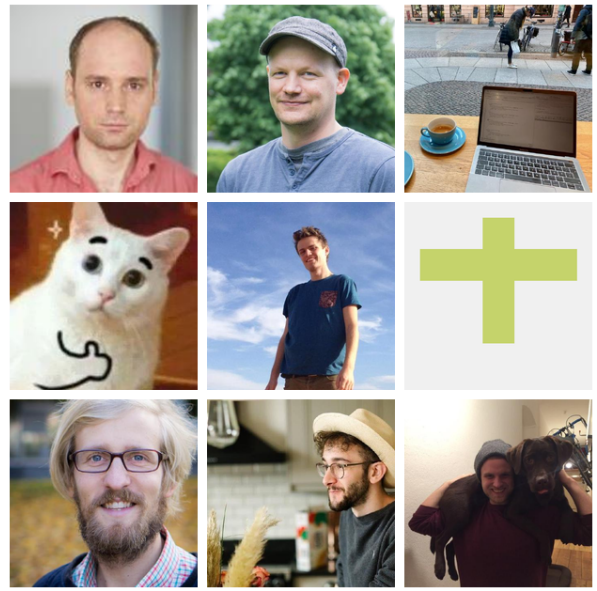
Modern Machine Learning in R

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

December 11, 2020

Intro

SO YOU WANT TO DO ML IN R

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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:

```r
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svm_model = e1071::svm(Species ~ ., data = iris)
```

vs.

```r
# 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)
```

MLR3 PHILOSOPHY

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  - Truly object-oriented: data and methods live in the same object
  - Make use of inheritance
  - Reference semantics

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  - List columns to arrange complex objects in tabular structure

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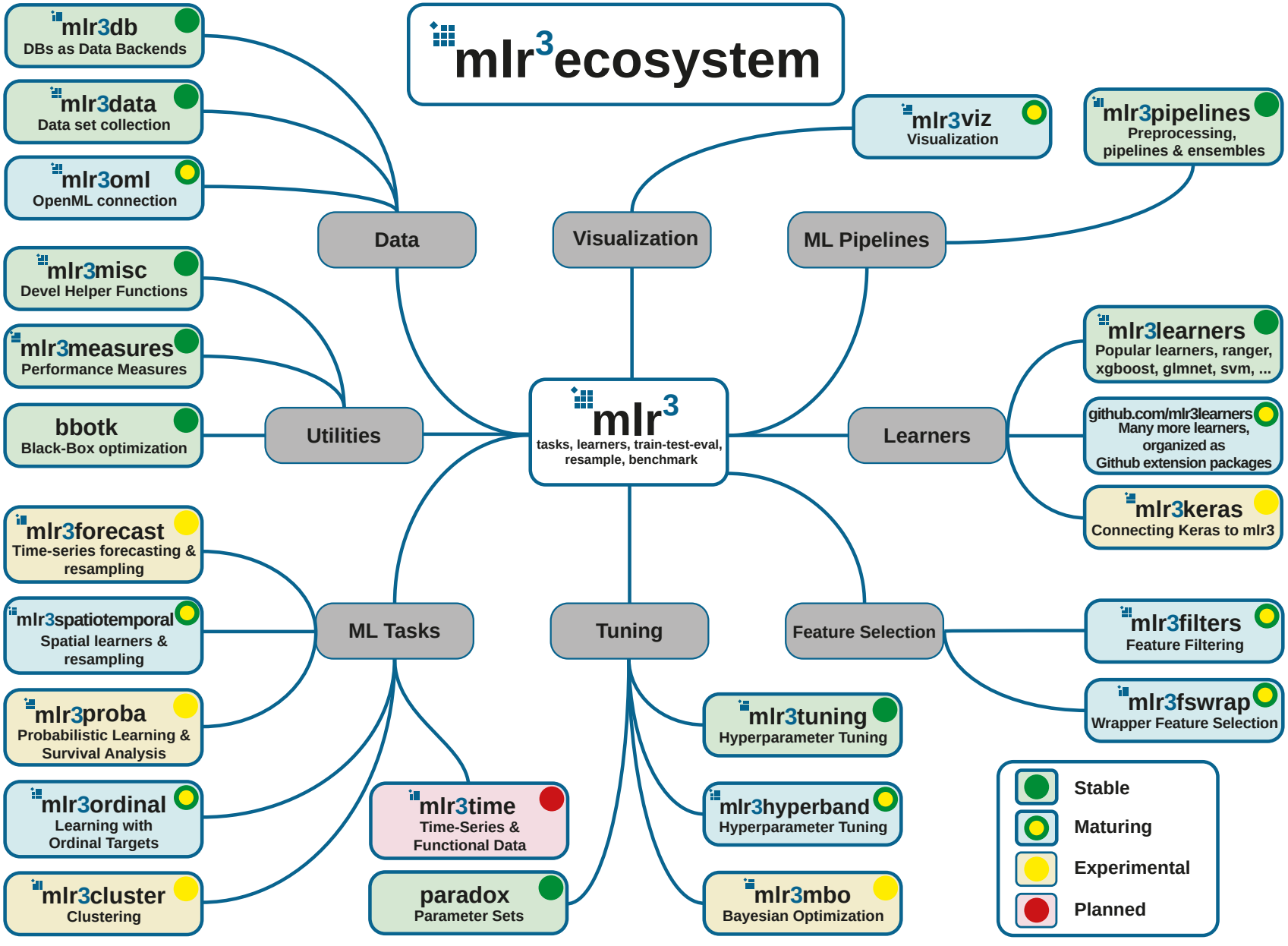
- Embrace **data.table**, both for arguments and internally
  - Fast operations for tabular data
  - List columns to arrange complex objects in tabular structure
- Be **light on dependencies**:
  - `R6`, `data.table`, `lgr`, `uuid`, `mlbench`, `digest`
  - Plus some of our own packages (`backports`,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


mlr3ecosystem
mlr3db
DBs as Data Backends
mlr3data
Data set collection
mlr3oml
OpenML connection
mlr3misc
Devel Helper Functions
mlr3measures
Performance Measures
bbotk
Black-Box optimization
mlr3forecast
Time-series forecasting & resampling
mlr3spatiotemporal
Spatial learners & resampling
mlr3proba
Probabilistic Learning & Survival Analysis
mlr3ordinal
Learning with Ordinal Targets
mlr3cluster
Clustering
Data
Utilities
ML Tasks
Visualization
ML Pipelines
Tuning
Learners
Feature Selection
mlr3
tasks, learners, train-test-eval, resample, benchmark
mlr3viz
Visualization
mlr3pipelines
Preprocessing, pipelines & ensembles
mlr3learners
Popular learners, ranger, xgboost, glmnet, svm, ...
github.com/mlr3learners
Many more learners, organized as Github extension packages
mlr3keras
Connecting Keras to mlr3
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

SO YOU WANT TO DO ML IN R

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

Ingredients:

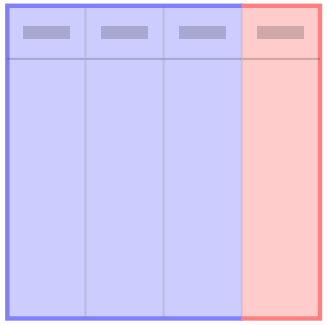
- Data / Task
- Learning Algorithms
- Performance Evaluation
- Performance Comparison

Data

DATA

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

  $\Rightarrow$ target determines the machine learning "Task"



```
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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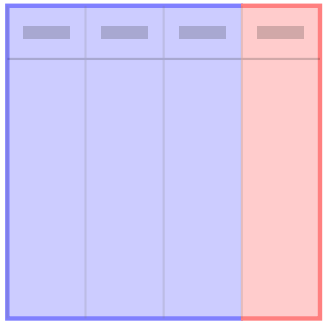

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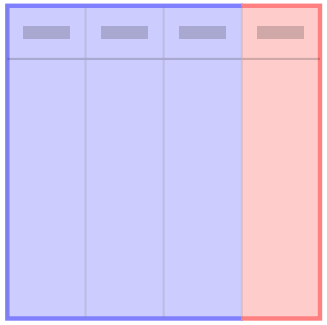

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```
task = TaskClassif$new("iris", iris, "Species")
```

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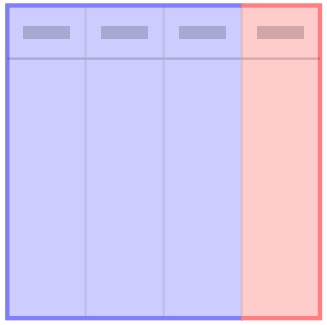

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#> 1          5.1         3.5          1.4         0.2  setosa
#> 2          4.9         3.0          1.4         0.2  setosa
#> ...
```

Task ID → "iris", data → iris, target name → "Species"

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

DATA

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

```
print(task)

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

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

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

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

Learning Algorithms

LEARNING ALGORITHMS

- Get a `Learner` provided by `mlr`

```
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learner$train(task)
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```
learner$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) *
```

