Hyperparameter Optimization

Foundations, Algorithms, Best Practices and Open Challenges

Martin Binder
LMU, MCML

Slides:
https://tinyurl.com/mlr3vfs

Modern Machine Learning in R

R-packages:

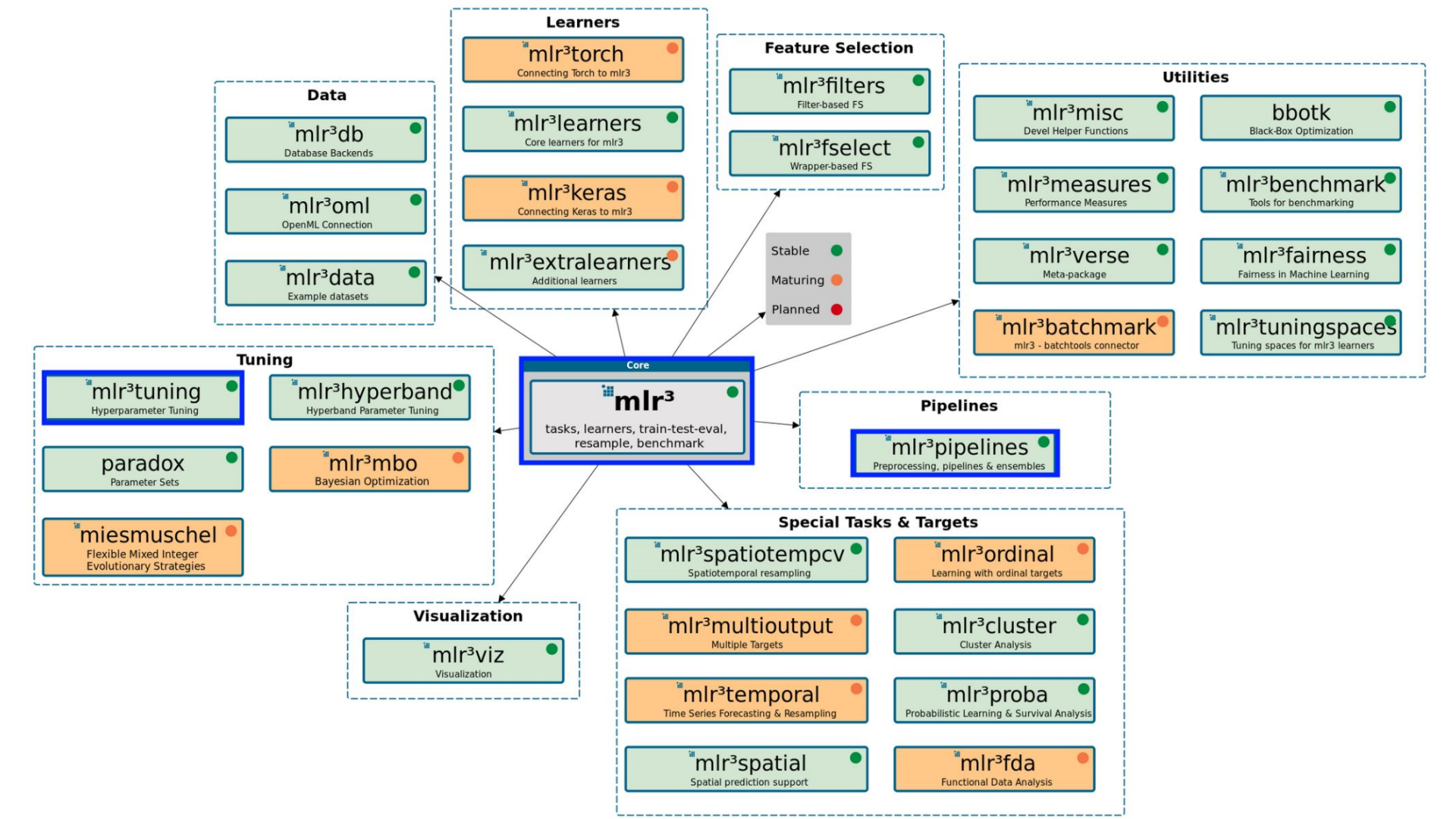
- **mlr3**
- **mlr3tuning**
- **mlr3pipelines**

(and others)

Modern Machine Learning in R

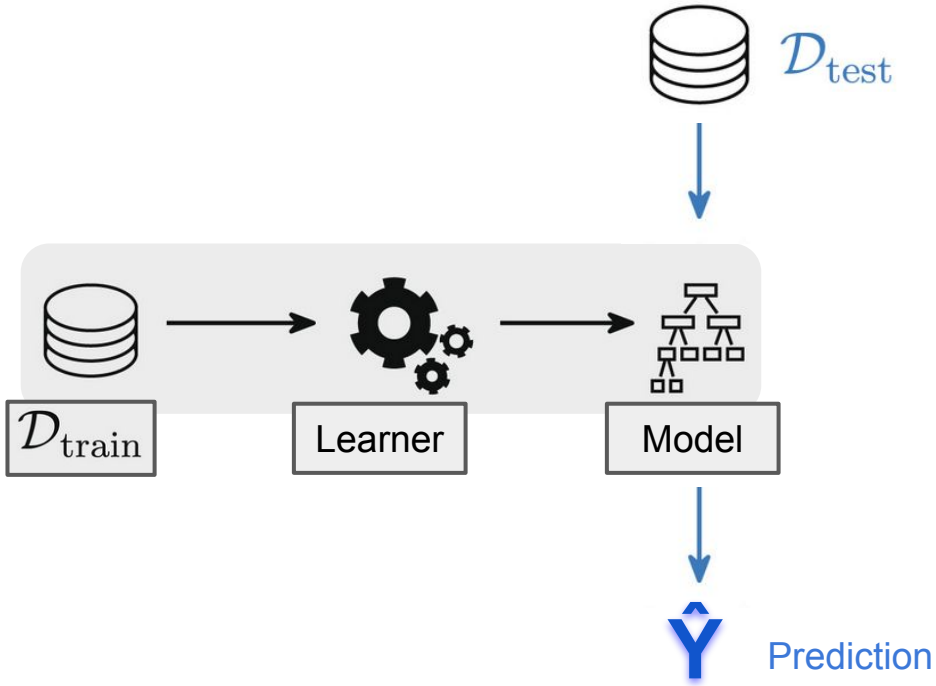
Principles of **`mlr3`**:

- Object oriented (R6)
  - algorithms are objects
  - ... with unified interfaces
  - ... that can be combined in a modular way
- Focus on AutoML
  - Hyperparameter-optimization
  - Machine-learning pipelines

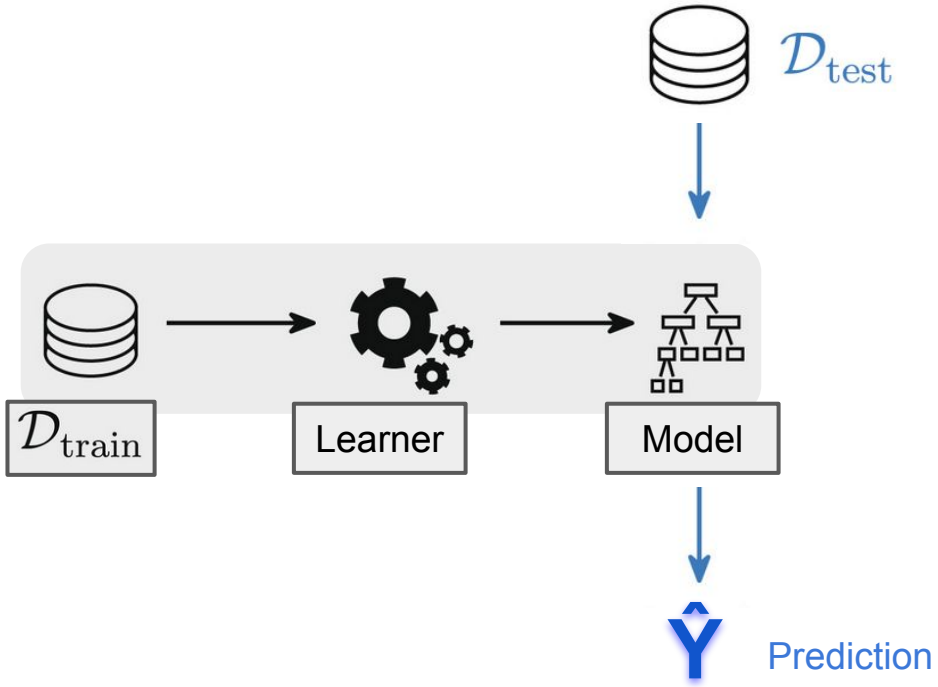

Learners
mlr³torch
Connecting Torch to mlr3
mlr³learners
Core learners for mlr3
mlr³keras
Connecting Keras to mlr3
mlr³extralearners
Additional learners
Feature Selection
mlr³filters
Filter-based FS
mlr³fselect
Wrapper-based FS
Utilities
mlr³misc
Devel Helper Functions
bbotk
Black-Box Optimization
mlr³measures
Performance Measures
mlr³benchmark
Tools for benchmarking
mlr³verse
Meta-package
mlr³fairness
Fairness in Machine Learning
mlr³batchmark
mlr3 - batchtools connector
mlr³tuningspaces
Tuning spaces for mlr3 learners
Data
mlr³db
Database Backends
mlr³oml
OpenML Connection
mlr³data
Example datasets
Stable
Maturing
Planned
Tuning
mlr³tuning
Hyperparameter Tuning
mlr³hyperband
Hyperband Parameter Tuning
paradox
Parameter Sets
mlr³mbo
Bayesian Optimization
miesmuschel
Flexible Mixed Integer
Evolutionary Strategies
Core
mlr³
tasks, learners, train-test-eval,
resample, benchmark
Pipelines
mlr³pipelines
Preprocessing, pipelines & ensembles
Visualization
mlr³viz
Visualization
Special Tasks & Targets
mlr³spatiotempcv
Spatiotemporal resampling
mlr³ordinal
Learning with ordinal targets
mlr³multioutput
Multiple Targets
mlr³cluster
Cluster Analysis
mlr³temporal
Time Series Forecasting & Resampling
mlr³proba
Probabilistic Learning & Survival Analysis
mlr³spatial
Spatial prediction support
mlr³fda
Functional Data Analysis

Machine Learning

Machine Learning



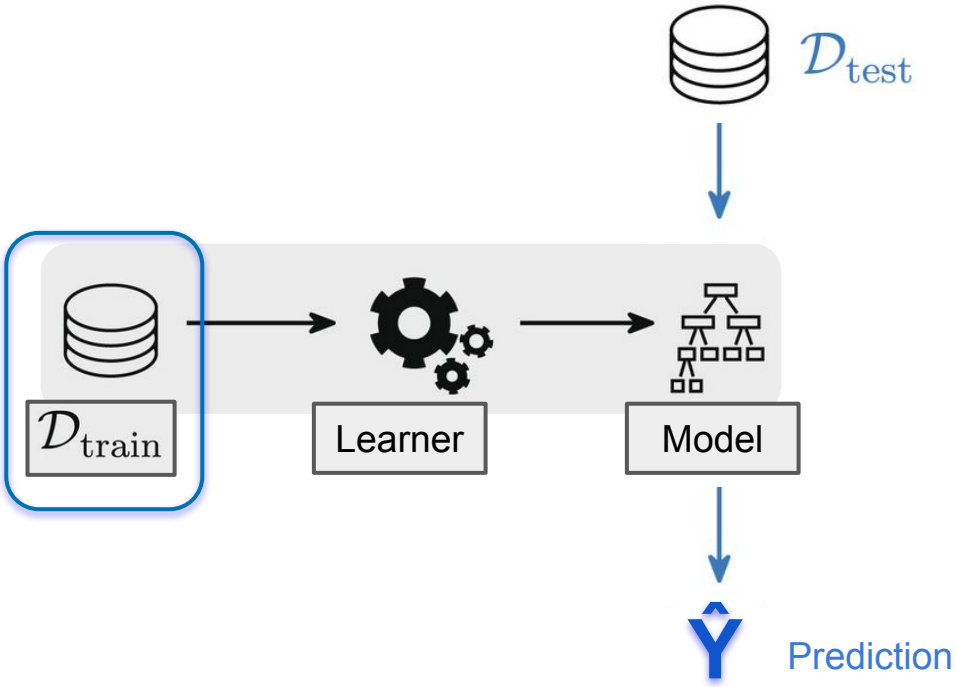
Machine Learning




```r
data("german", package = "rchallenge")

library("mlr3")
```

Machine Learning

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library("mlr3")

