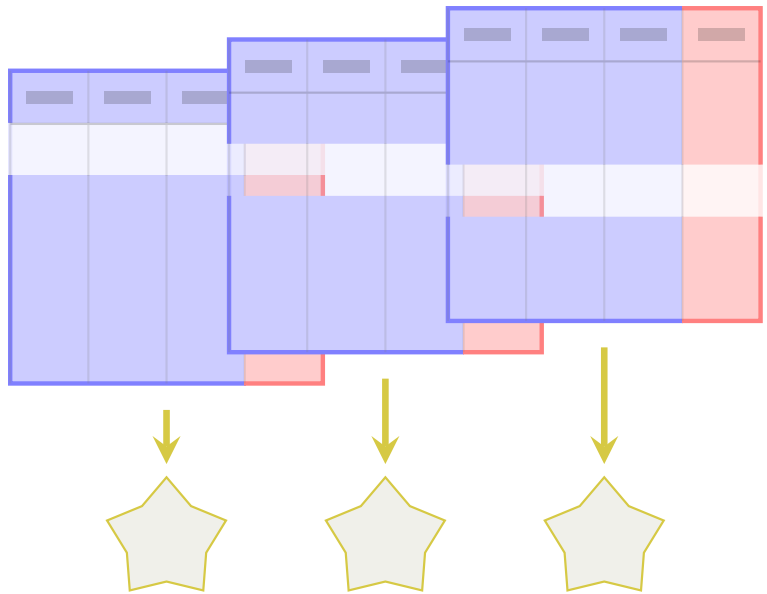

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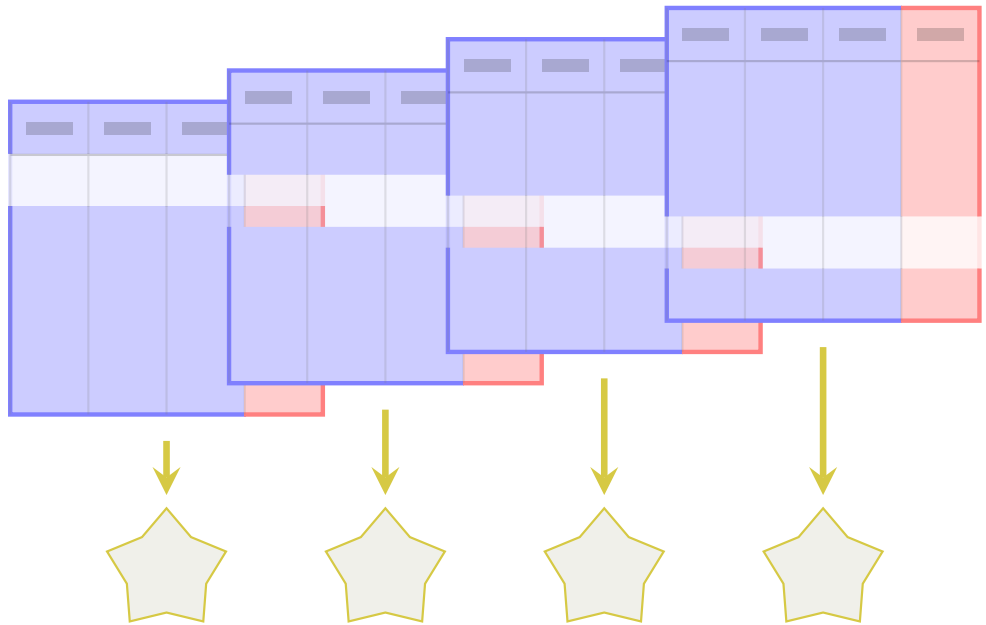