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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# 2            2           2            3           2
```

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

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

- We get a `Prediction` object:

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

HYPERPARAMETERS

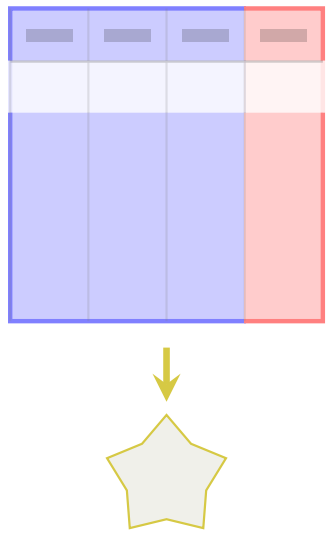
- Learners have *hyperparameters*

```
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
```

Resampling

RESAMPLING



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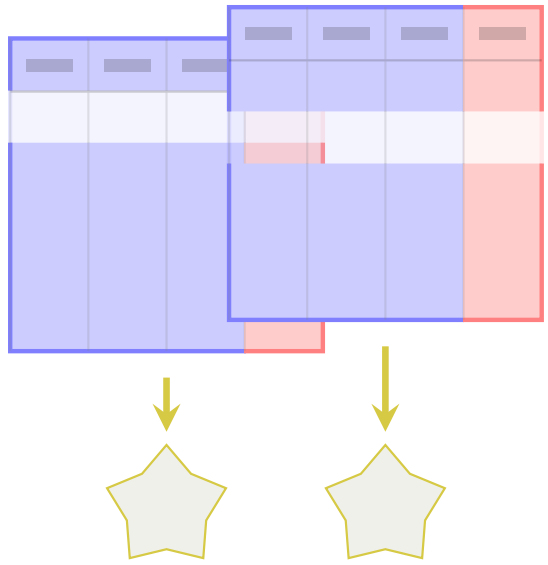

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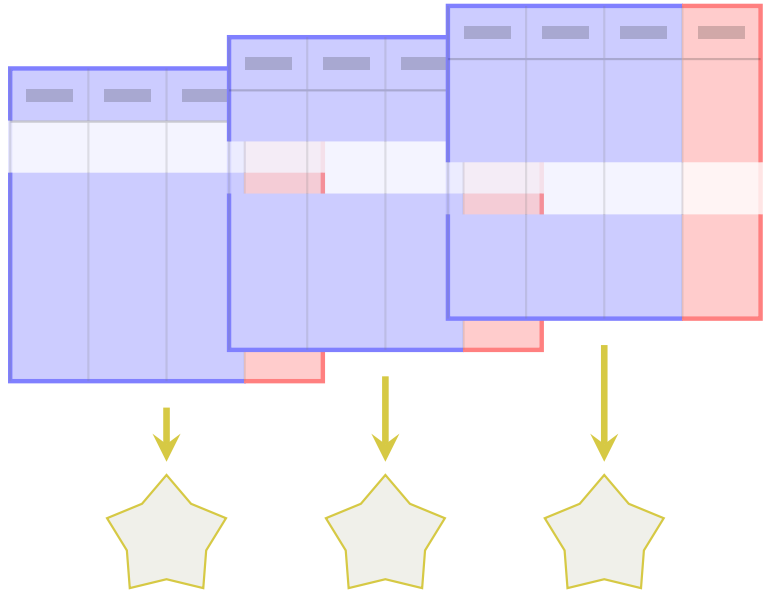

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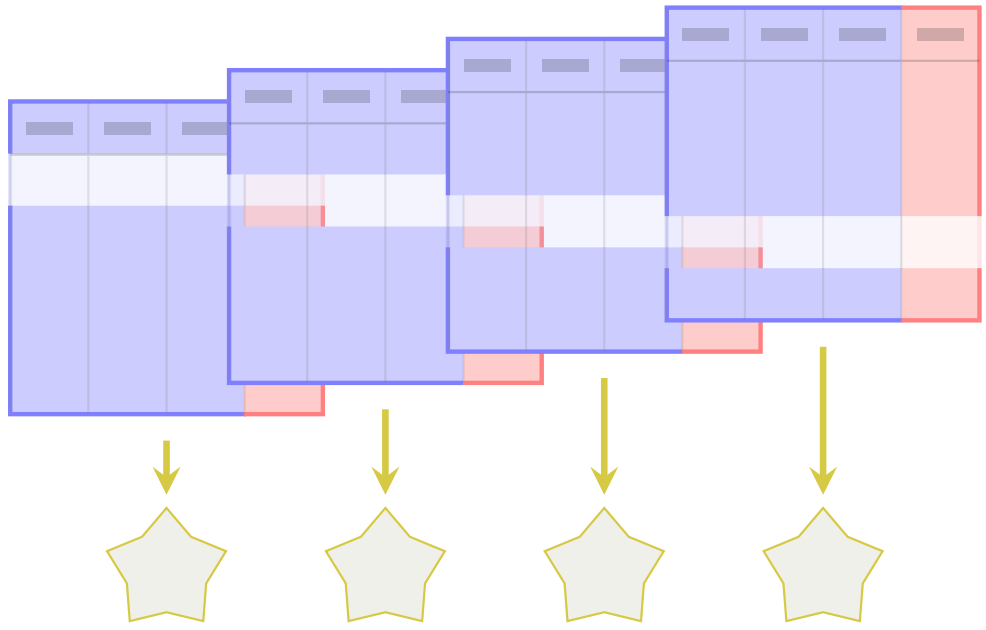
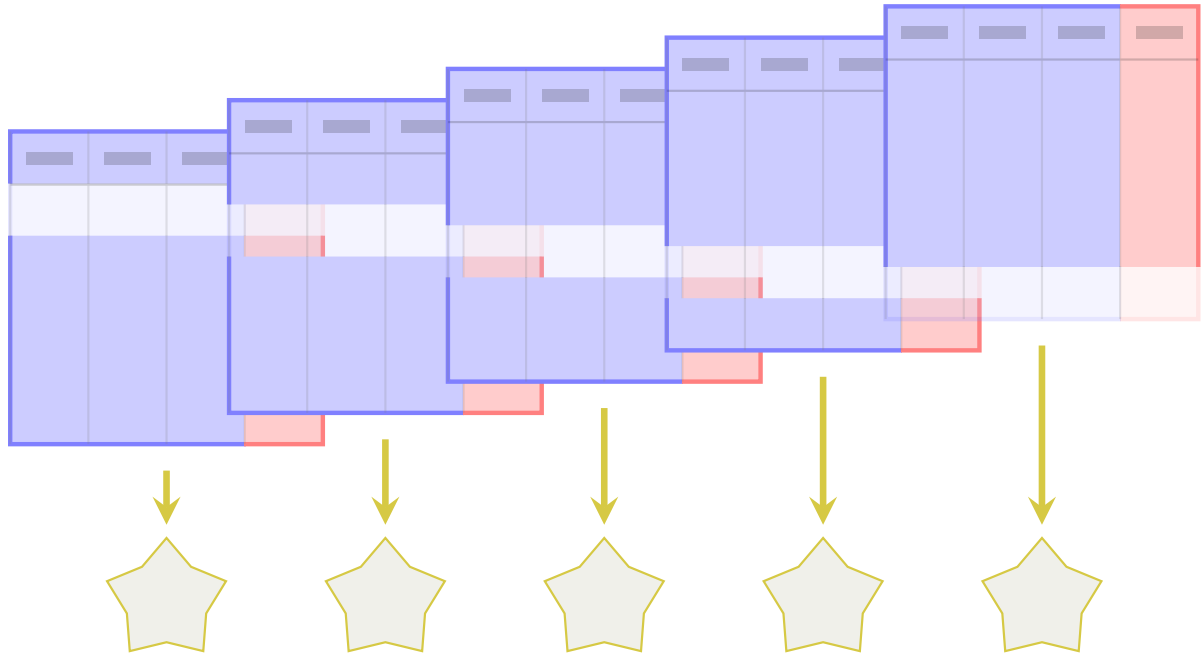


RESAMPLING



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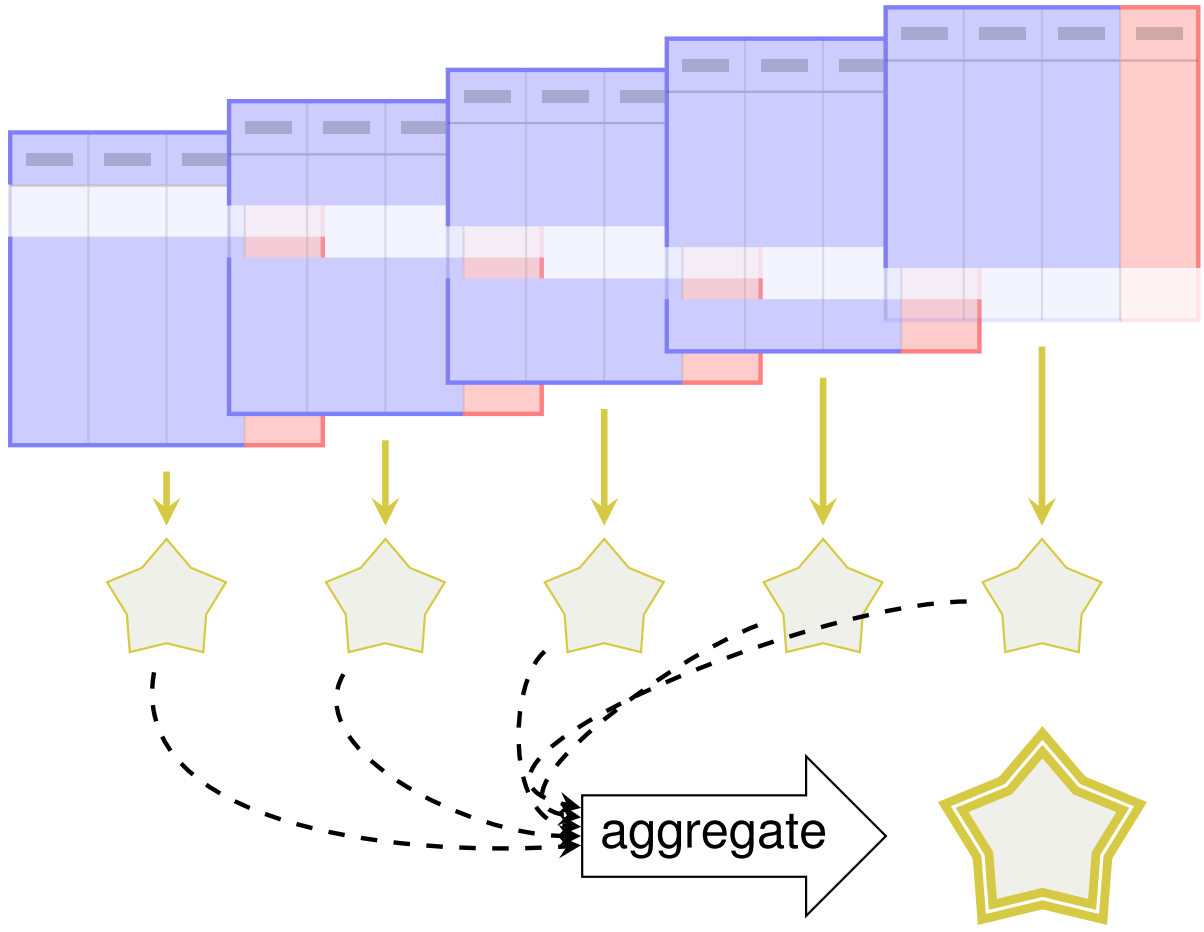

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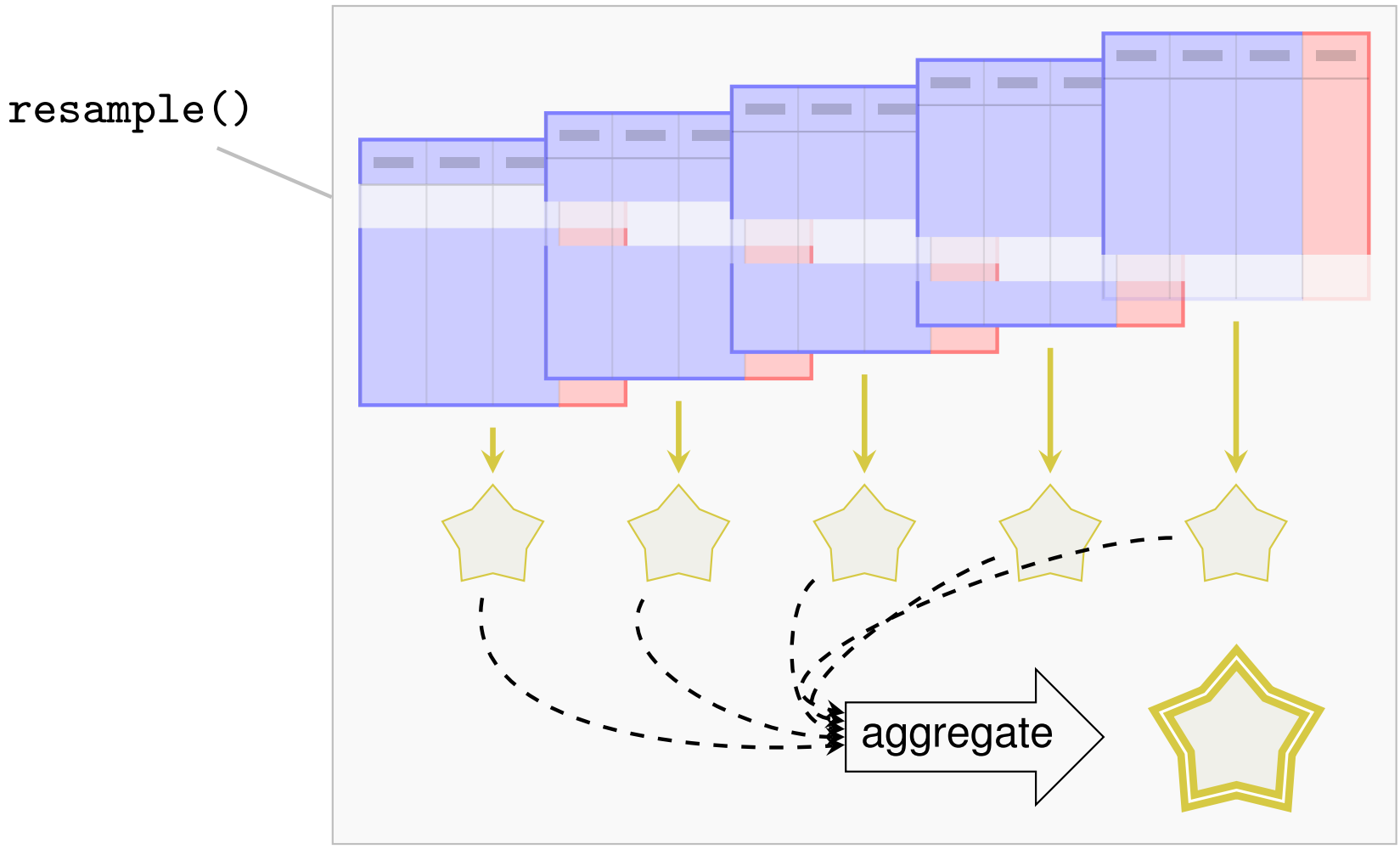

RESAMPLING

- Resample description: How to split the data

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```

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

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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

- Calculate performance:

```
rr$aggregate(msr("classif.ce"))
#> classif.ce
#>      0.067
```

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```
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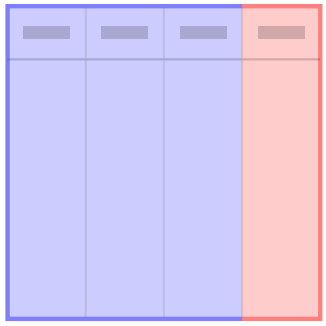
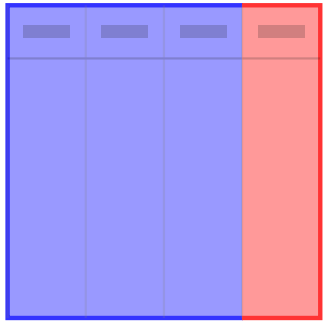
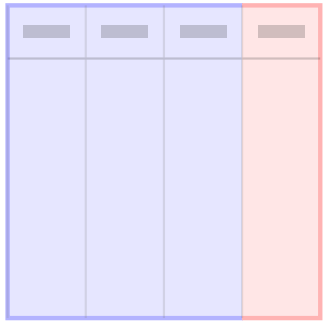
- Get predictions

```
rr$prediction()
#> <PredictionClassif> for 150 observations:
#>     row_id     truth   response
#>          3    setosa     setosa
#>         13    setosa     setosa
#>         14    setosa     setosa
#> ---
#>        136 virginica  virginica
#>        139 virginica versicolor
#>        141 virginica  virginica
```

Benchmark

PERFORMANCE COMPARISON

	Learner 1	Learner 2	Learner 3
	?	?	?
	?	?	?
	?	?	?

PERFORMANCE COMPARISON

- Multiple Learners, multiple Tasks:

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

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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)
```