task <- as_task_classif(
  german,
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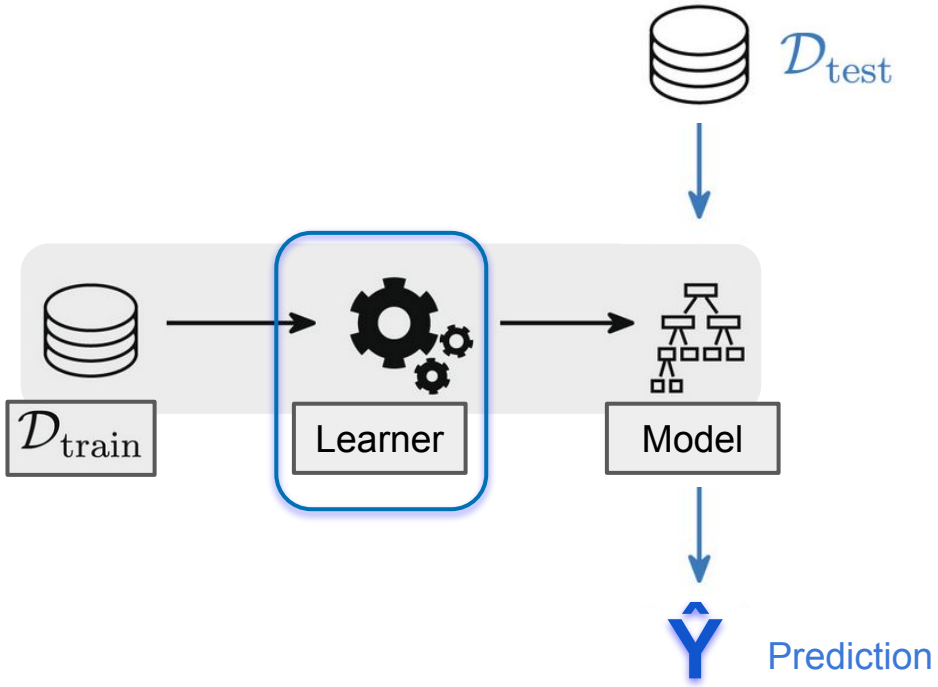
)
```

Machine Learning

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library("mlr3learners")
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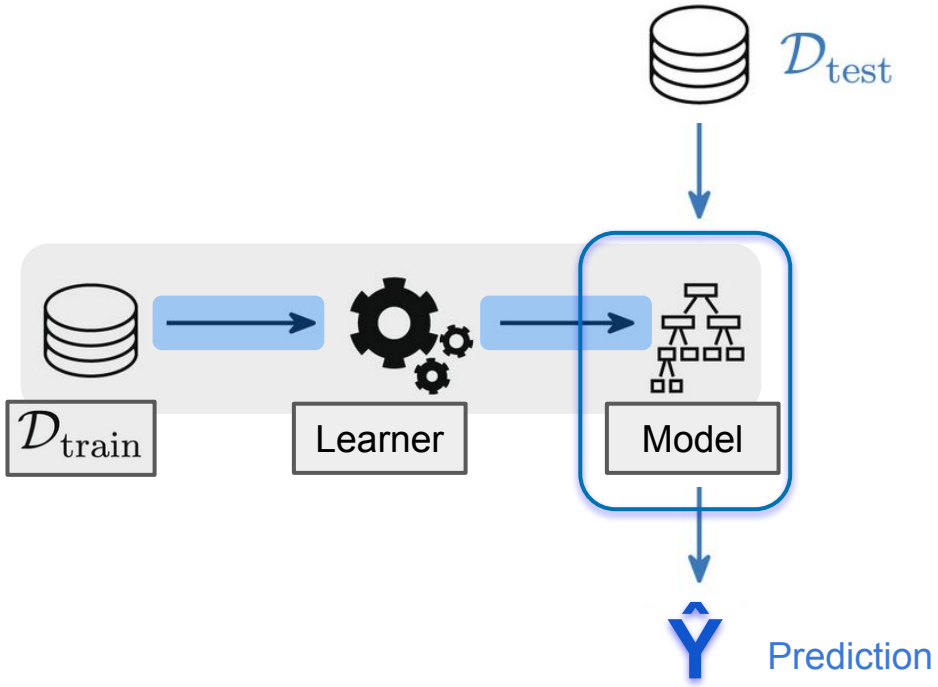
Machine Learning

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splits <- partition(task)
learner$train(task, row_ids = splits$train)
```
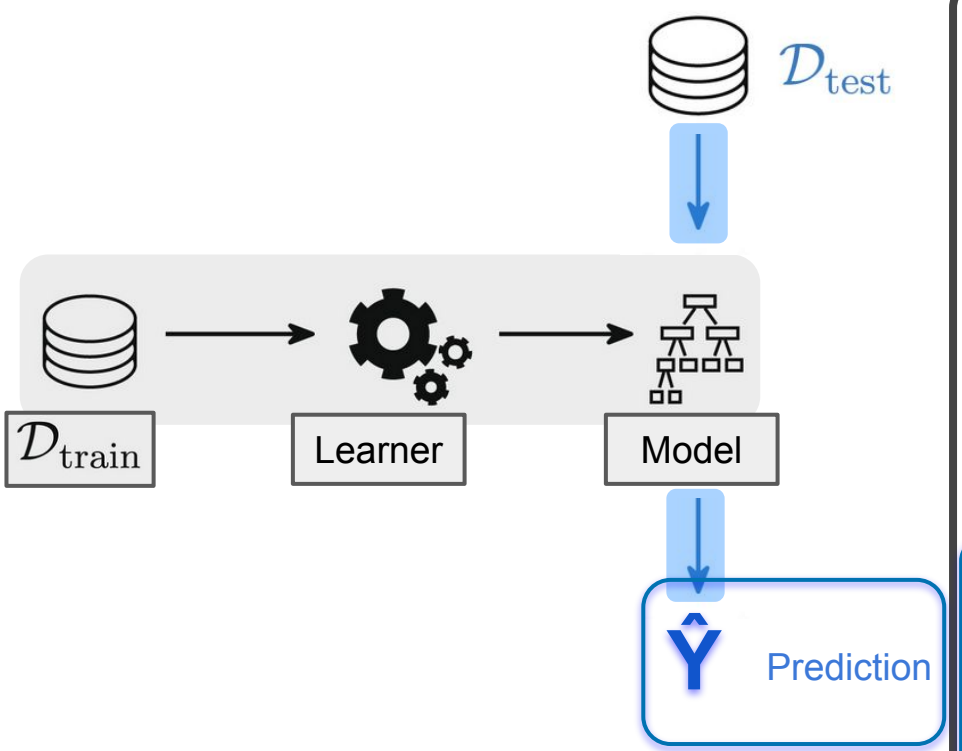

Machine Learning

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learner <- lrn("classif.kknn")

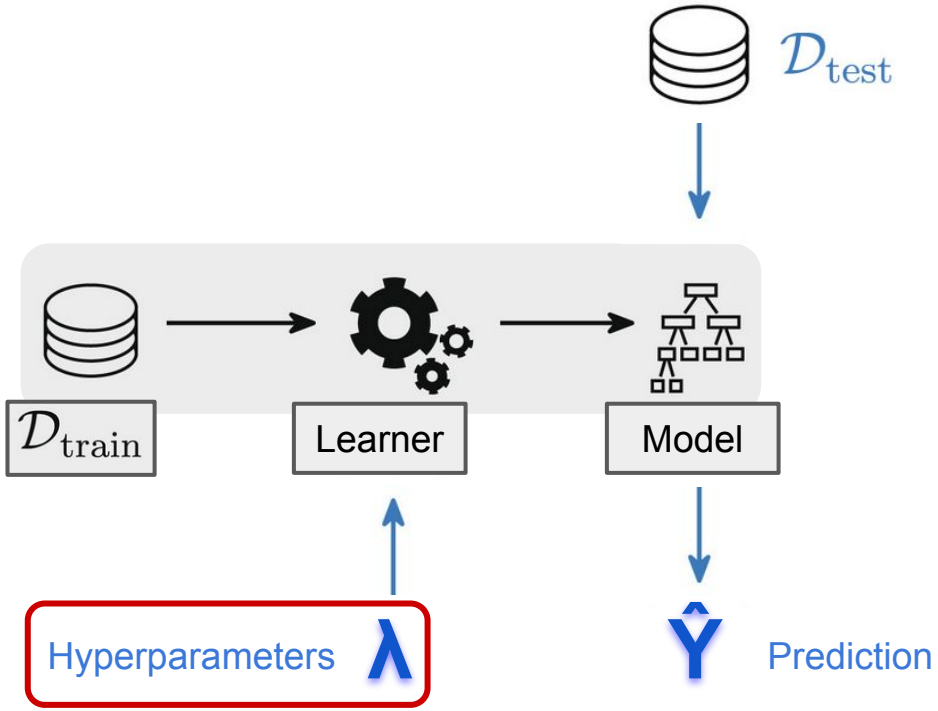
splits <- partition(task)
learner$train(task, row_ids = splits$train)

learner$predict(task, row_ids = splits$predict)
#> <PredictionClassif> for 1000 observations:
#>     row_ids truth response
#>           1  good     good
#>           2  good     good
#>           3  good     good
```

Machine Learning: It's Not That Easy

- Hyperparameters
- Preprocessing

Machine Learning -- Not That Easy (I)

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#> <PredictionClassif> for 1000 observations:
#>     row_ids truth response
#>           1  good     good
#>           2  good     good
#>           3  good     good
```
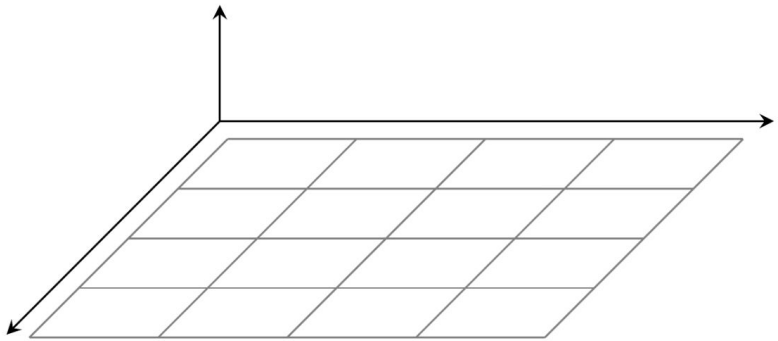
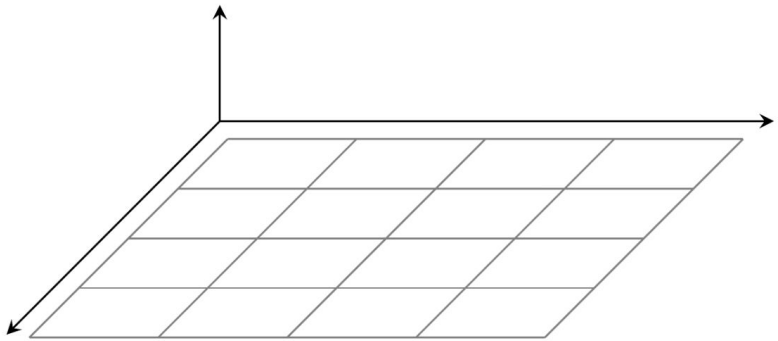

k = ?
other Methods?

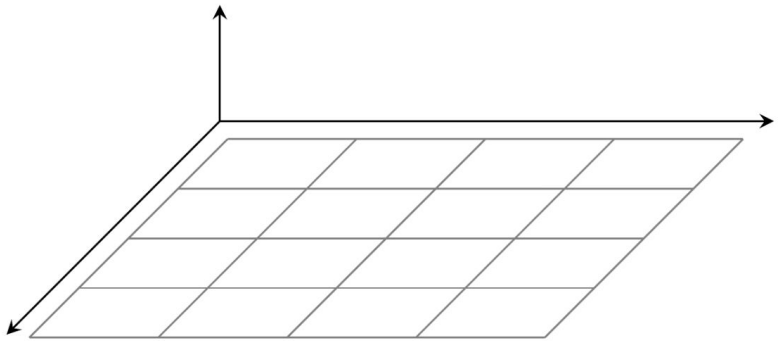
Hyperparameter Optimization

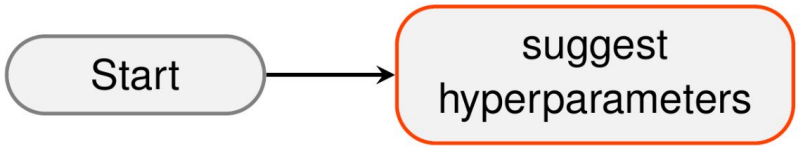
"Try out different values,
see what works best"