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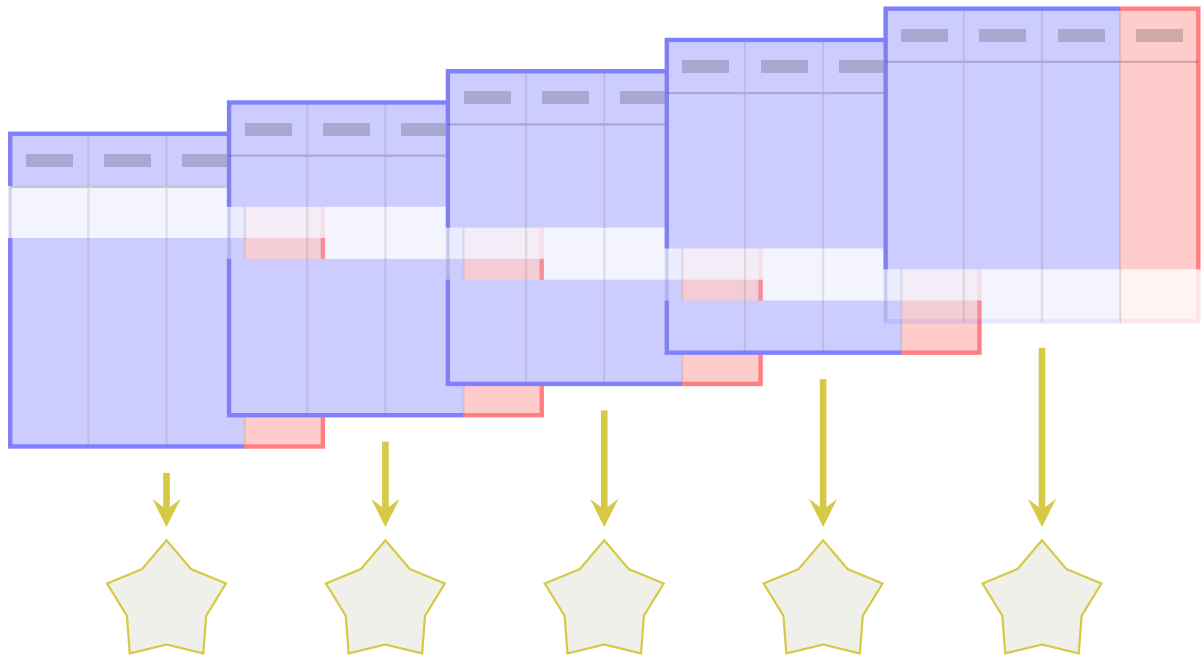