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```
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bmr = benchmark(design)
```

- We get a `BenchmarkResult` object which shows that `kknn` outperforms `rpart`:

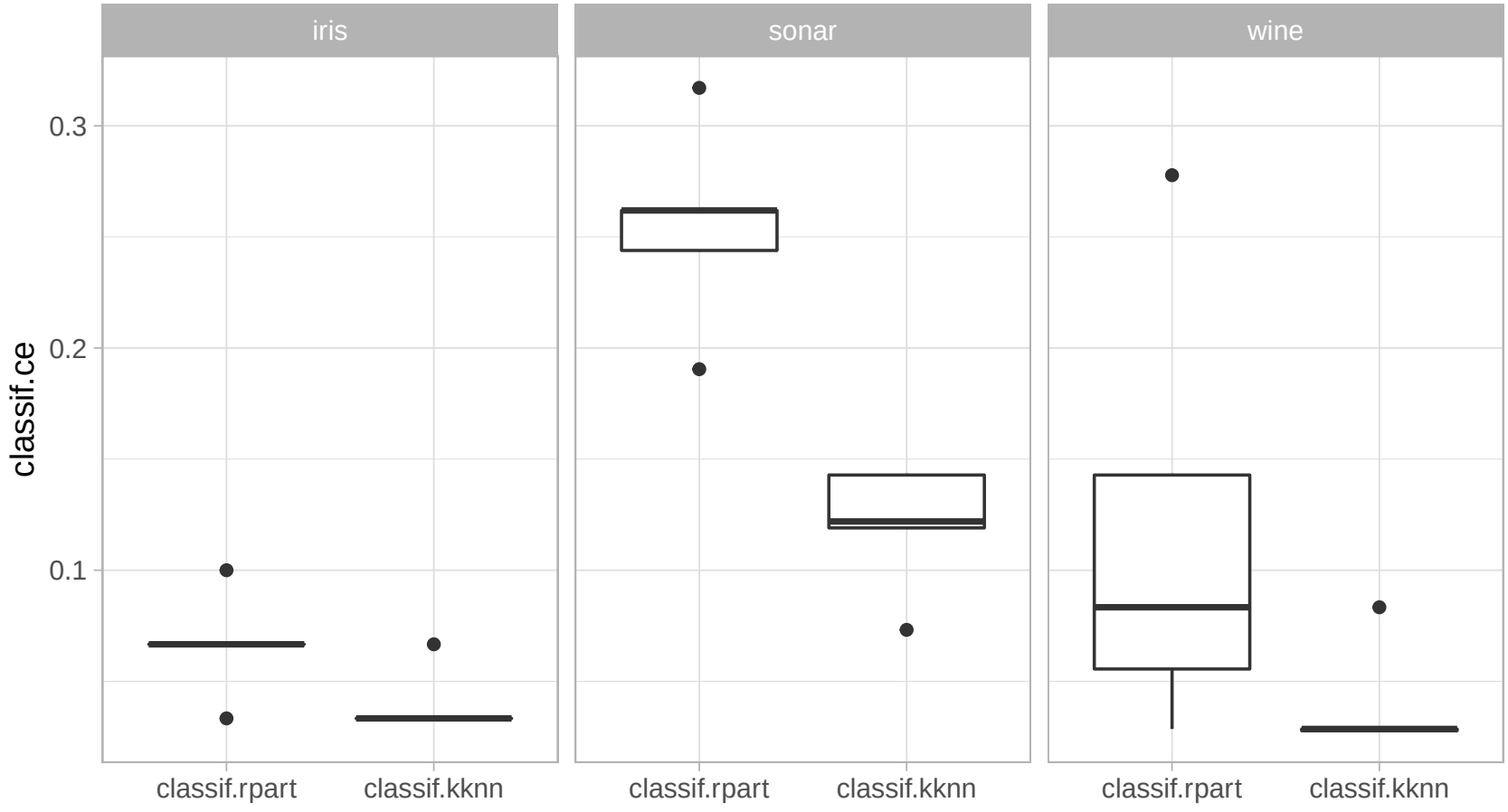
```
bmr_ag = bmr$aggregate()
bmr_ag[, c("task_id", "learner_id", "classif.ce")]
```

```
#>    task_id    learner_id classif.ce
#> 1:    iris classif.rpart      0.067
#> 2:    iris  classif.kknn      0.040
#> 3:   sonar classif.rpart      0.255
#> 4:   sonar  classif.kknn      0.120
#> 5:    wine classif.rpart      0.118
#> 6:    wine  classif.kknn      0.039
```

BENCHMARK RESULT

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

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



Dictionaries

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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 10 stored values
#> Keys: boston_housing, breast_cancer, german_credit, iris,
#>   mtcars, 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
```

Tuning

TUNING

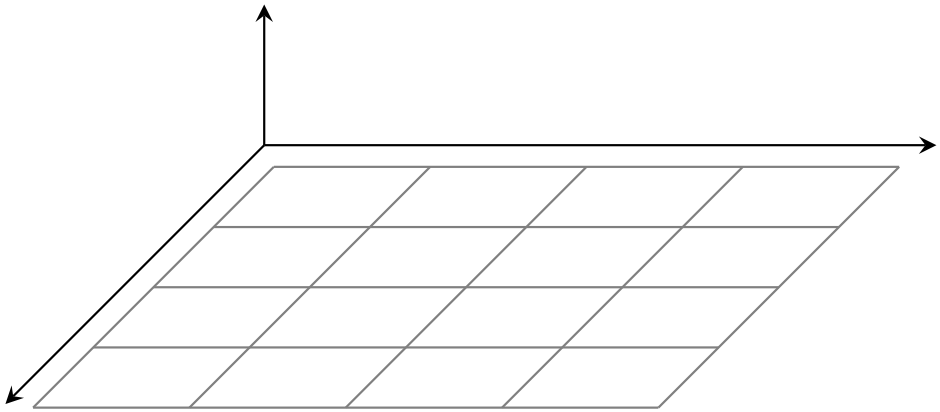
- Behavior of most methods depends on *hyperparameters*
- We want to choose them so our algorithm performs well
- Good hyperparameters are data-dependent

$\Rightarrow$ We do *black box optimization* ("Try stuff and see what works")

Tuning toolbox for `mlr3`:

```
library("bbotk")
library("mlr3tuning")
```

TUNING



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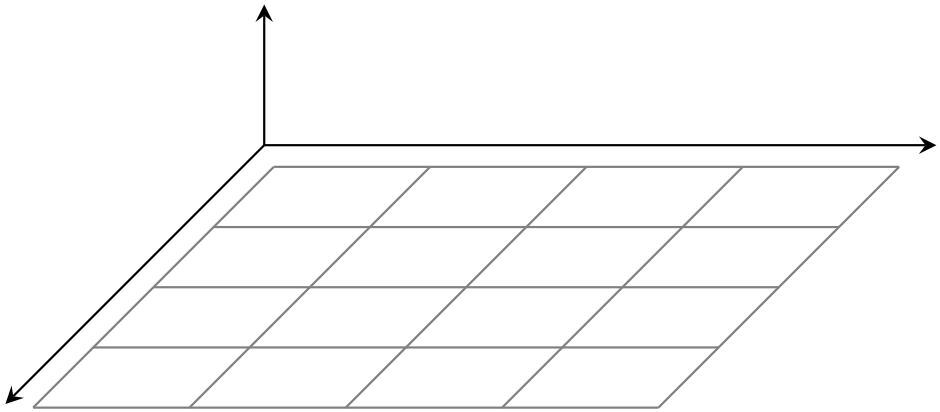
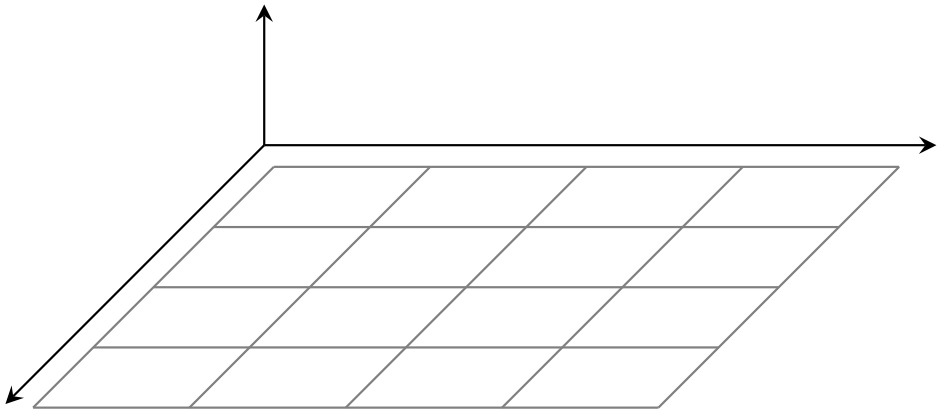
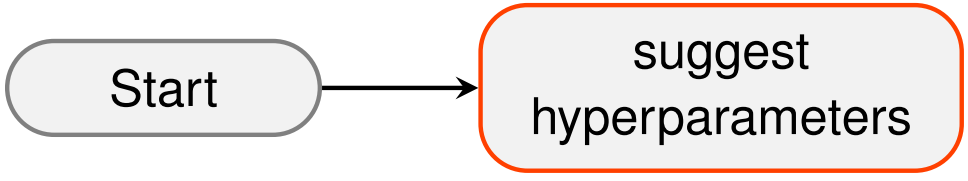