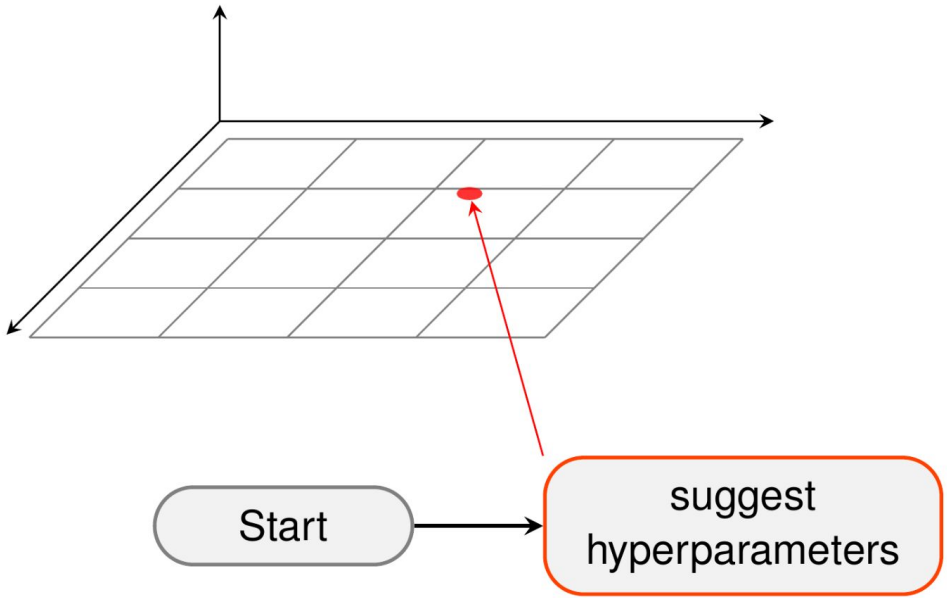


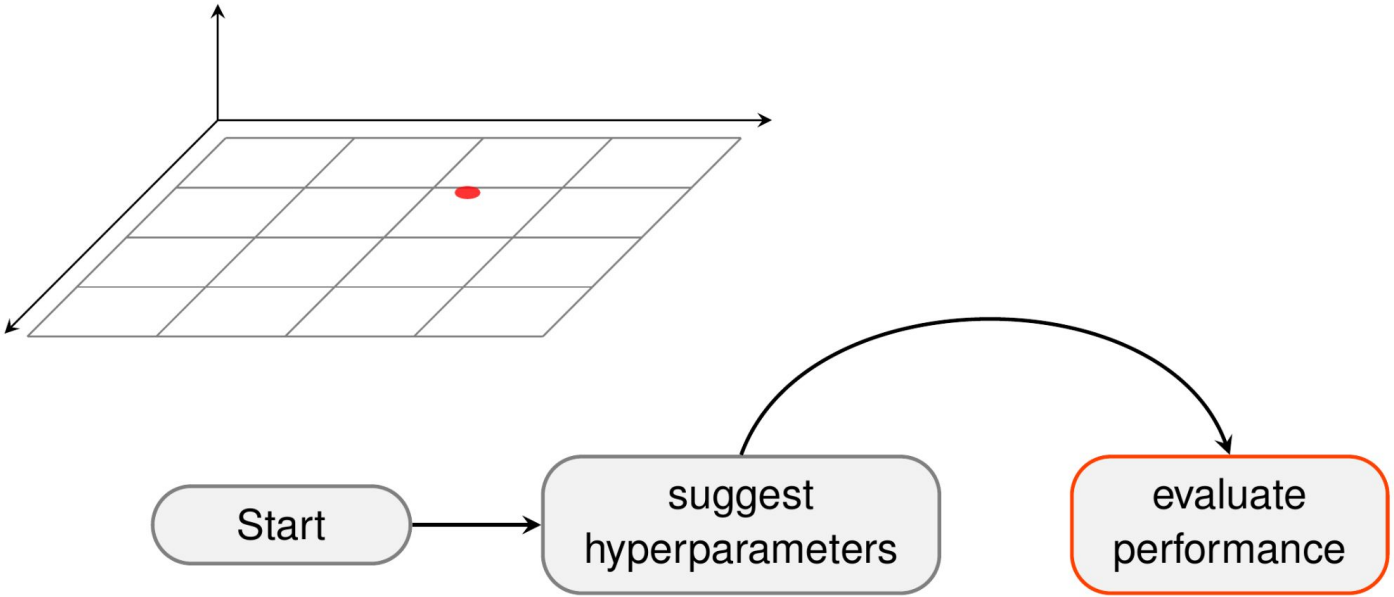


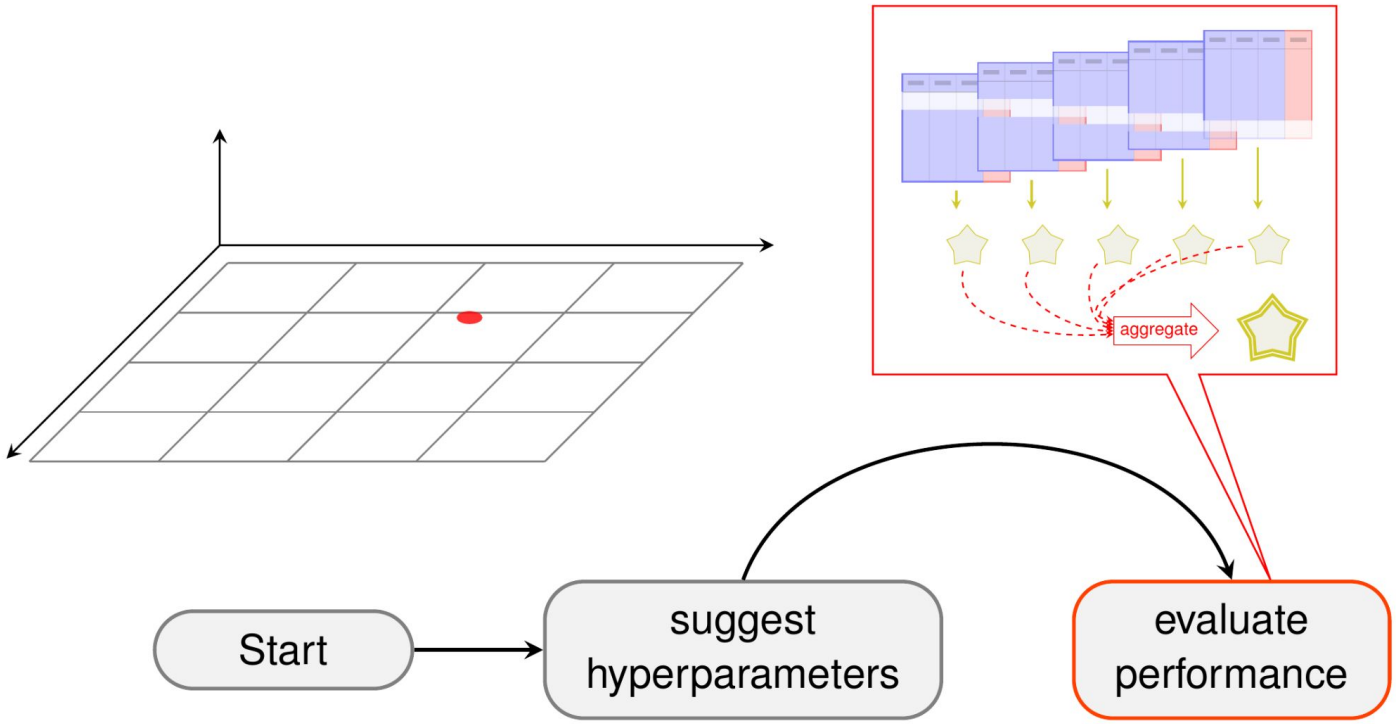
Start

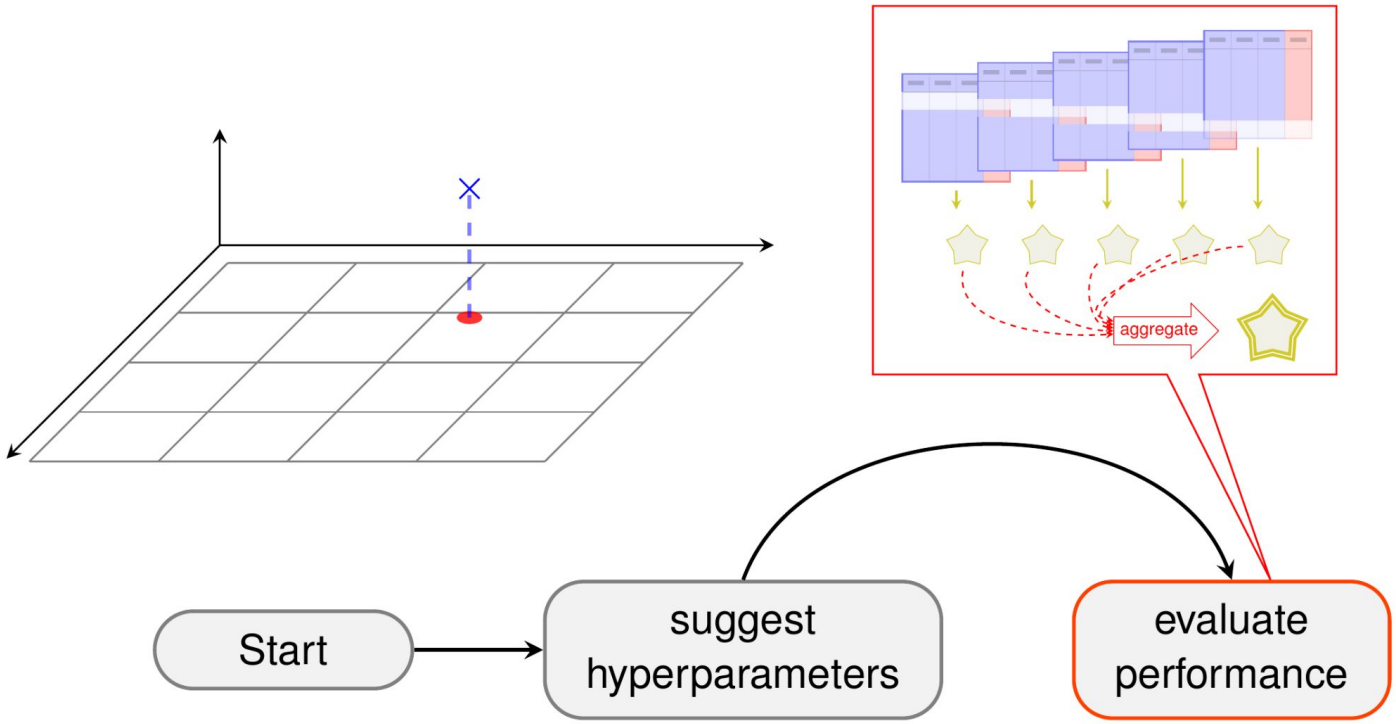



Start
suggest
hyperparameters


Start
suggest
hyperparameters


Start
suggest
hyperparameters
evaluate
performance


aggregate
Start
suggest
hyperparameters
evaluate
performance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Start
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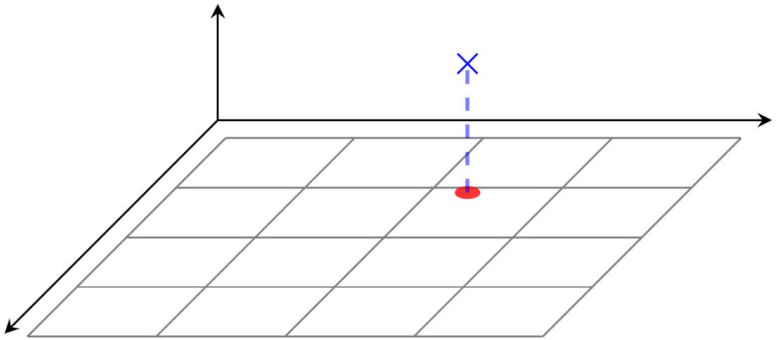