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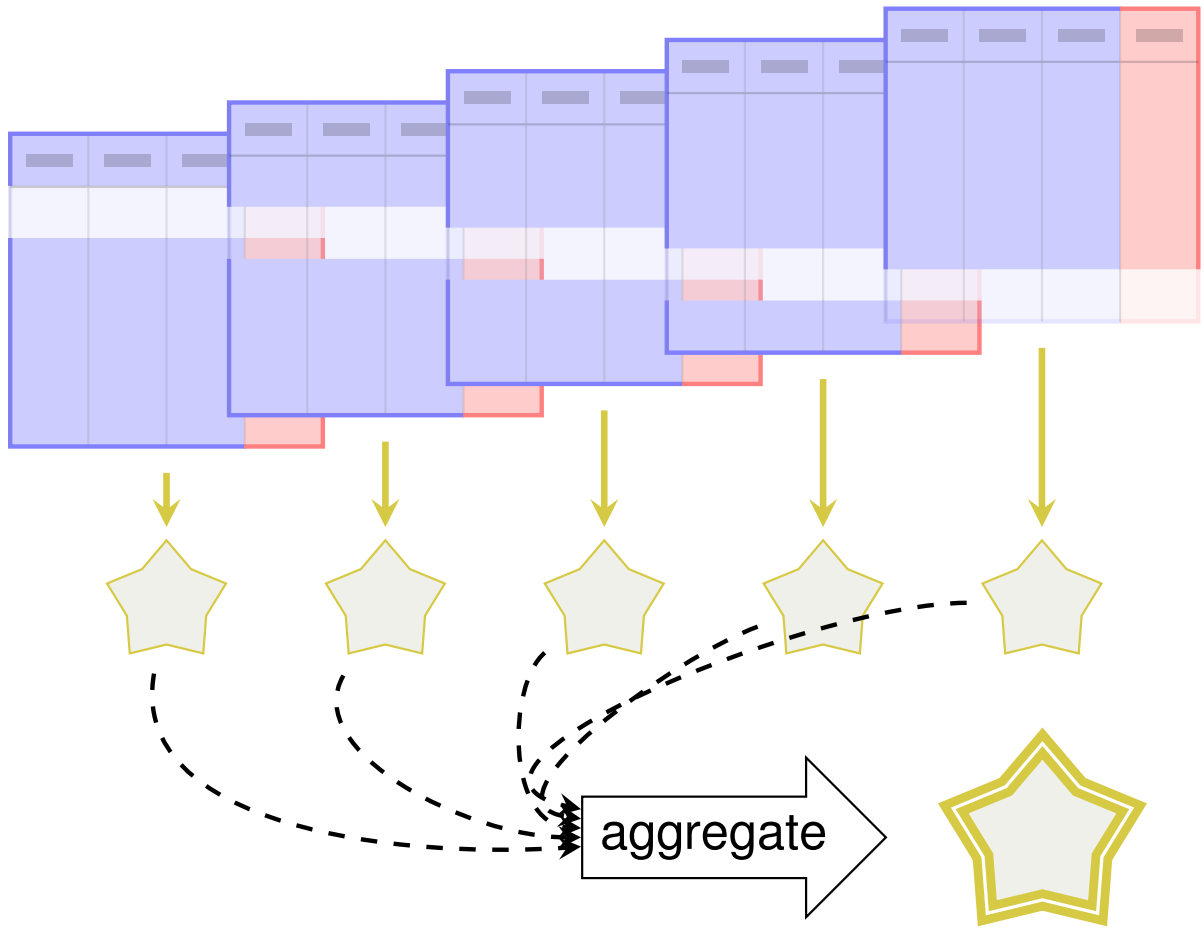
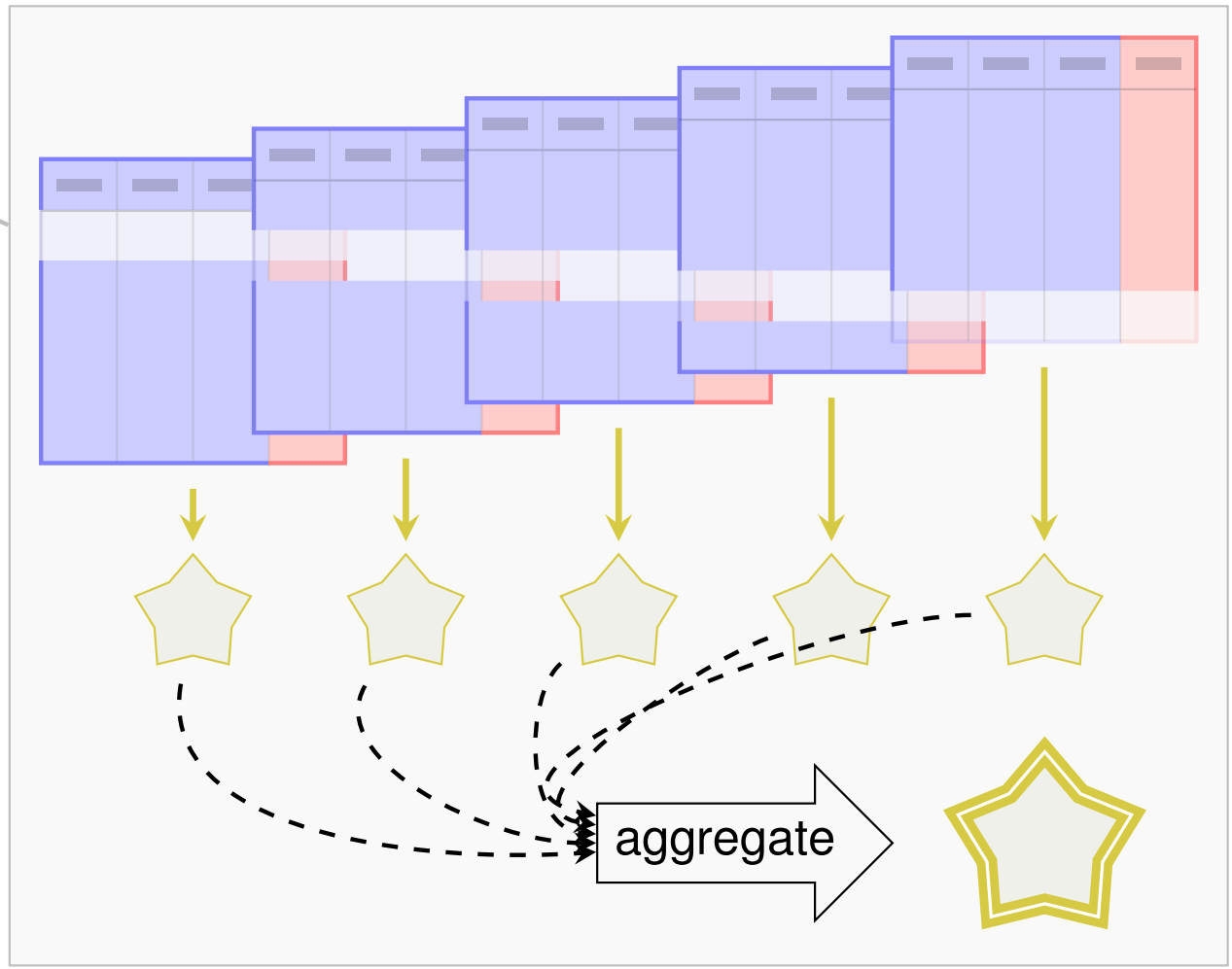