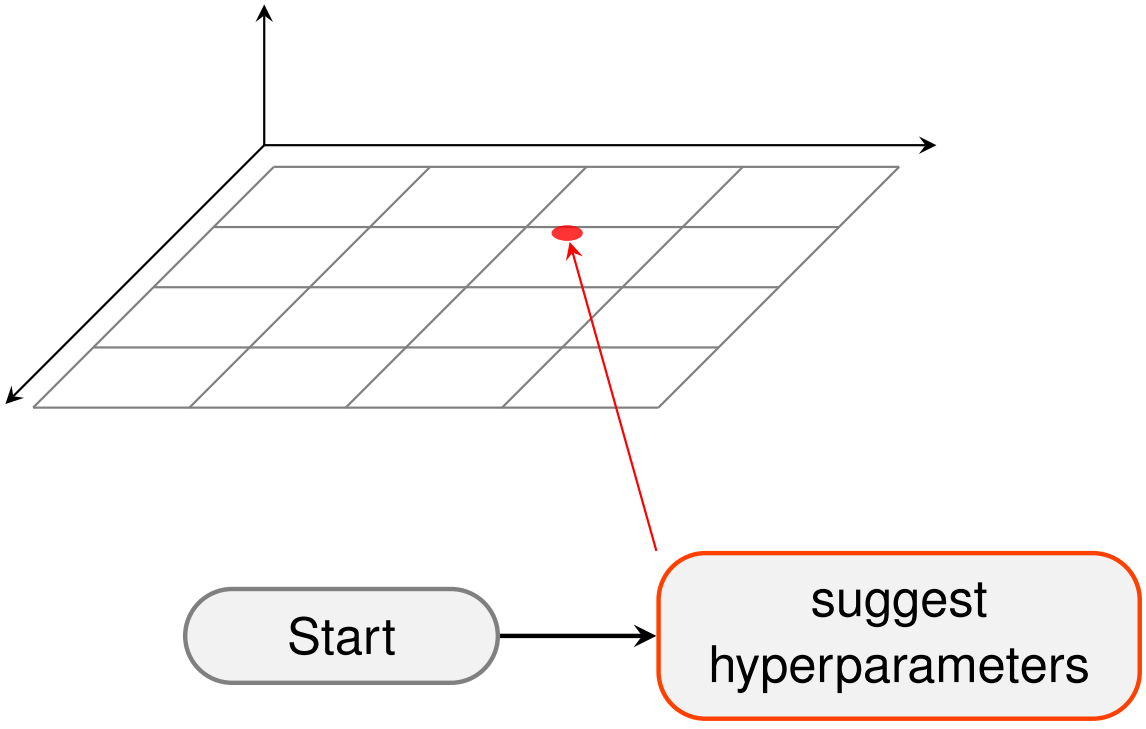
Start

TUNING

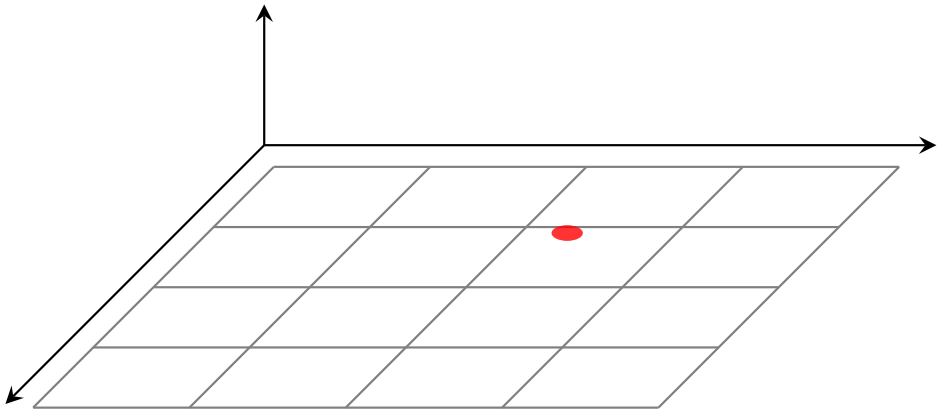


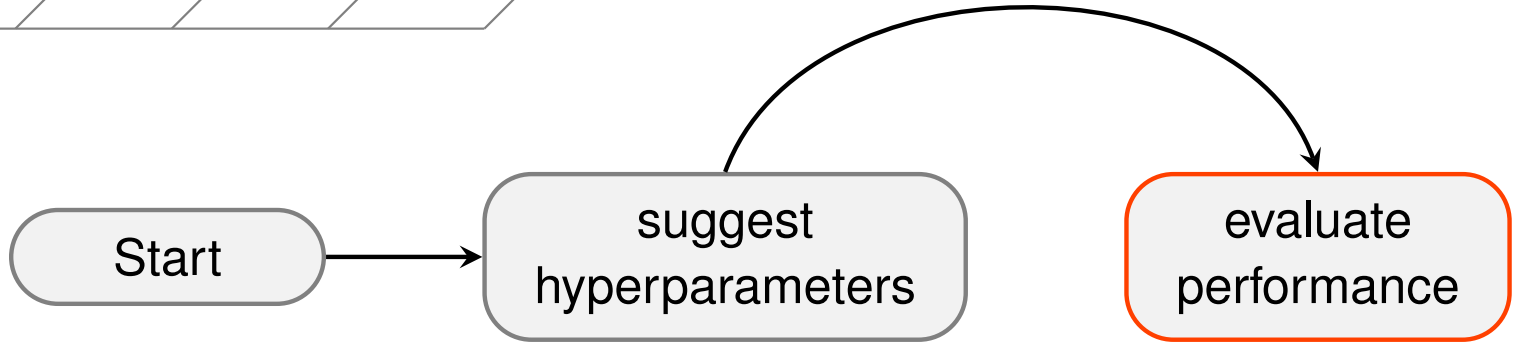


TUNING

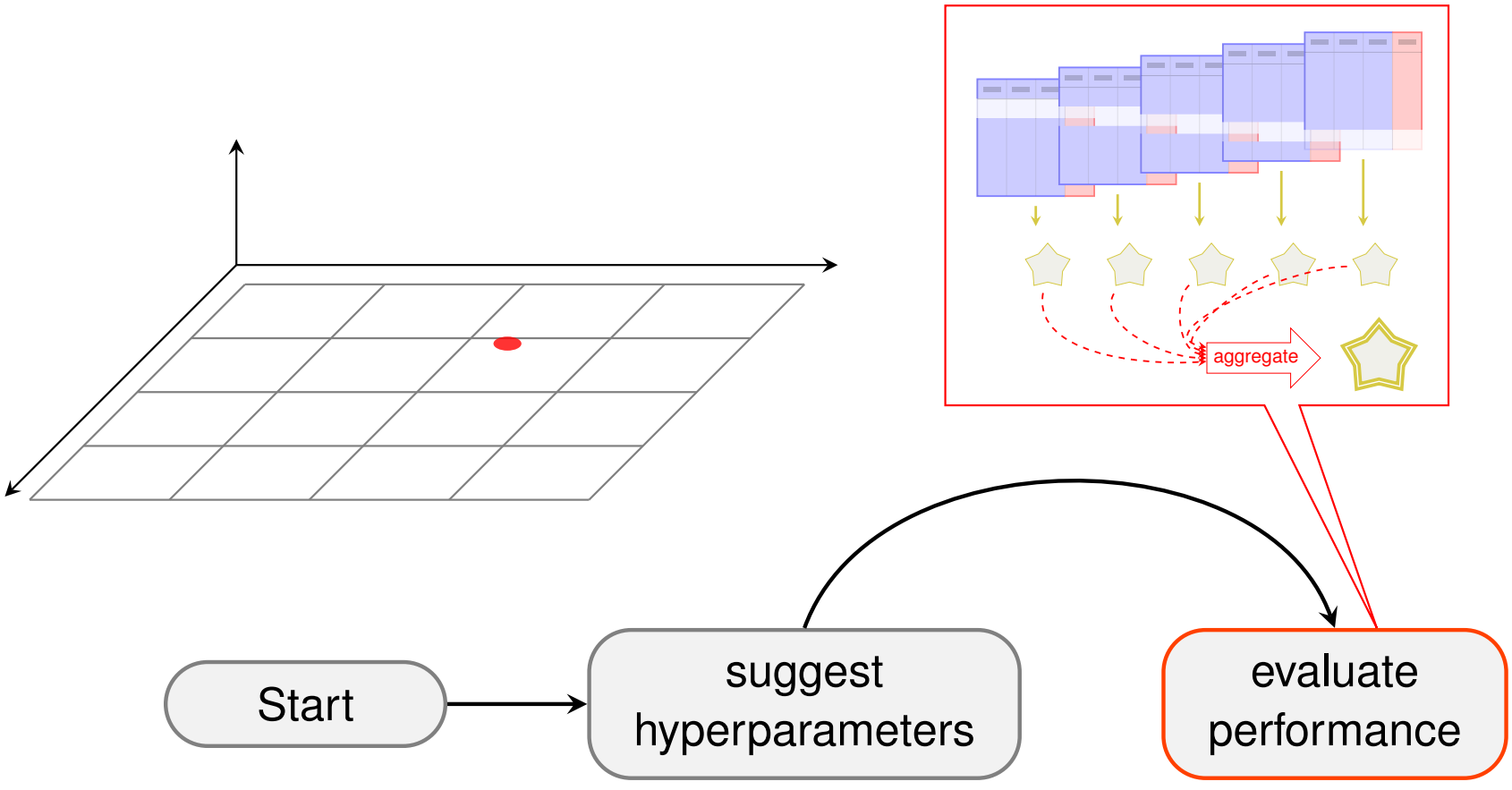


TUNING

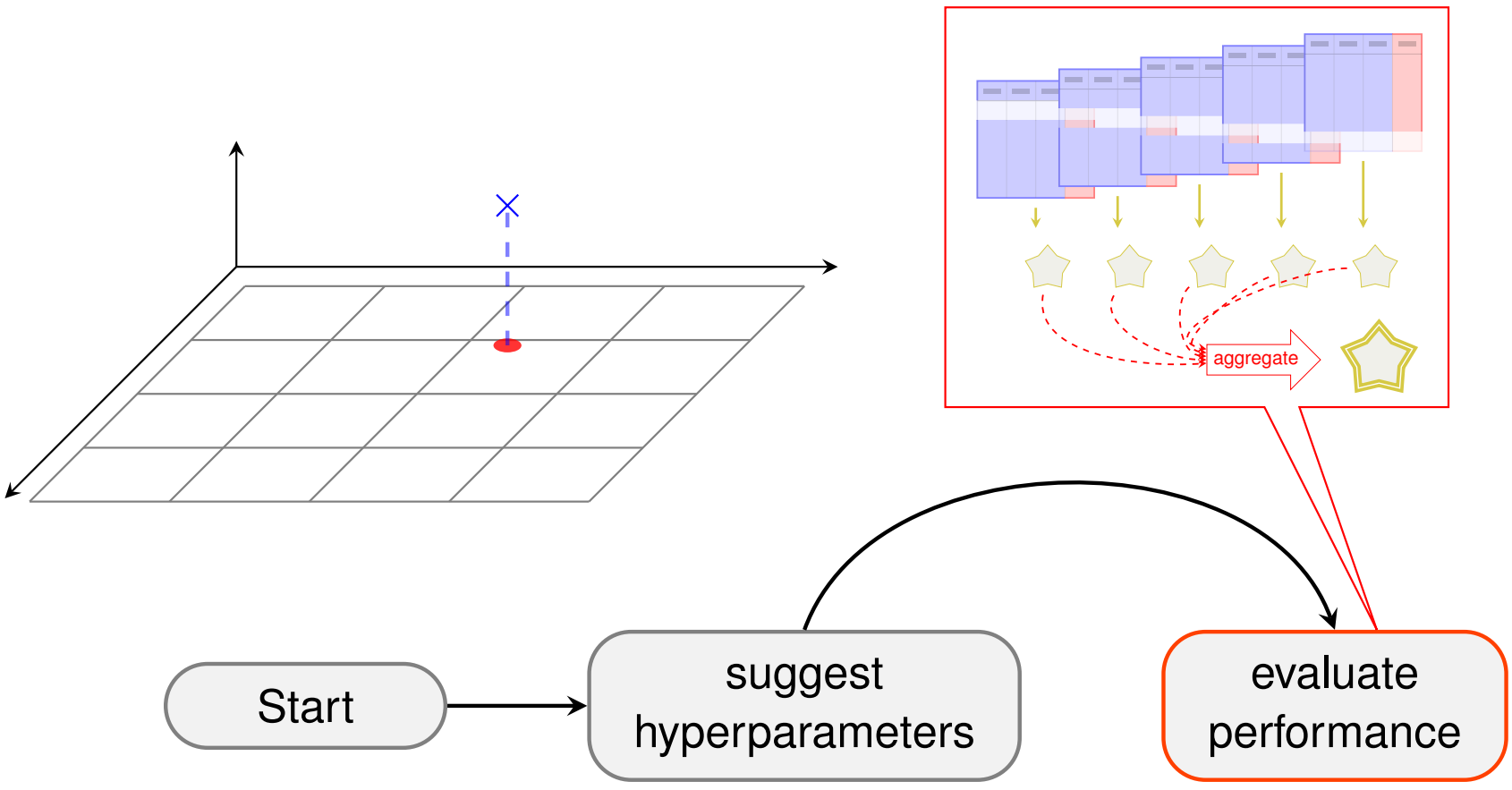