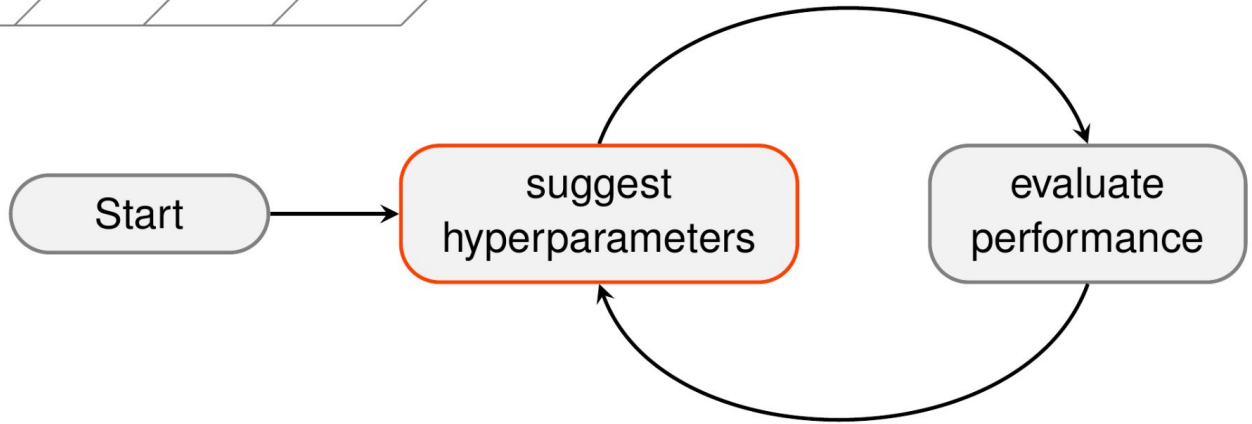
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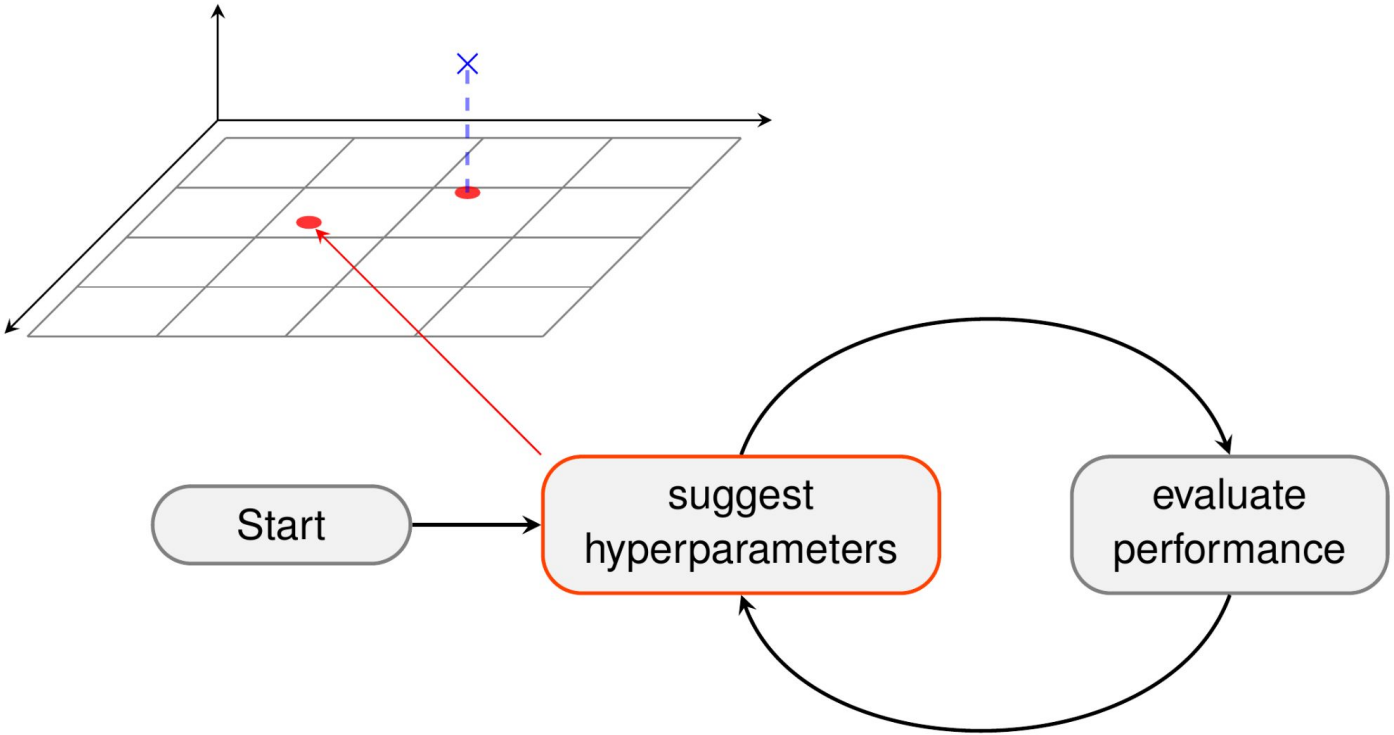
Start
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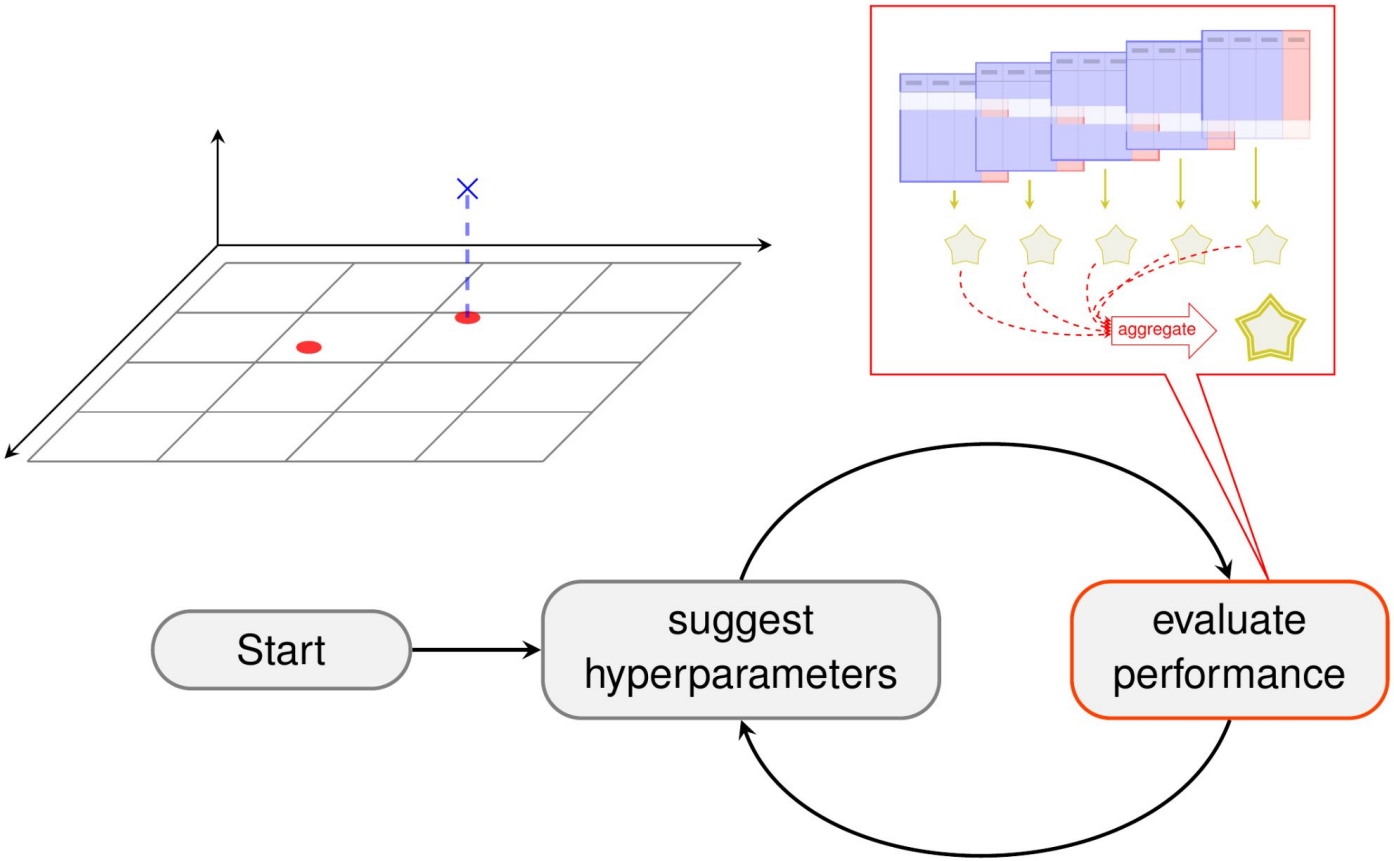
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Start
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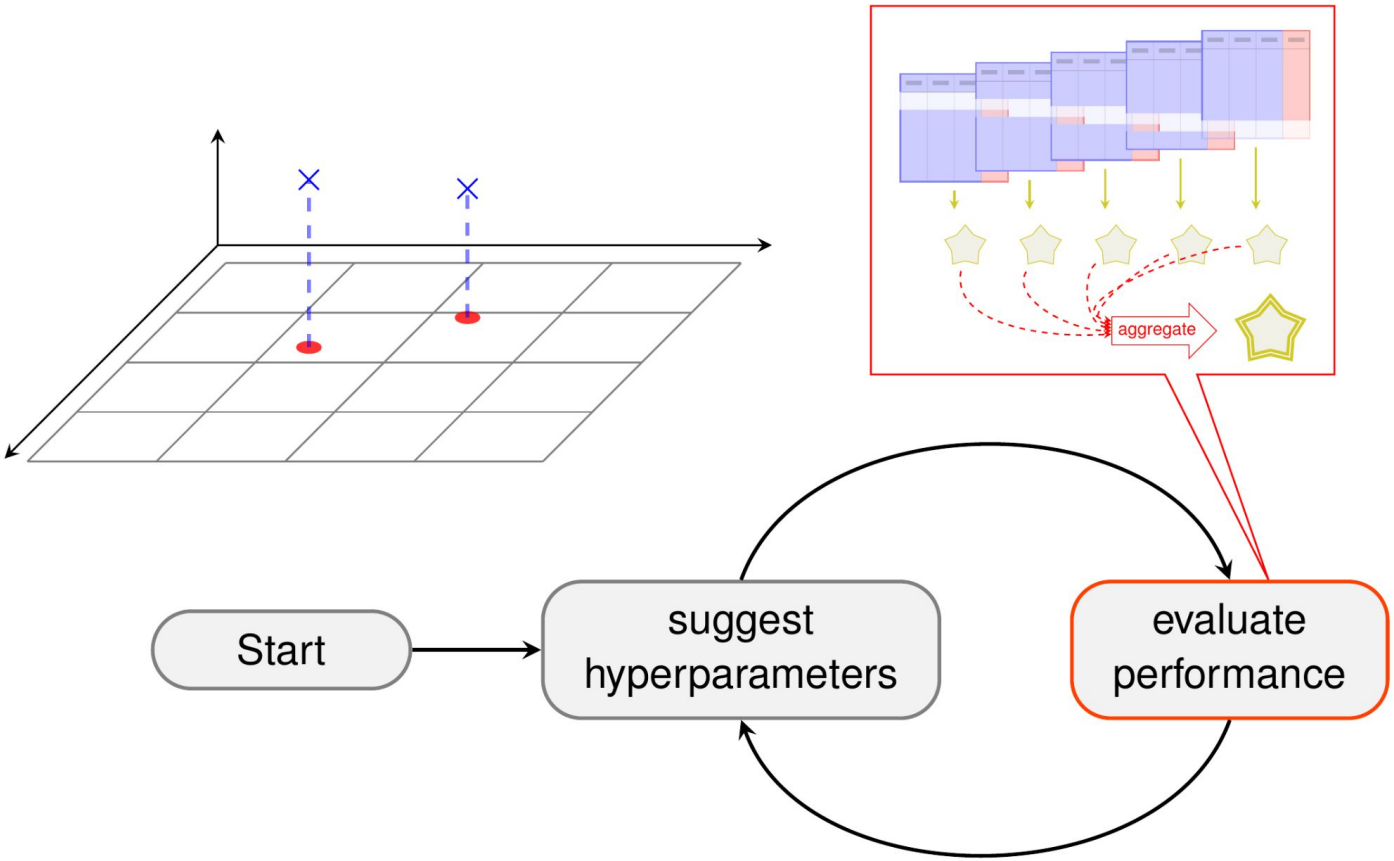
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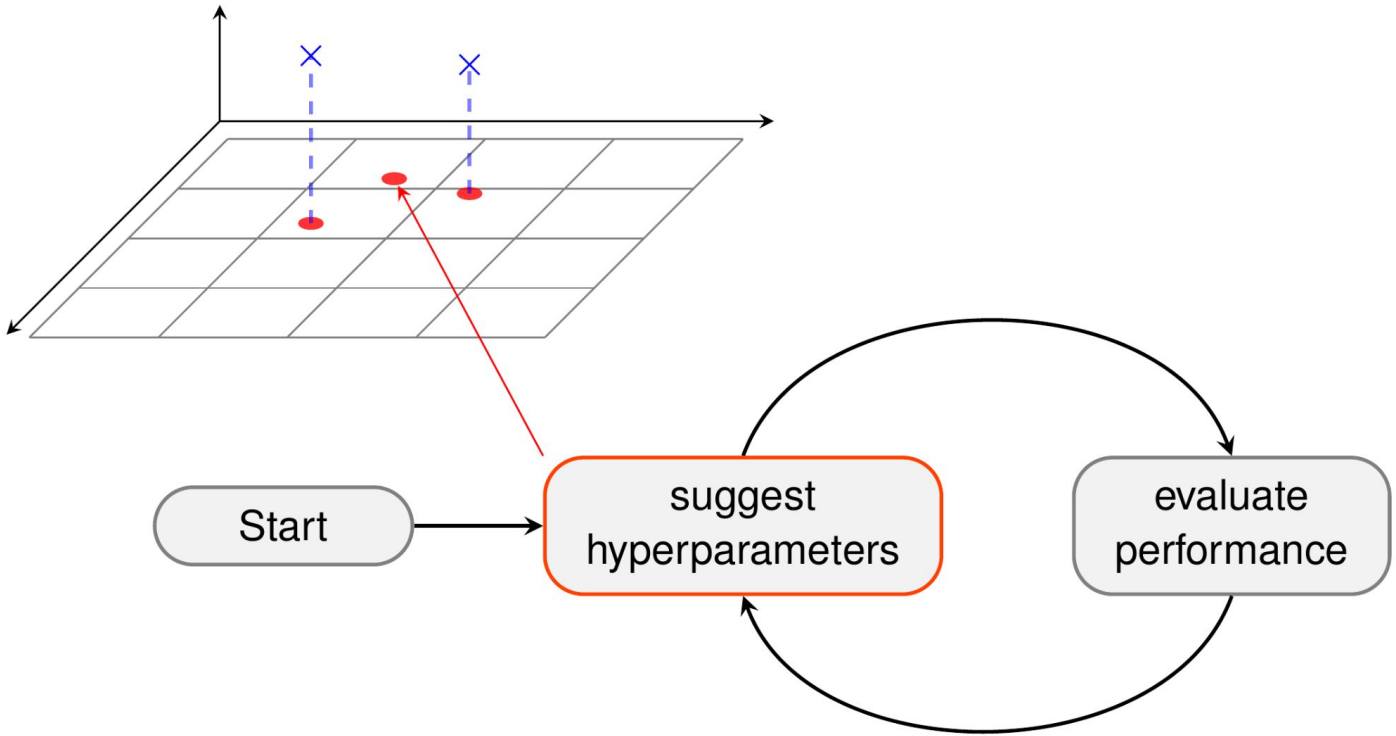
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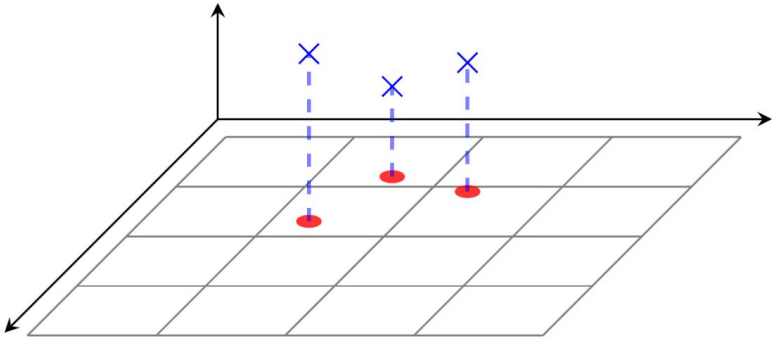

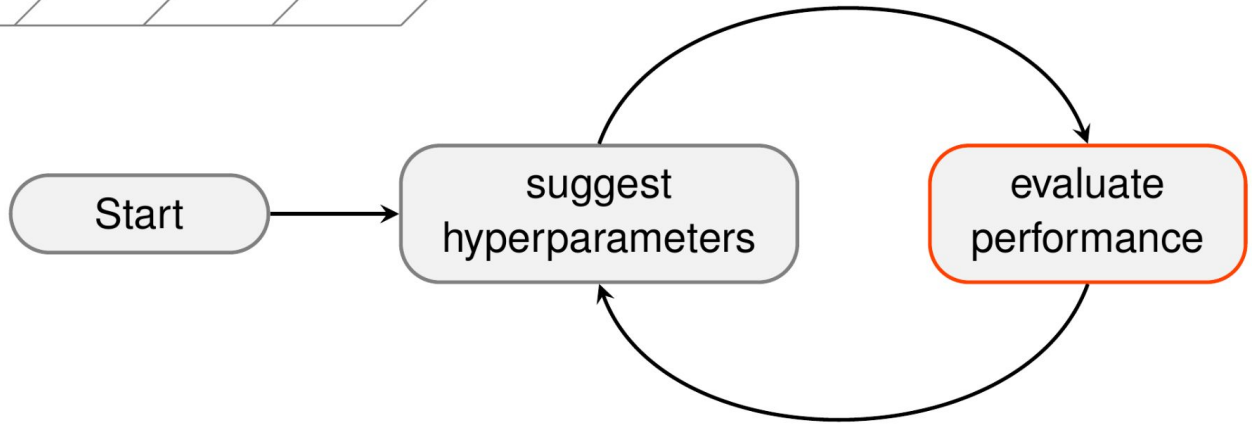
Start
suggest
hyperparameters
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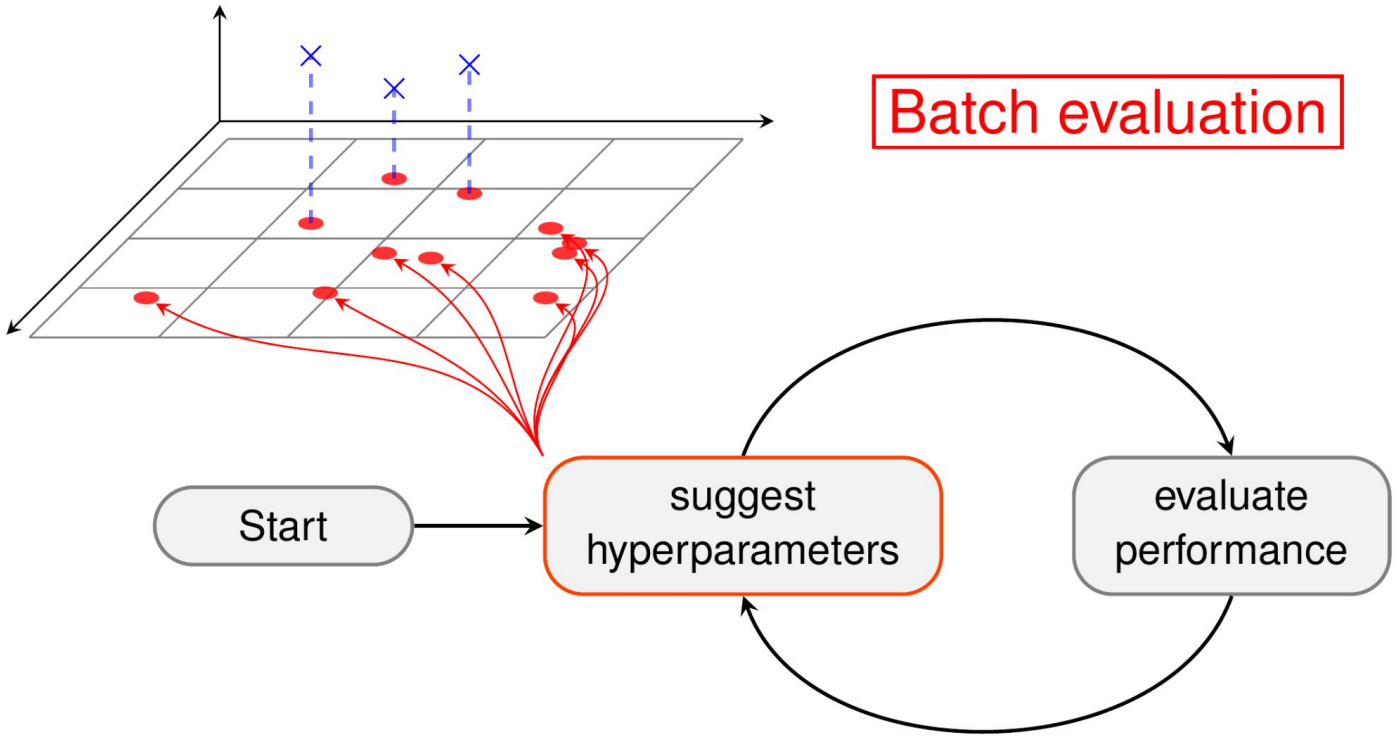
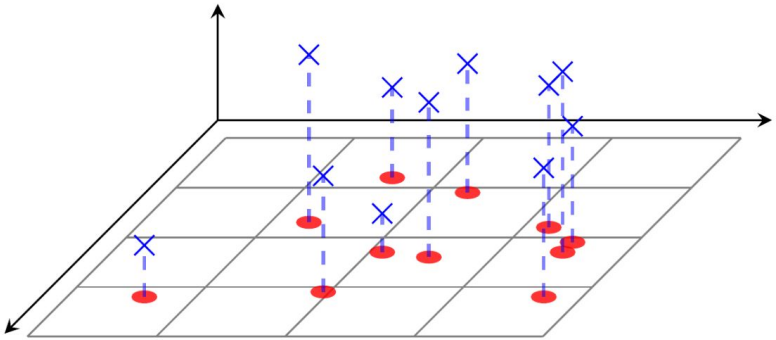
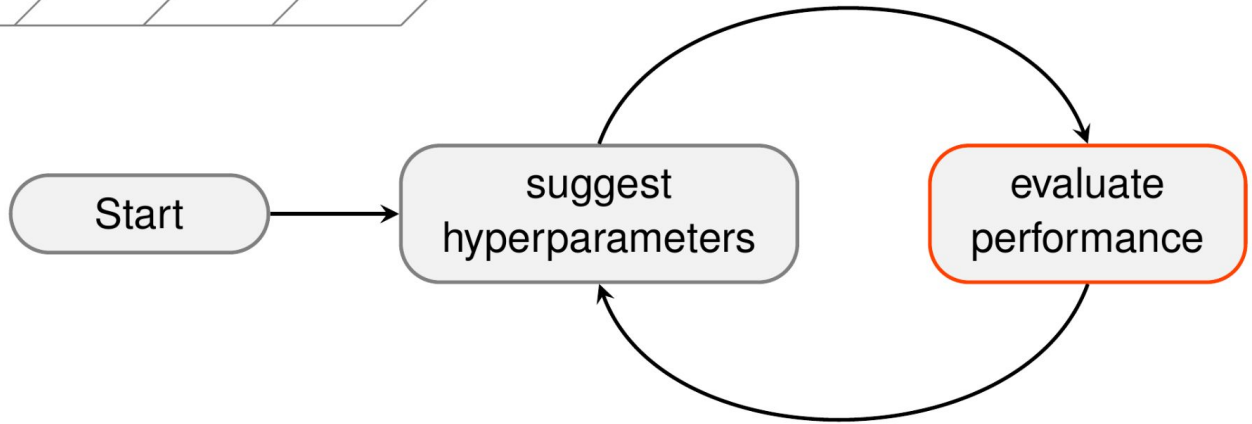
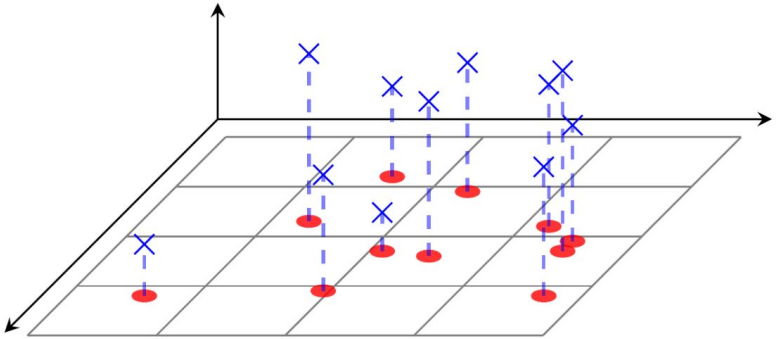
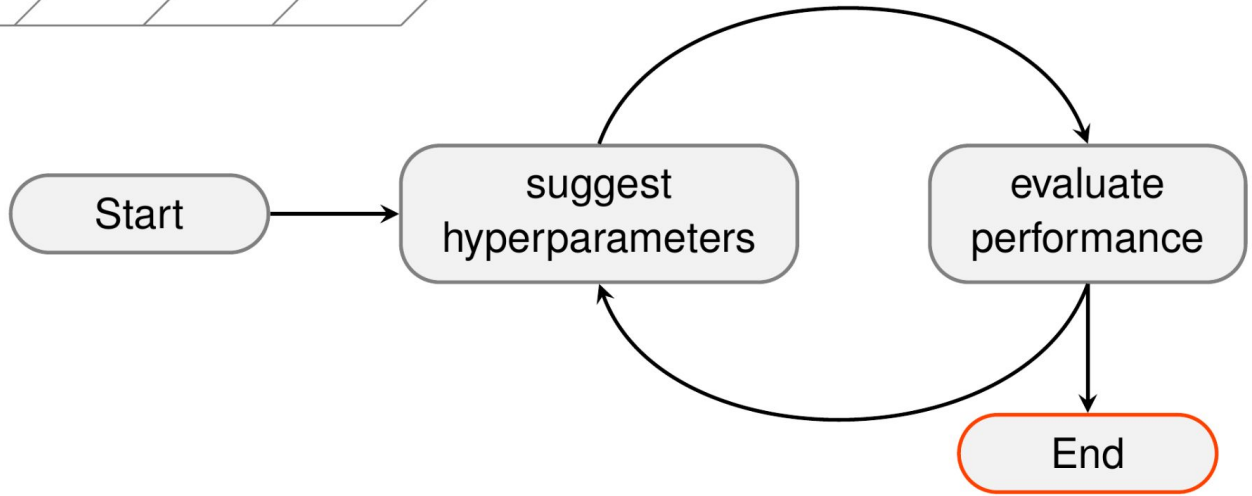