RESAMPLING

`resample()`



RESAMPLING

- Resample description: How to split the data

```
cv5 = rsmp("cv", folds = 5)
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- Use the `resample()` function for resampling:

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task = TaskClassif$new("iris", iris, "Species")
learner = lrn("classif.rpart")
rr = resample(task, learner, cv5)
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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

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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
# 1: <TaskClassif[45]> <LearnerClassifRpart[34]> <ResamplingCV[19]>
# 2: <TaskClassif[45]> <LearnerClassifRpart[34]> <ResamplingCV[19]>
# 3: <TaskClassif[45]> <LearnerClassifRpart[34]> <ResamplingCV[19]>
# 4: <TaskClassif[45]> <LearnerClassifRpart[34]> <ResamplingCV[19]>
# 5: <TaskClassif[45]> <LearnerClassifRpart[34]> <ResamplingCV[19]>
#    iteration              prediction
# 1:         1 <PredictionClassif[19]>
# 2:         2 <PredictionClassif[19]>
# 3:         3 <PredictionClassif[19]>
# 4:         4 <PredictionClassif[19]>
# 5:         5 <PredictionClassif[19]>
```

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```

- Active bindings and functions that make information easily accessible

RESAMPLING RESULTS

- Calculate performance:

```
rr$aggregate(msr("classif.ce"))
#> classif.ce
#>       0.06
```

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```
rr$aggregate(msr("classif.ce"))
#> classif.ce
#>       0.06
```

- Get predictions

```
rr$prediction()
#> <PredictionClassif> for 150 observations:
#>     row_id     truth  response
#>          3    setosa    setosa
#>          8    setosa    setosa
#>         10    setosa    setosa
#> ---
#>        143 virginica virginica
#>        144 virginica virginica
#>        145 virginica virginica
```

RESAMPLING

- Predictions of individual folds

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

```
#> <PredictionClassif> for 30 observations:
#>     row_id     truth  response
#>          3    setosa    setosa
#>          8    setosa    setosa
#>         10    setosa    setosa
#> ---
#>        136 virginica virginica
#>        140 virginica virginica
#>        142 virginica virginica
```

RESAMPLING

- Predictions of individual folds

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predictions = rr$predictions()
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```

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#>          3    setosa    setosa
#>          8    setosa    setosa
#>         10    setosa    setosa
#> ---
#>        136 virginica virginica
#>        140 virginica virginica
#>        142 virginica virginica
```