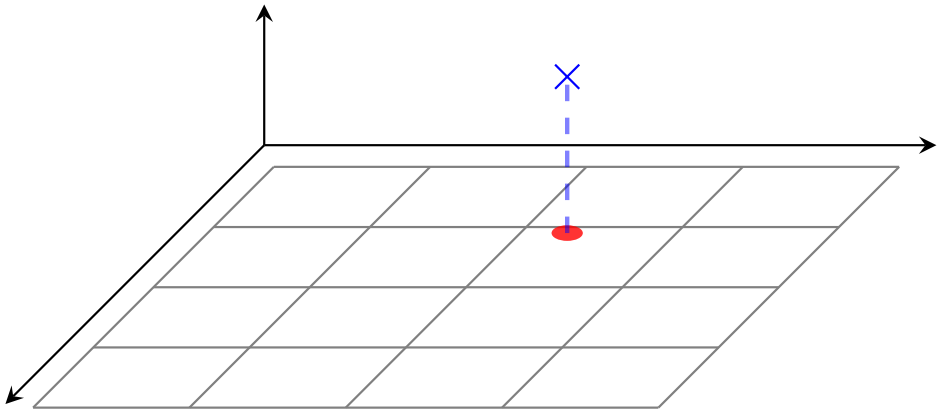
TUNING

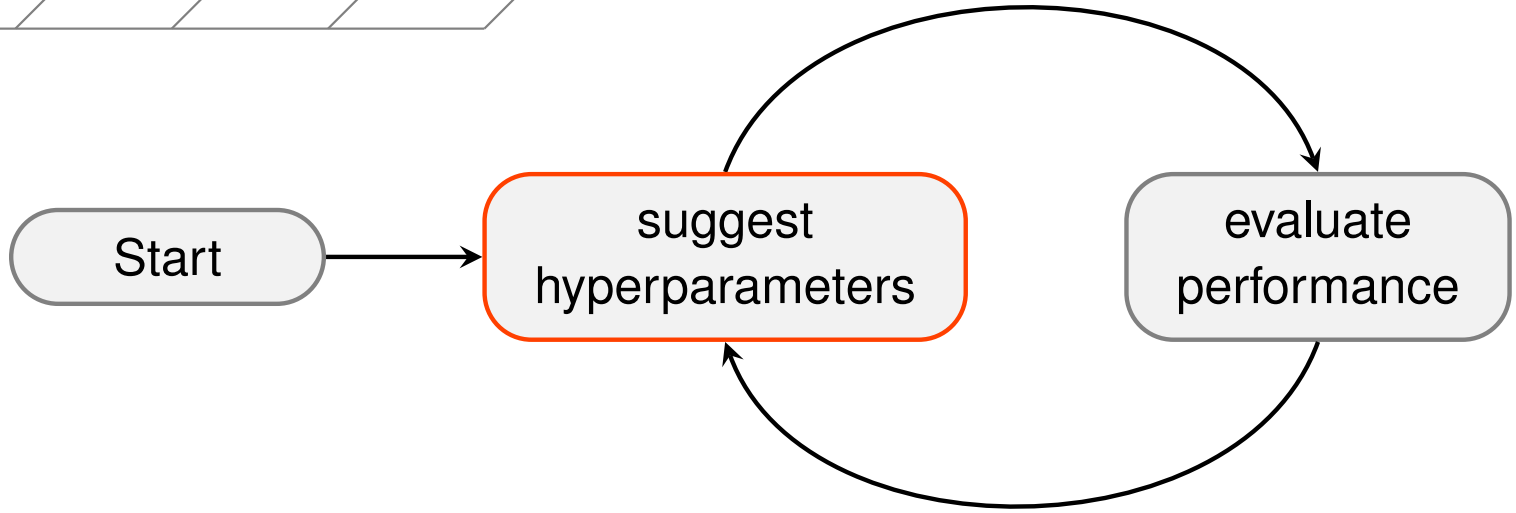

aggregate
Start
suggest
hyperparameters
evaluate
performance

TUNING

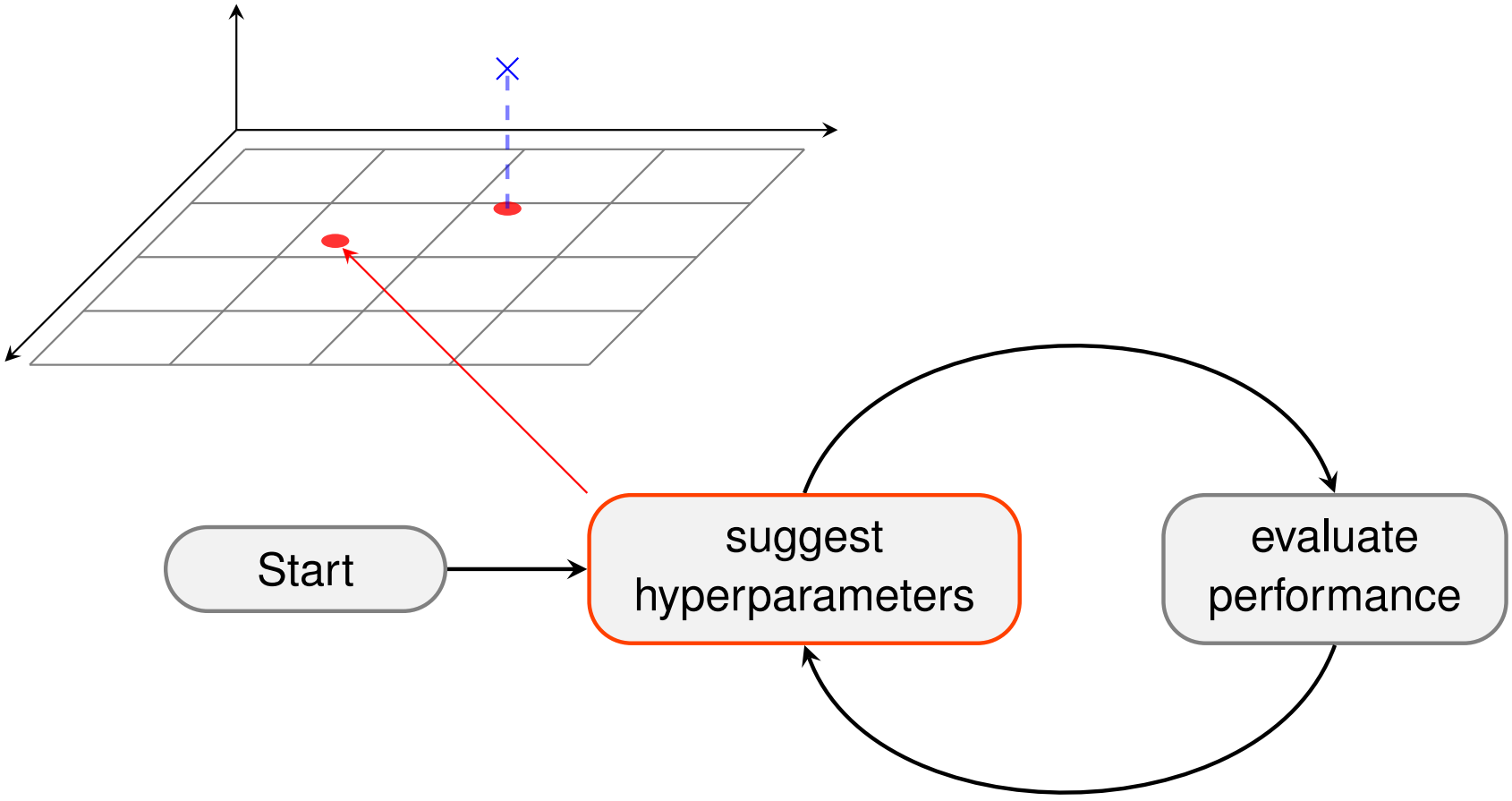

aggregate
Start