Batch evaluation
Start
suggest hyperparameters
evaluate performance



Batch evaluation






Start
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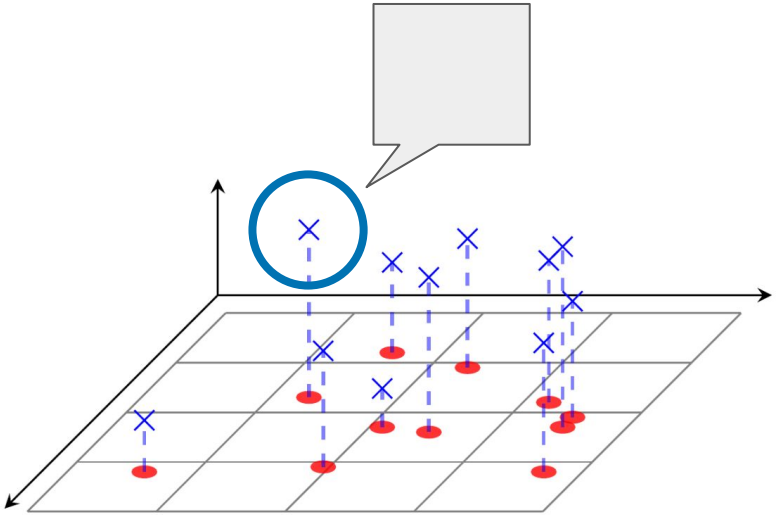
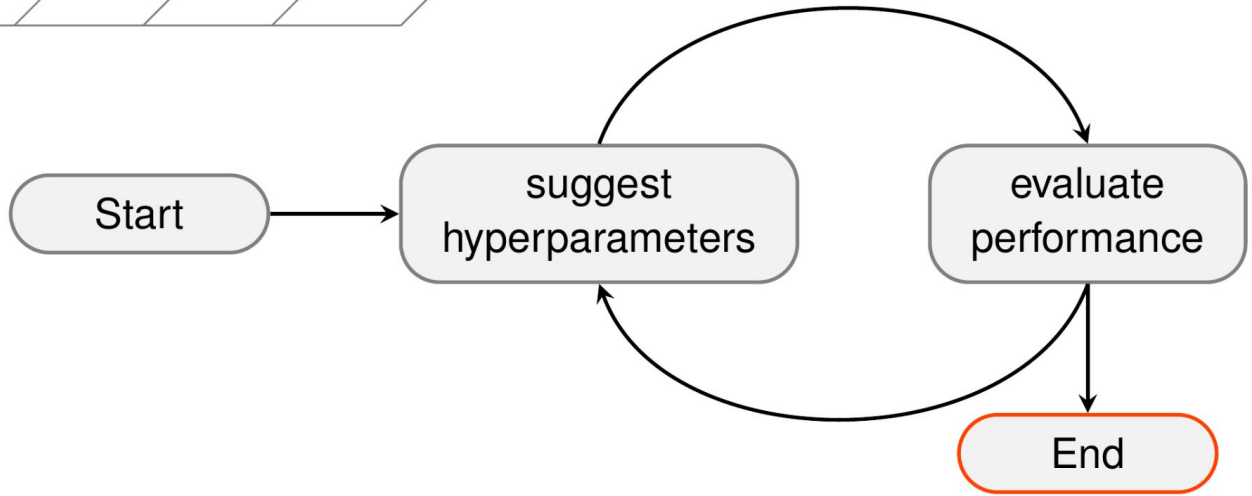
End




Start
suggest
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End

Tuning in mlr3

```
library("mlr3tuning")
lgr::get_logger("mlr3")$set_threshold("warn")
lgr::get_logger("bbotk")$set_threshold("warn")
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Tuning in mlr3

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library("mlr3tuning")
lgr::get_logger("mlr3")$set_threshold("warn")
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learner$param_set$values$k <- to_tune(2, 100, logscale = TRUE)
```

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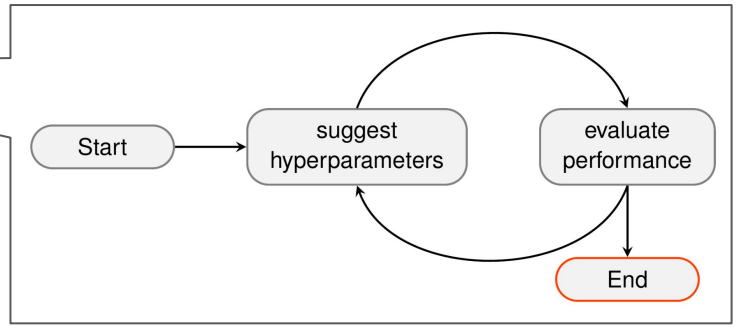
```

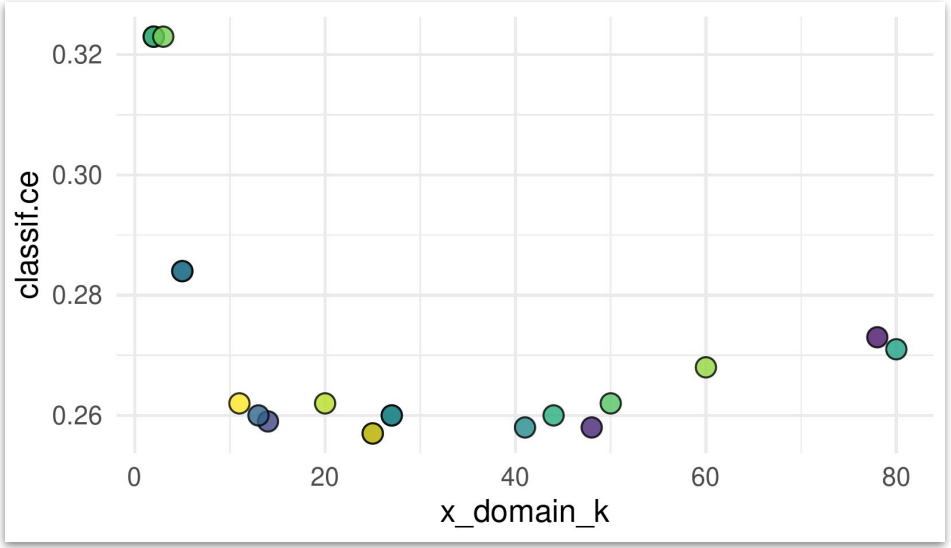
```
ti <- tune(
  tuner = tnr("random_search"),
  task = task,
  learner = learner,
  resampling = rsmp("cv", folds = 10),
  measures = msr("classif.ce"),
  term_evals = 20
)
```



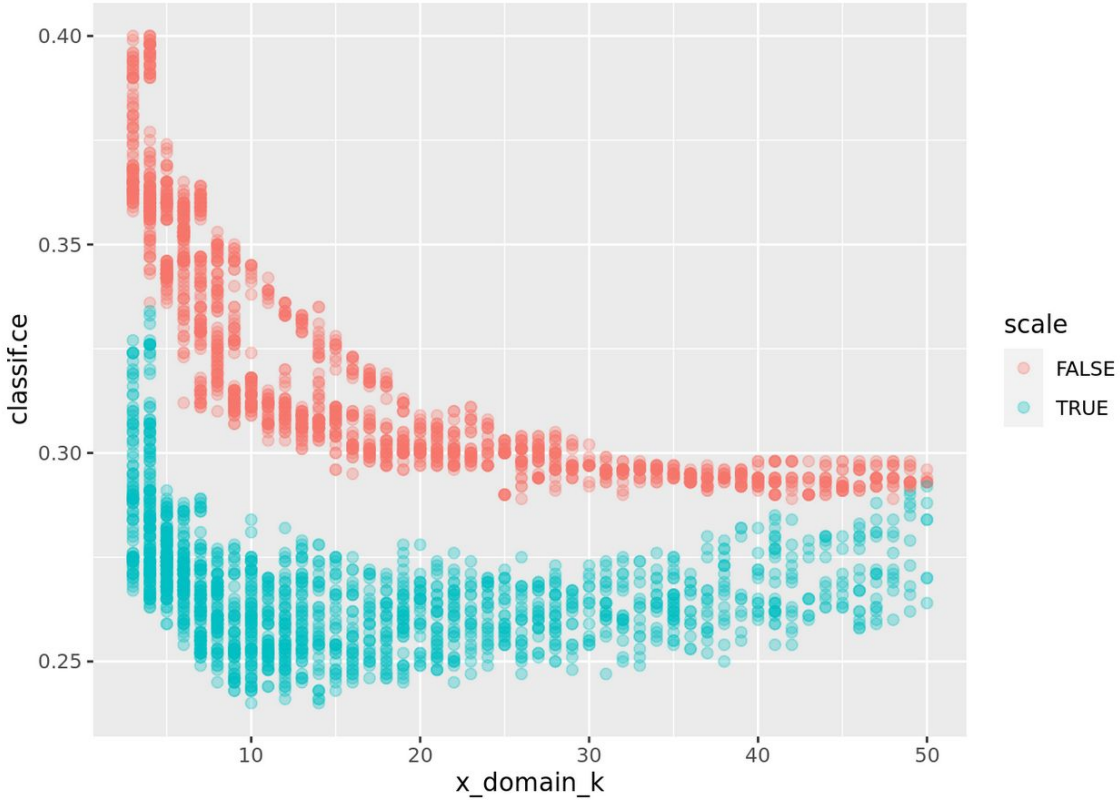
Tuning in mlr3

```
#> <TuningInstanceSingleCrit>
#> * State:  Optimized
#> * Objective: <ObjectiveTuning:classif.kknn_on_german>
#> * Search Space:
#>    id    class     lower    upper nlevels
#> 1:  k ParamDbl 0.6931472 4.615121     Inf
#> * Terminator: <TerminatorEvals>
#> * Result:
#>          k classif.ce
#> 1: 3.252434      0.257
#> * Archive:
#>           k classif.ce
#>  1: 3.252434      0.257
#>  2: 4.363433      0.273
#>  3: 3.888727      0.258
```