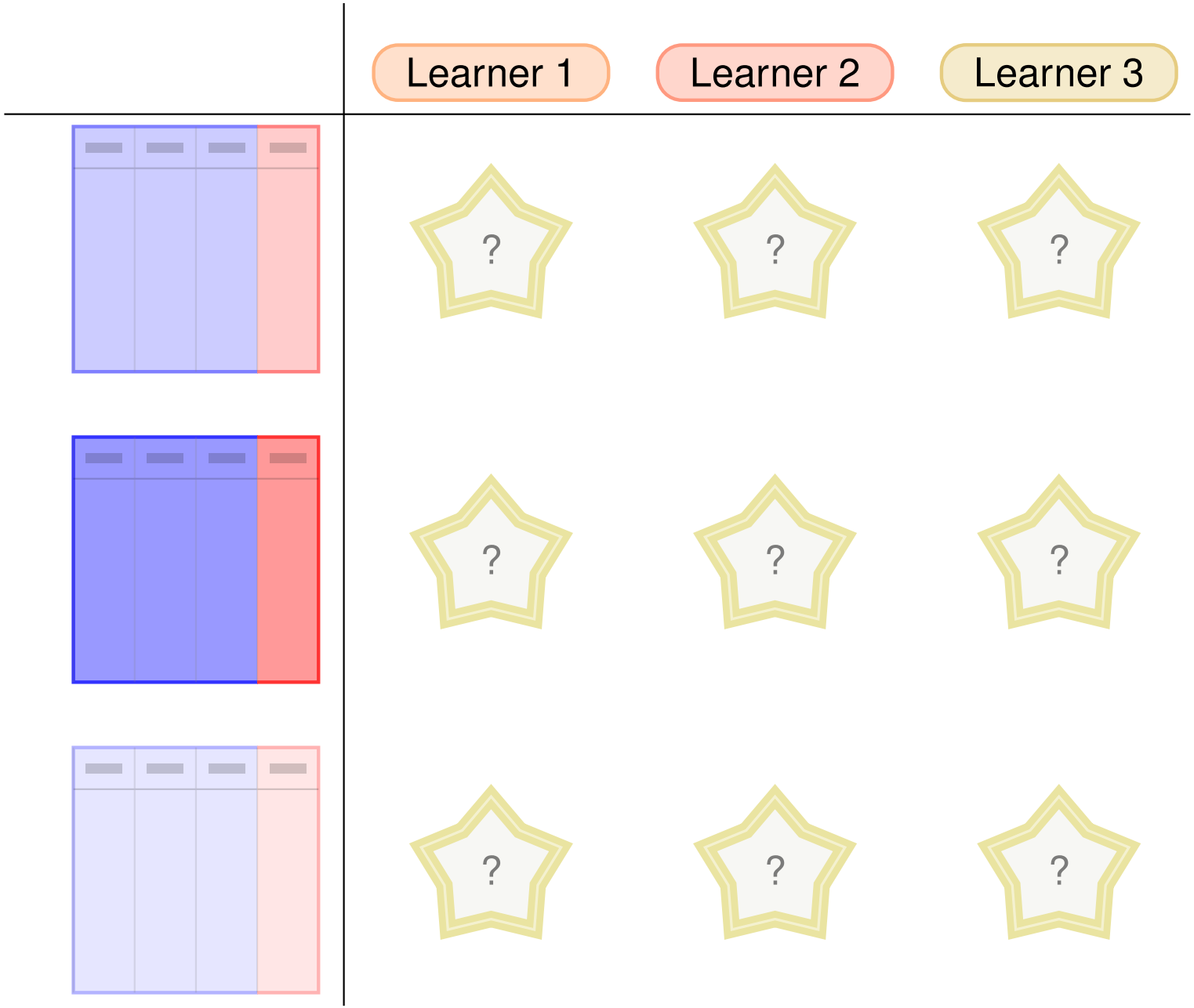
- Score of individual folds

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

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

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"))
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```