suggest
hyperparameters
evaluate
performance

TUNING

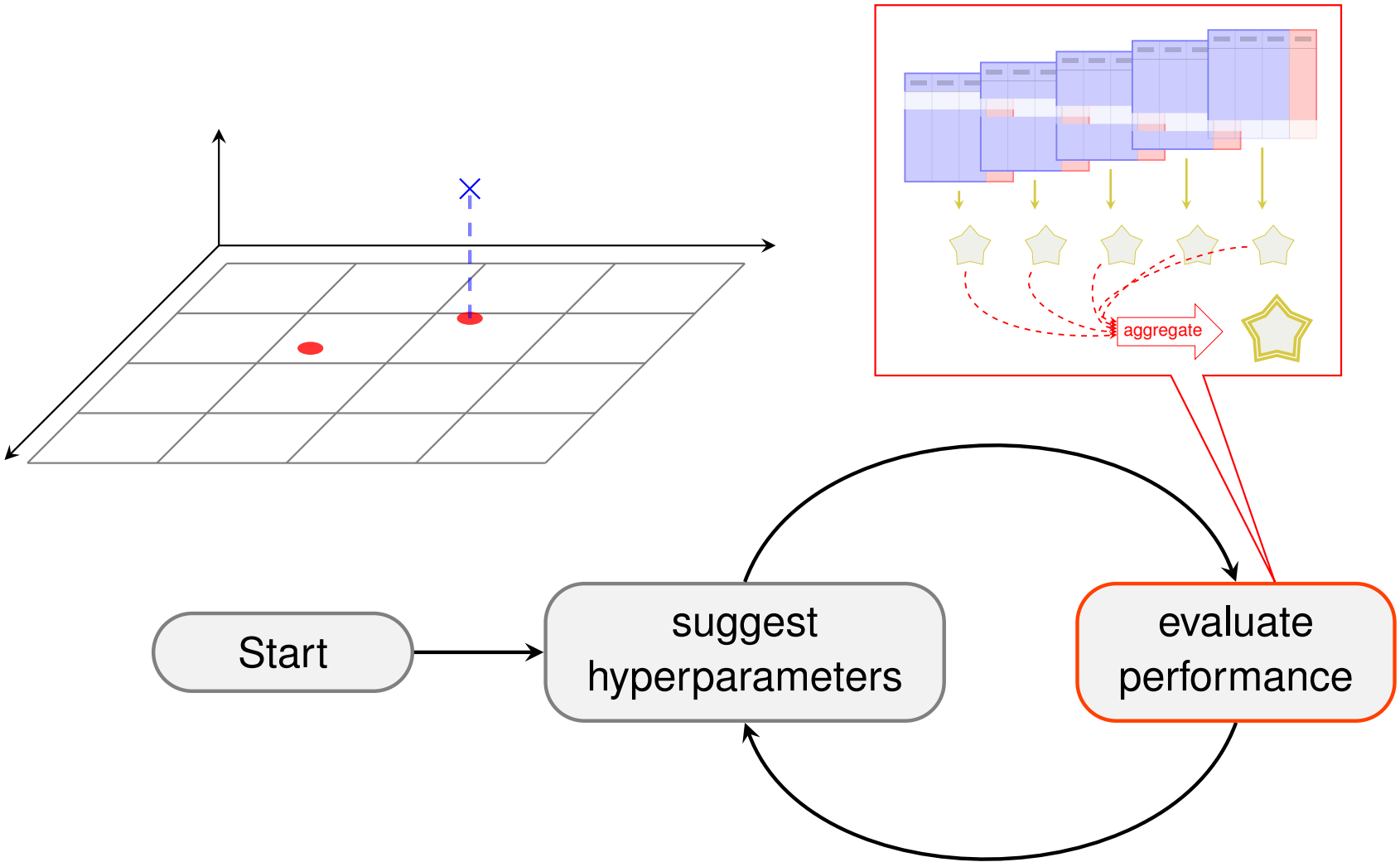




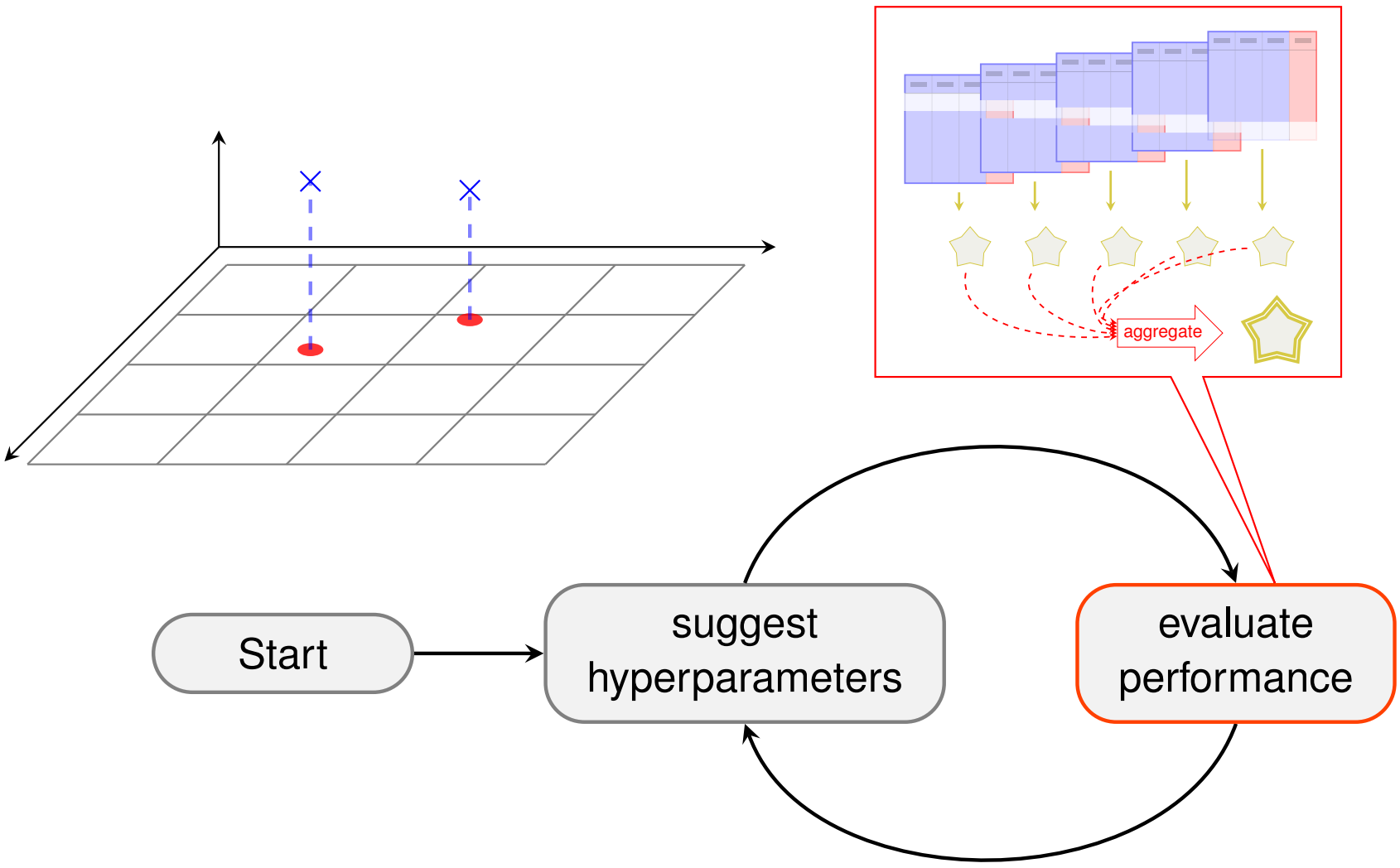
TUNING



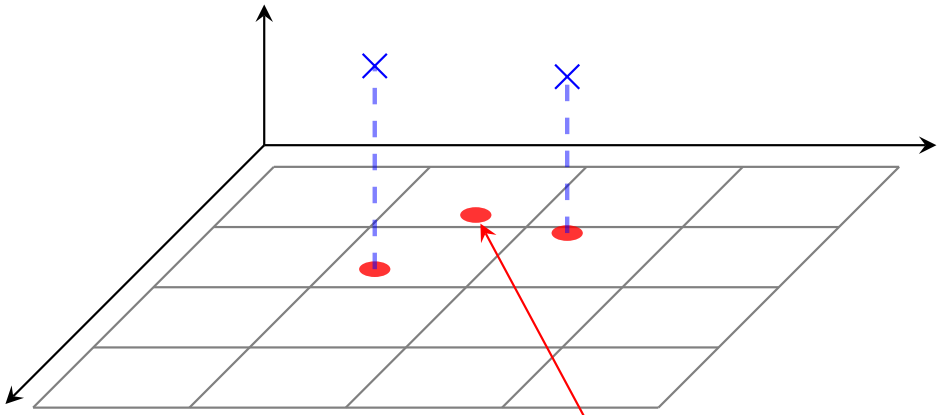
TUNING

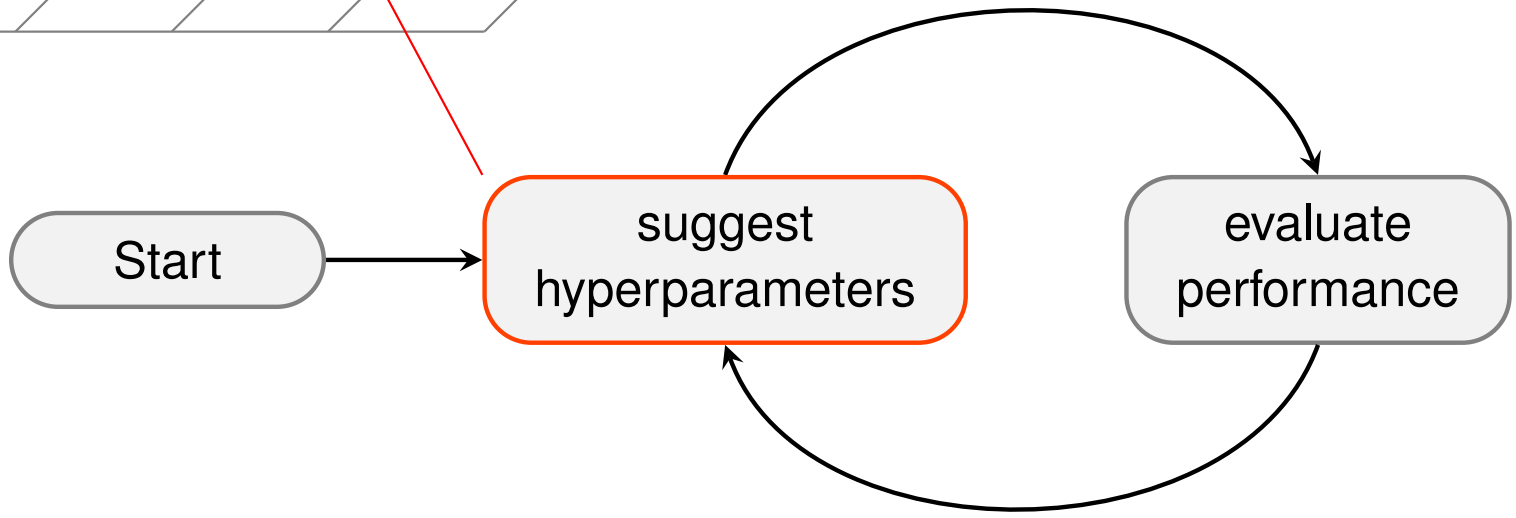