```
library("mlr3viz")
autoplot(ti, trafo = TRUE)
```



Tuning in mlr3

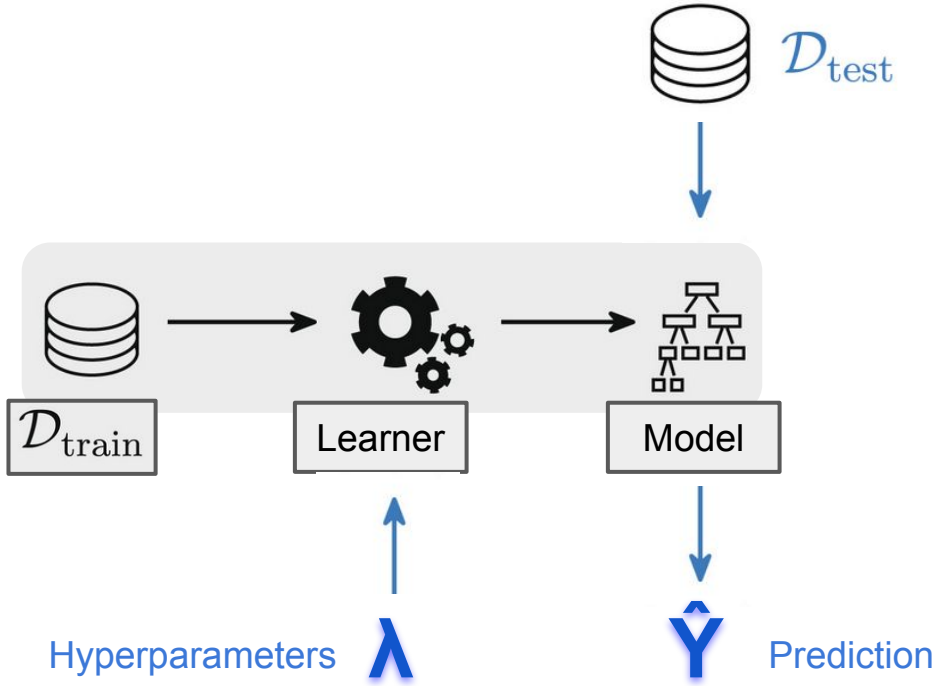


Tuning in mlr3

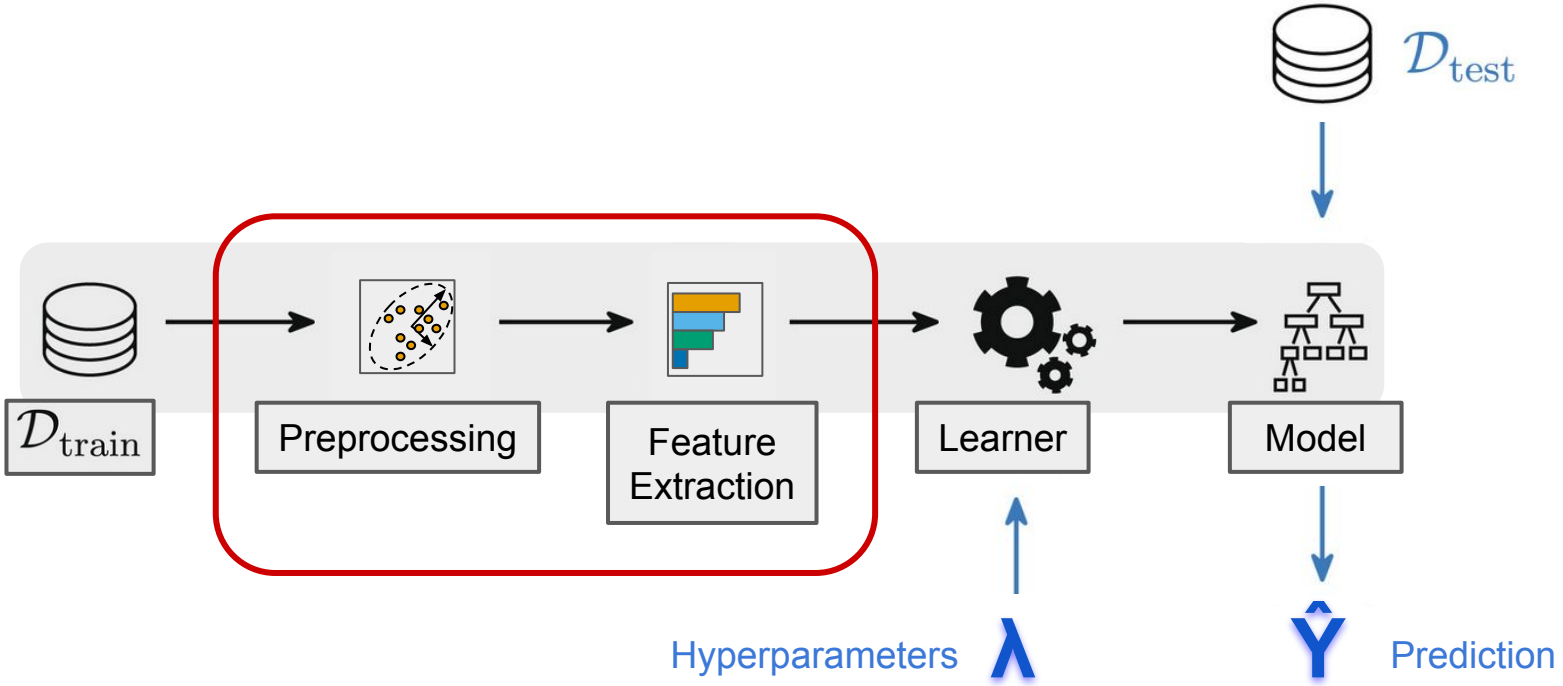
- Optimization algorithms are just objects, accessed through `tnr()`
- Common search spaces in the `mlr3tuningspaces` package
- Nested resampling for unbiased performance evaluation using the `AutoTuner`
- Transparent parallelization using the `future` package

Machine Learning:
It's Not That Easy

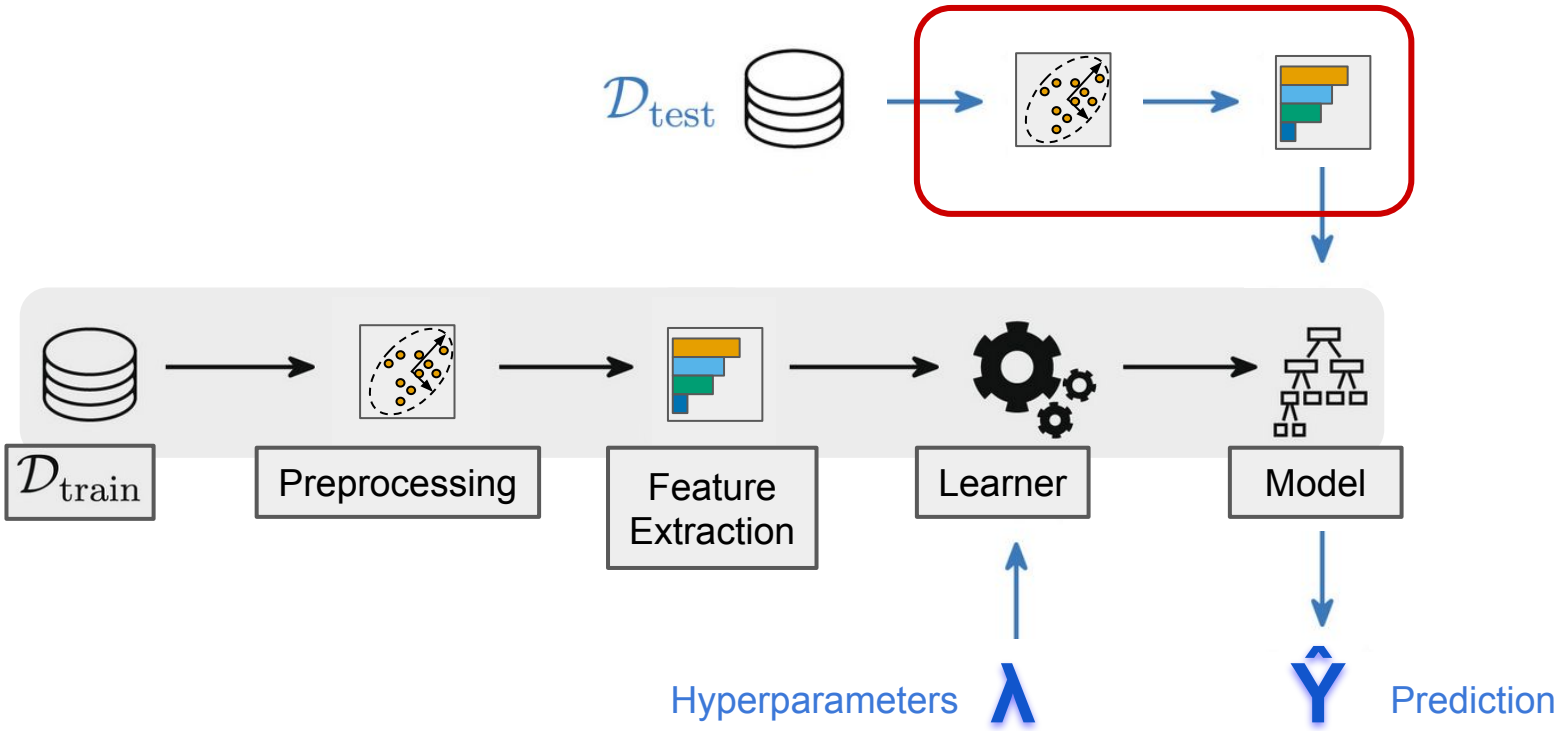
Machine Learning -- Not That Easy (II)



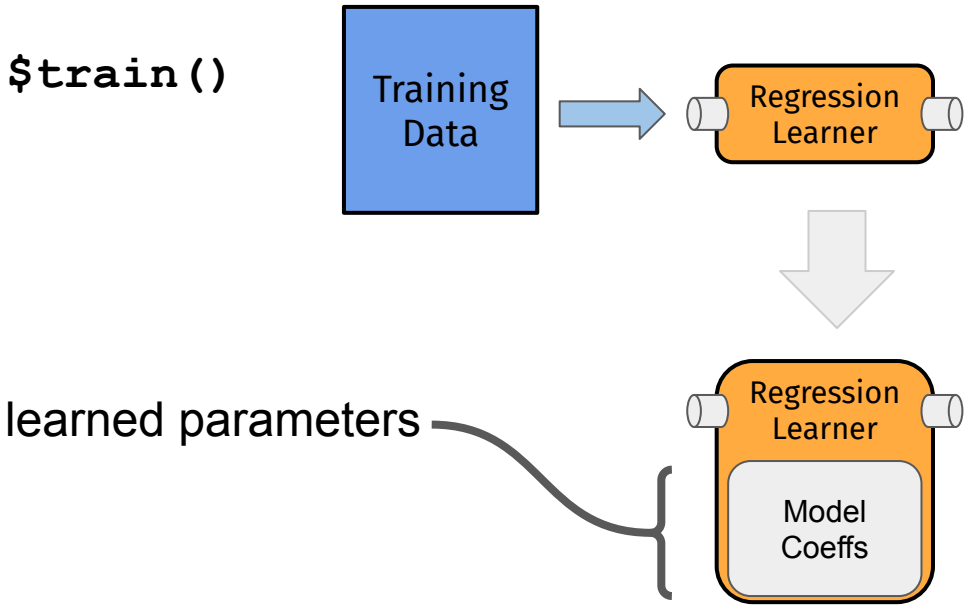
Machine Learning -- Not That Easy (II)



Machine Learning -- Not That Easy (II)



From Learner to Pipeline



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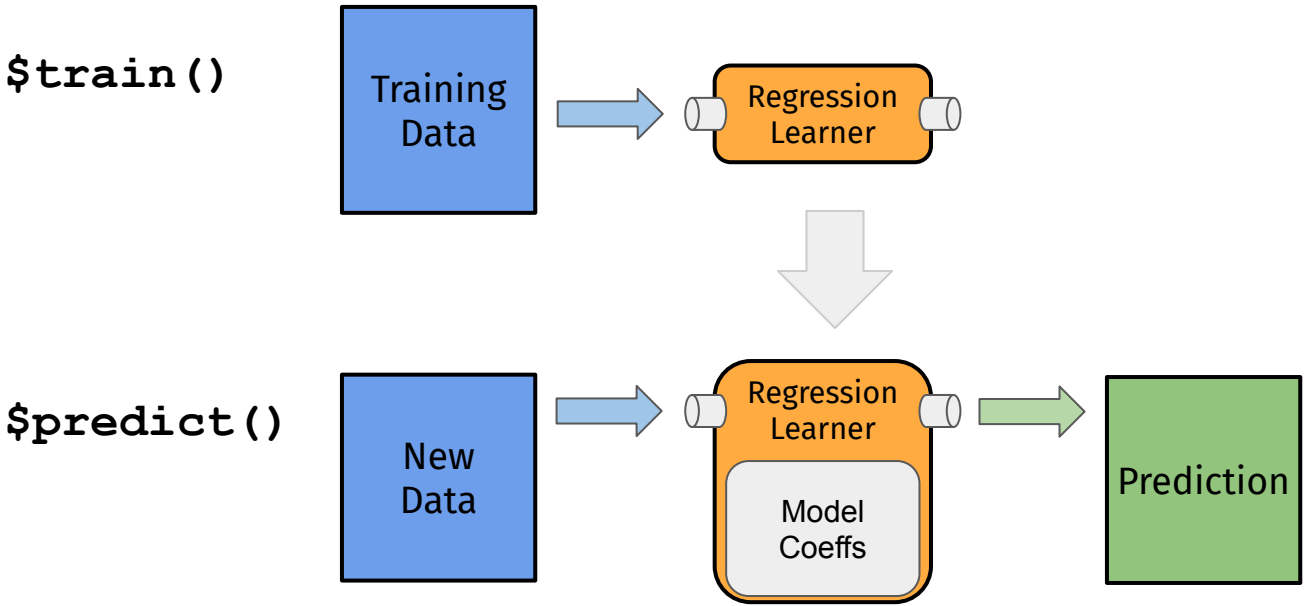

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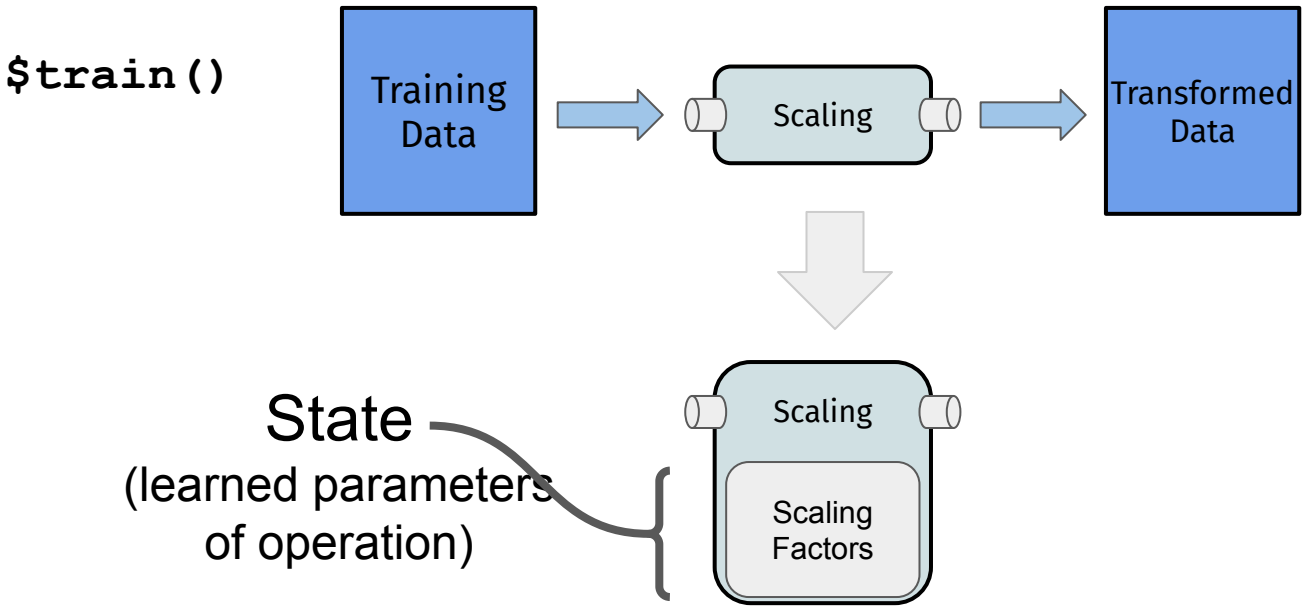
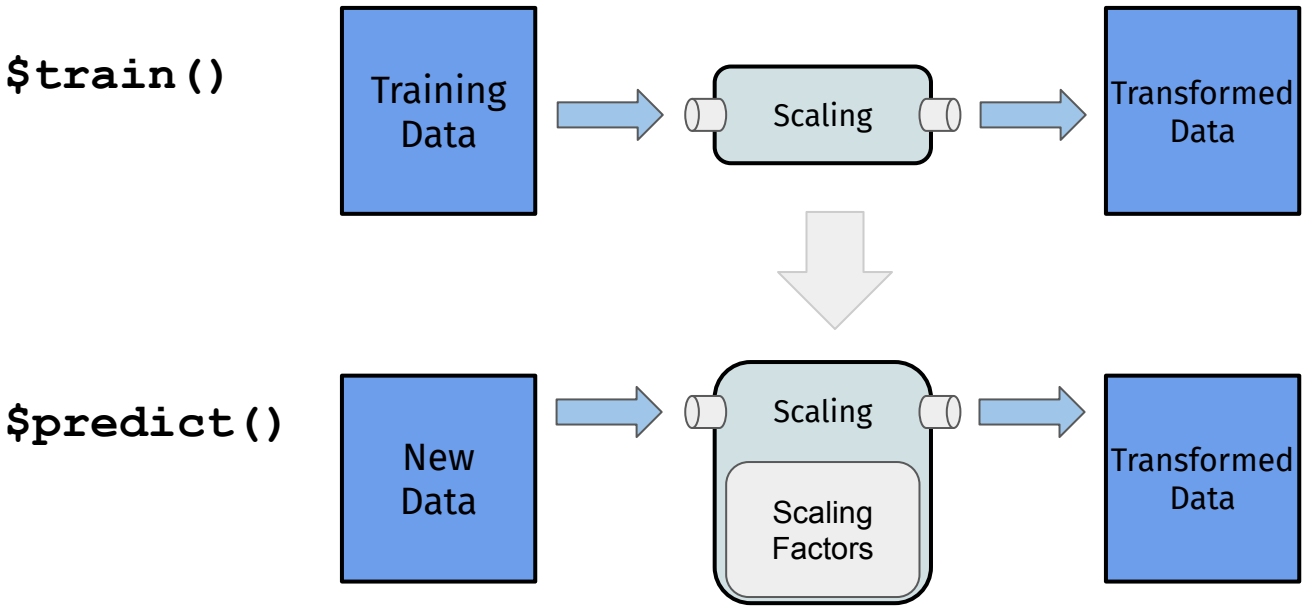


From Learner to Pipeline



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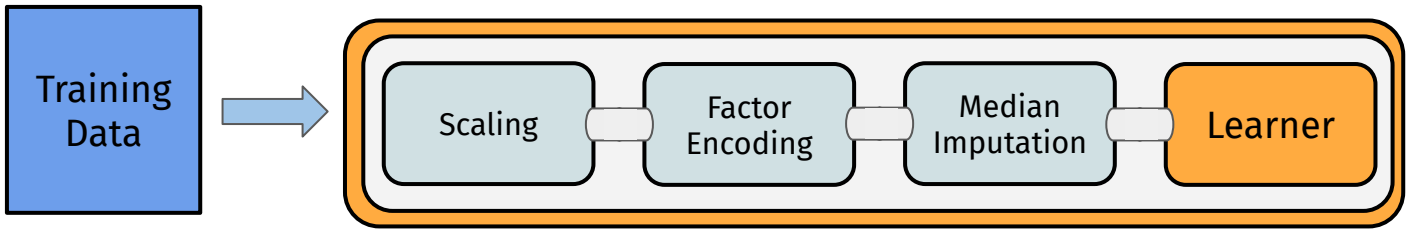
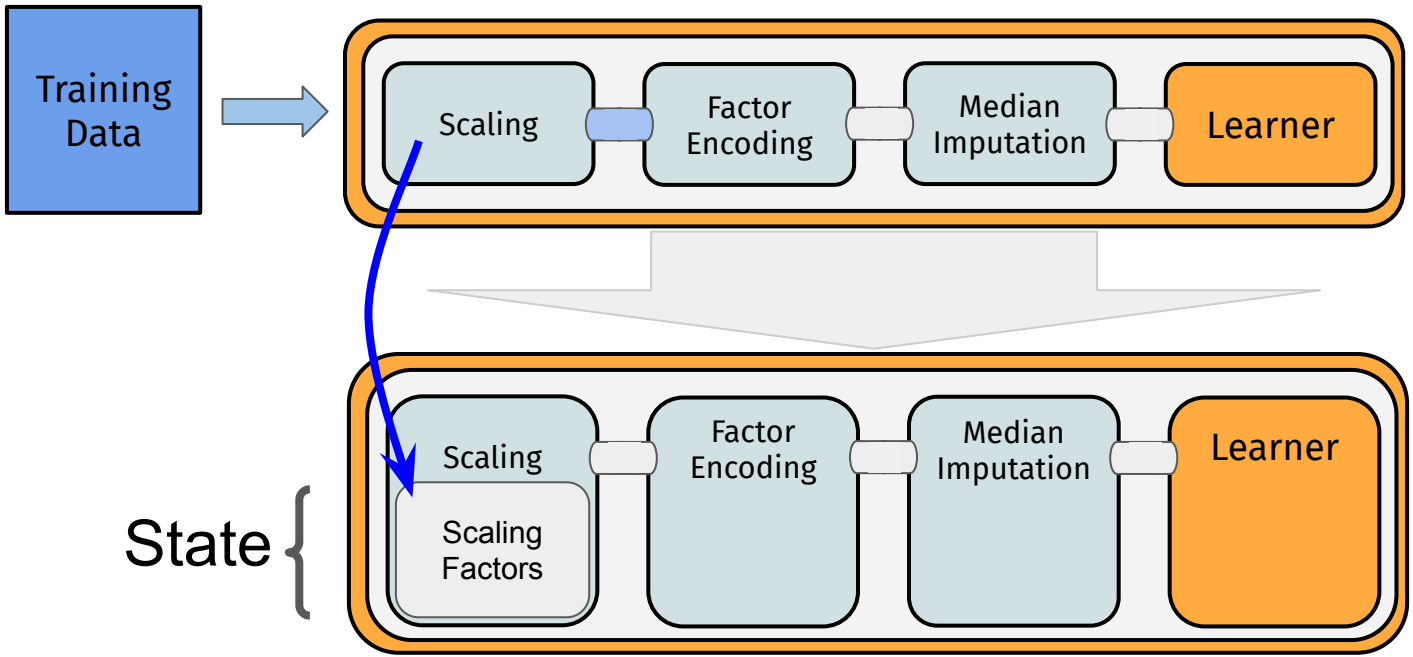
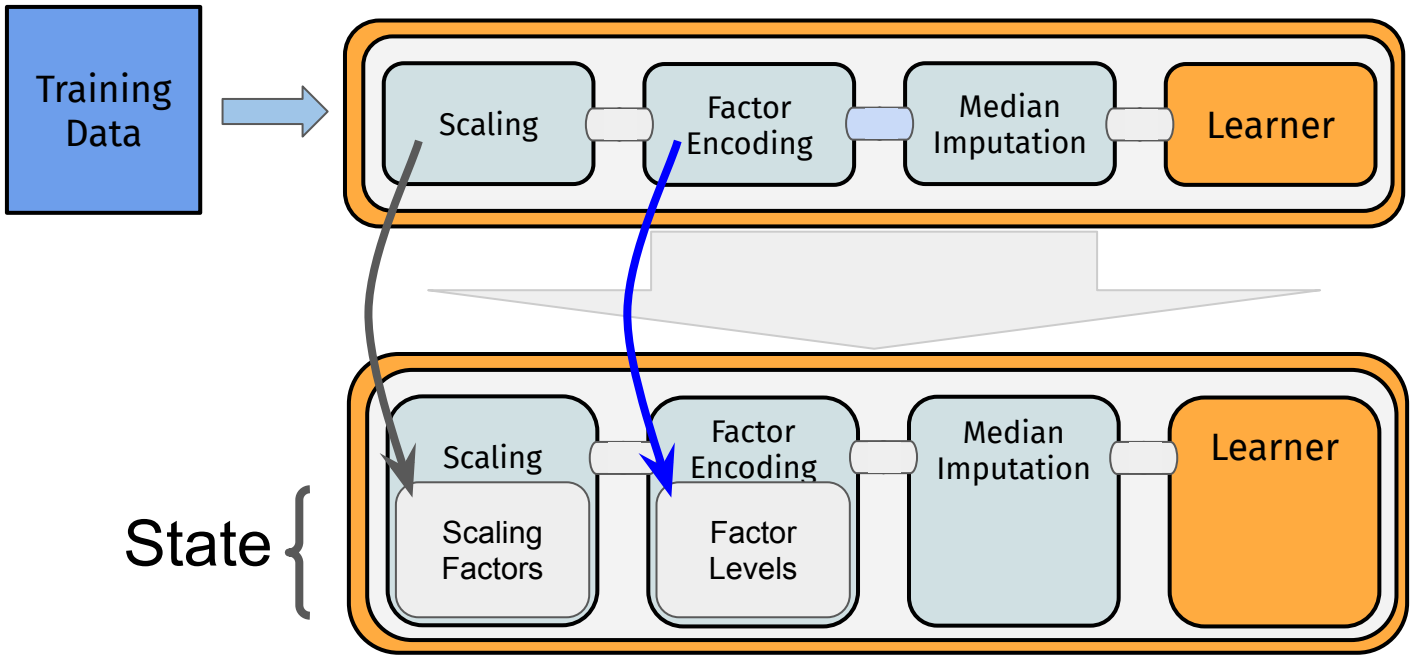


From Learner to Pipeline



From Learner to Pipeline



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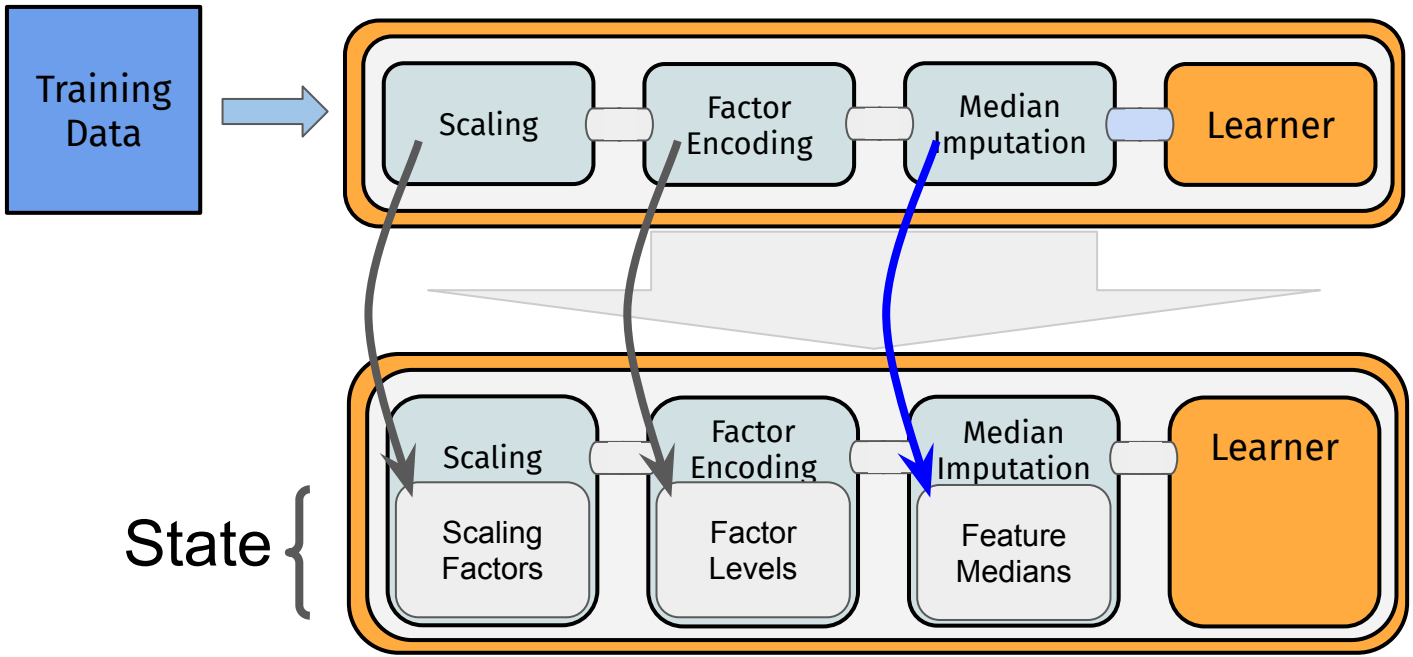
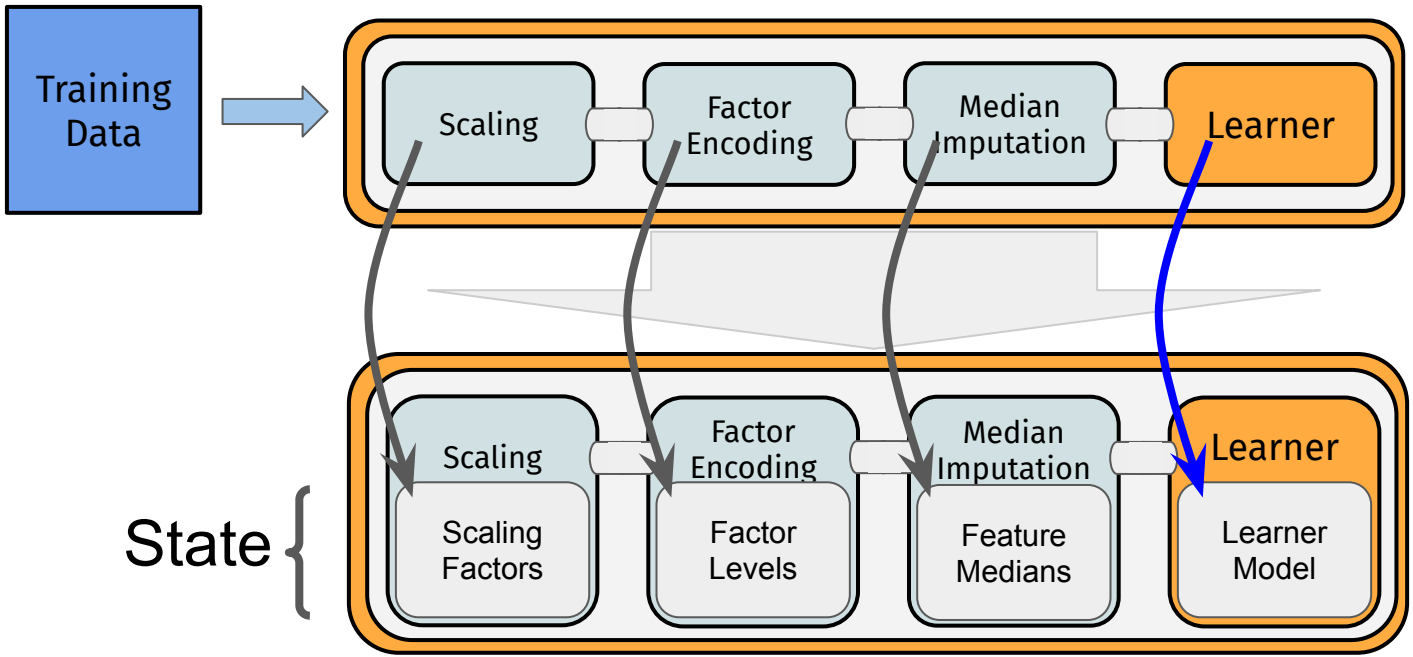
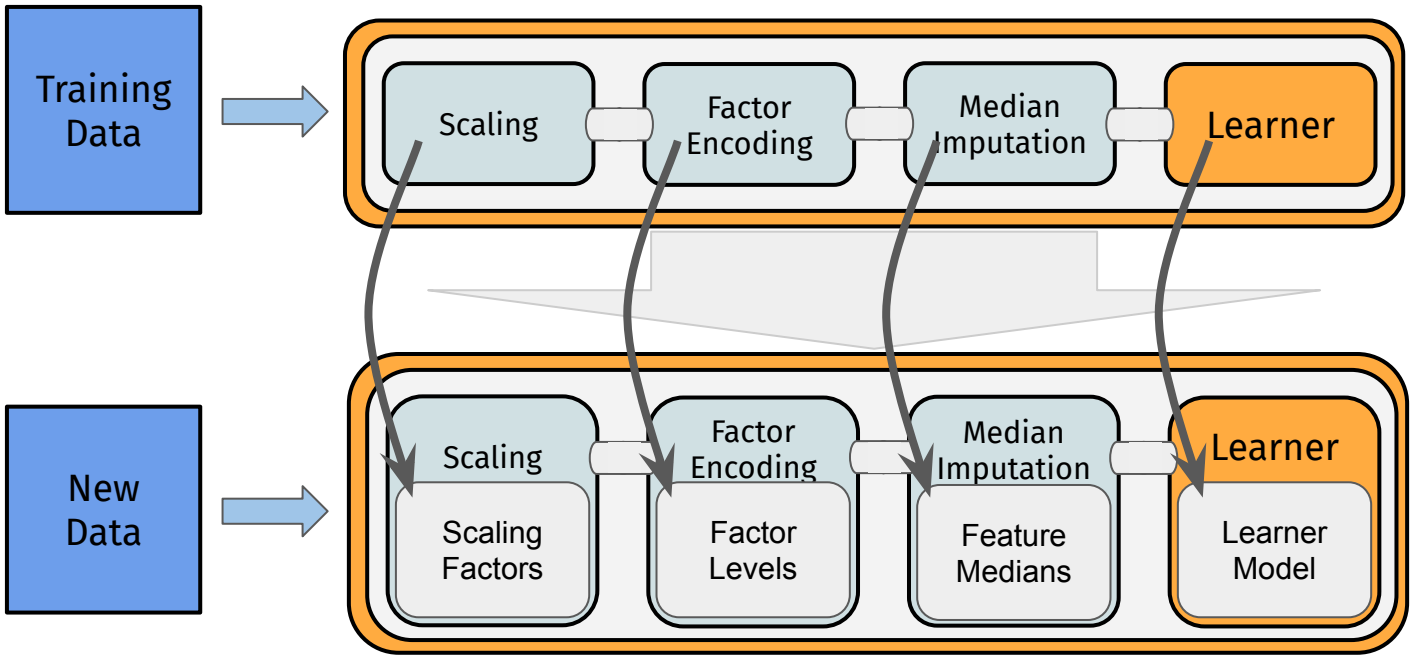