- 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      0.067
#> 2:    iris  classif.kknn      0.060
#> 3:   sonar classif.rpart      0.269
#> 4:   sonar  classif.kknn      0.164
#> 5:    wine classif.rpart      0.130
#> 6:    wine  classif.kknn      0.028
```

BENCHMARK RESULT

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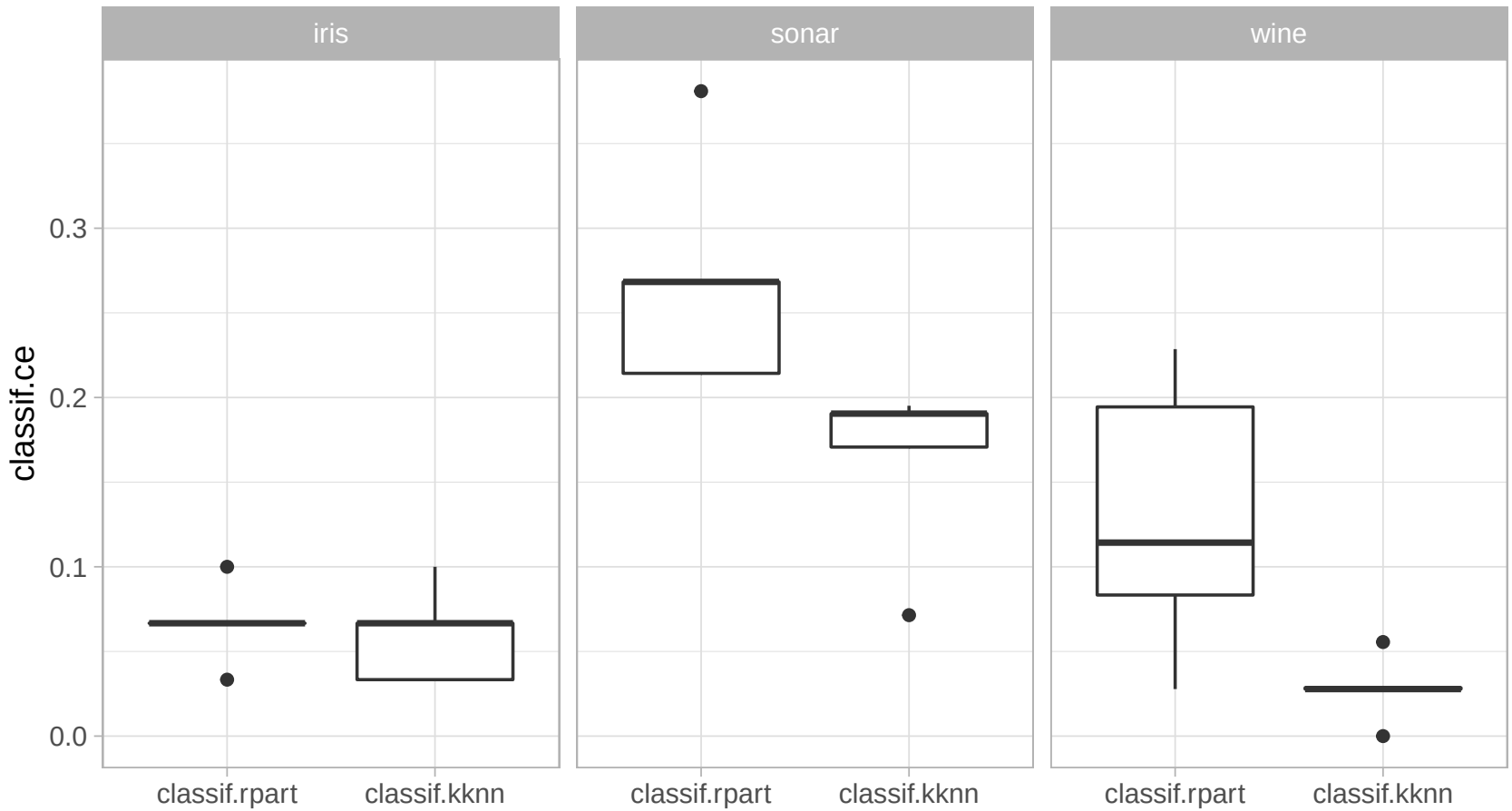
- Active bindings and functions that make information easily accessible

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**

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  - **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

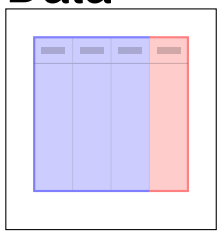
```
learner$help()
```

Outro

OVERVIEW

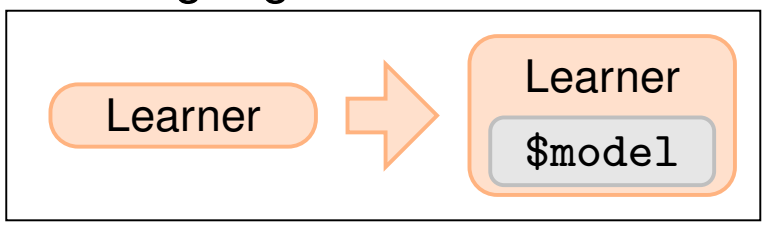
Ingredients:

Data



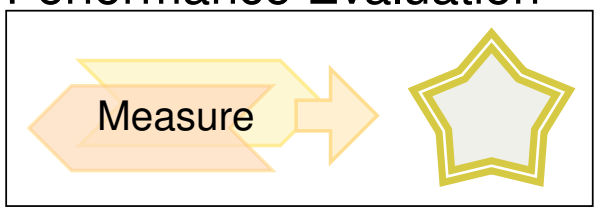
`TaskClassif`,
`TaskRegr`,
`tsk()`

Learning Algorithms



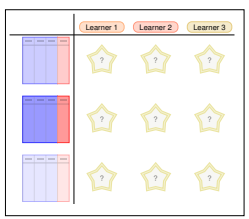
`lrn()` ⇒ `Learner`,
↪`Learner$train()`,
↪`Learner$predict()` ⇒ `Prediction`

Performance Evaluation



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

Performance Comparison



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