From Learner to Pipeline



From Learner to Pipeline



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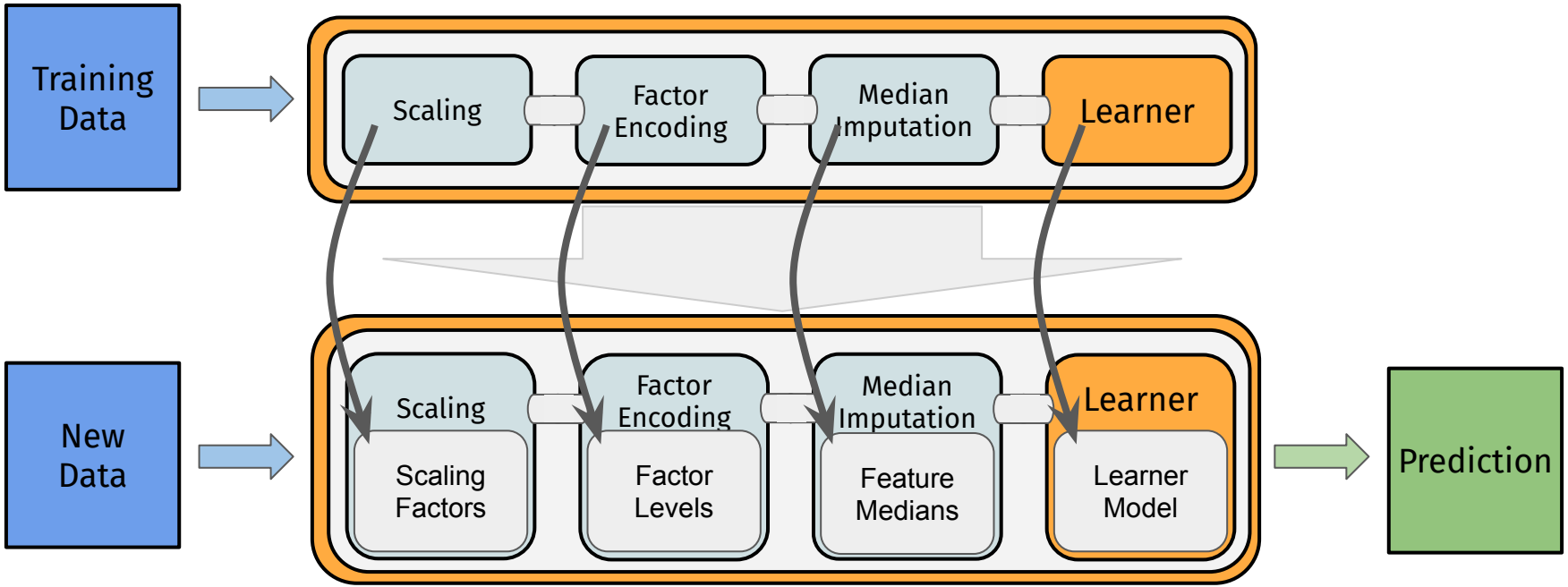

Pipelines in mlr3: mlr3pipelines

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library("mlr3pipelines")
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library("mlr3pipelines")
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pipeline <- as_learner(
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  lrn("classif.log_reg")
)
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)

pipeline$train(task)

pipeline$base_learner()$model
#> Call:  stats::glm(formula = task$formula(), family = "binomial", data = data,
#>     model = FALSE)

#> Coefficients:
#>                                     (Intercept)
#>                                       -8.237e-01
#>                                          amount
#>                                       2.705e-05
#>                                        duration
#>                                       3.342e-02
#>                                 status... < 0 DM
#>                                       -5.020e-01
#>                           status0<= ... < 200 DM
#>                                       -1.100e+00
#> status... >= 200 DM / salary for at least 1 year
#>                                       -2.025e+00
```
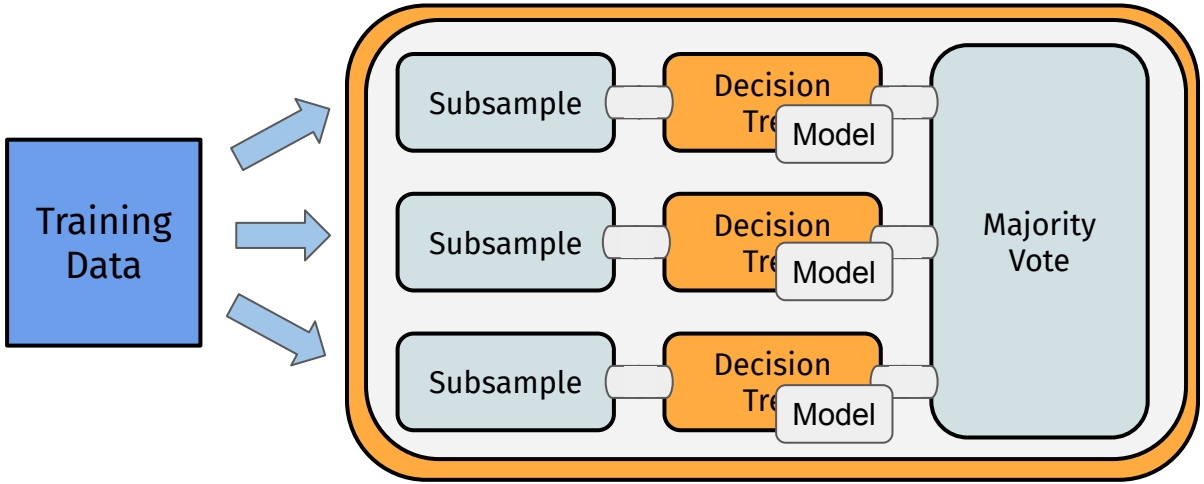

Pipelines in mlr3: mlr3pipelines

- Large library of common preprocessing operations
- Automatically avoids leaking test-set information into the training set
- Pipelines convert to `Learners`, work transparently with the rest of `mlr3`
- Advanced graph-structures: model ensembling



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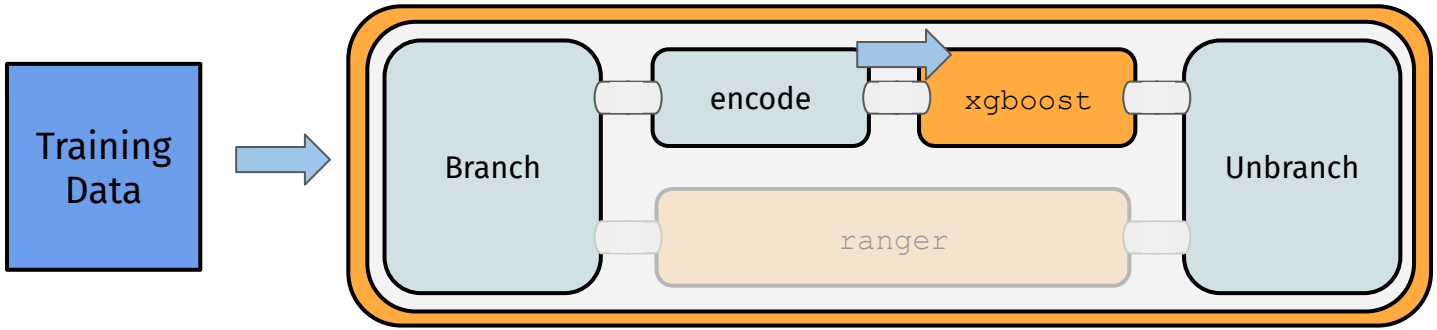
- Pipelines convert to **`Learners`**, work transparently with the rest of **`mlr3`**
- Advanced graph-structures: model ensembling
- Advanced graph-structures: alternative path branching -- control (and optimize) data-flow through hyperparameters



Next Steps

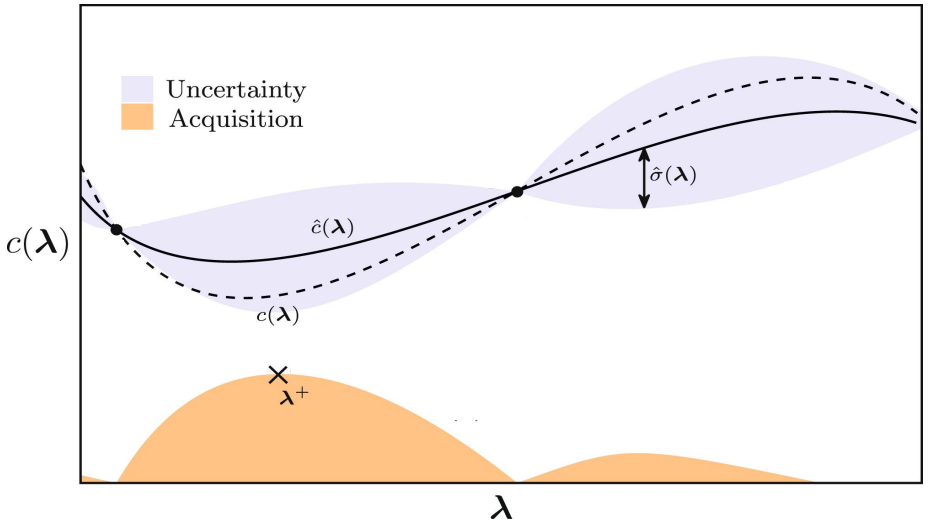
Going Beyond

More sophisticated optimization methods:

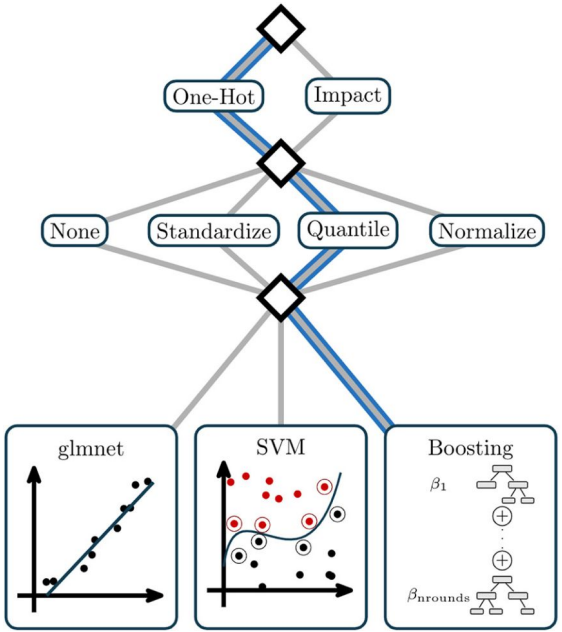
mlr³hyperband
Hyperband Parameter Tuning

mlr³mbo
Bayesian Optimization

miesmuschel
Flexible Mixed Integer Evolutionary Strategies



Optimizing pipeline-configurations and hyperparameters simultaneously



Learn More!

Free online `mlr3` book:

mlr3book.mlr-org.com

(physical copy is on the way)

- Examples from this talk: https://tinyurl.com/mlr3germancredit
- Slides: https://tinyurl.com/mlr3vfs