aggregate
Start
suggest
hyperparameters
evaluate
performance

TUNING

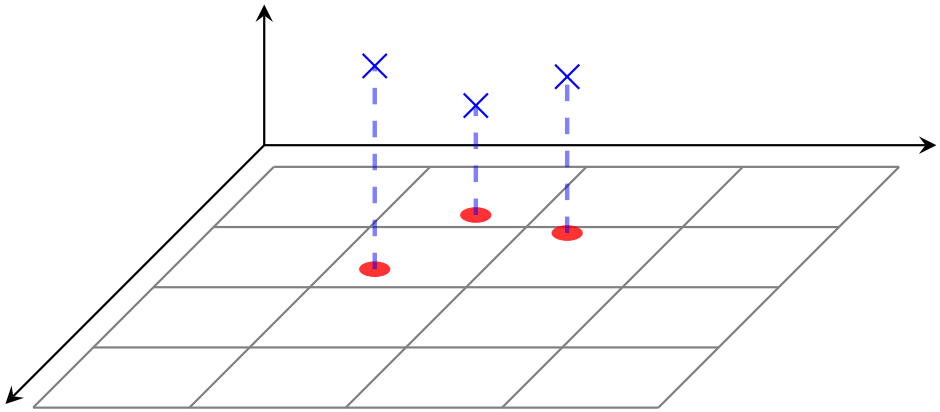

aggregate
Start
suggest
hyperparameters
evaluate
performance

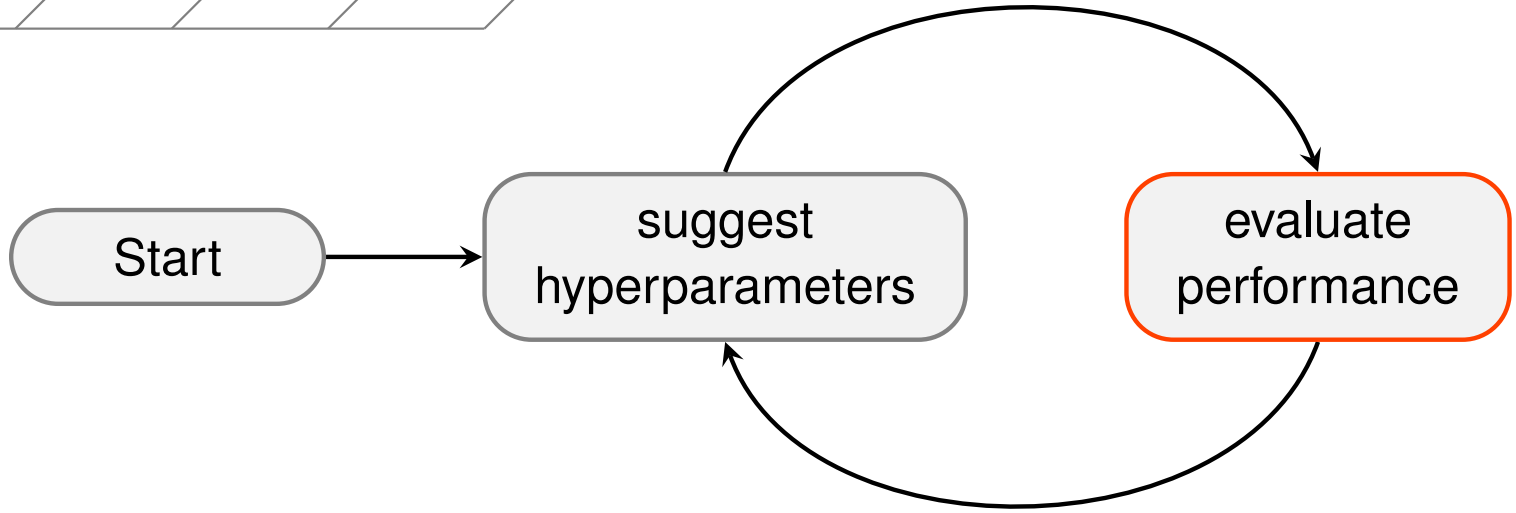
TUNING



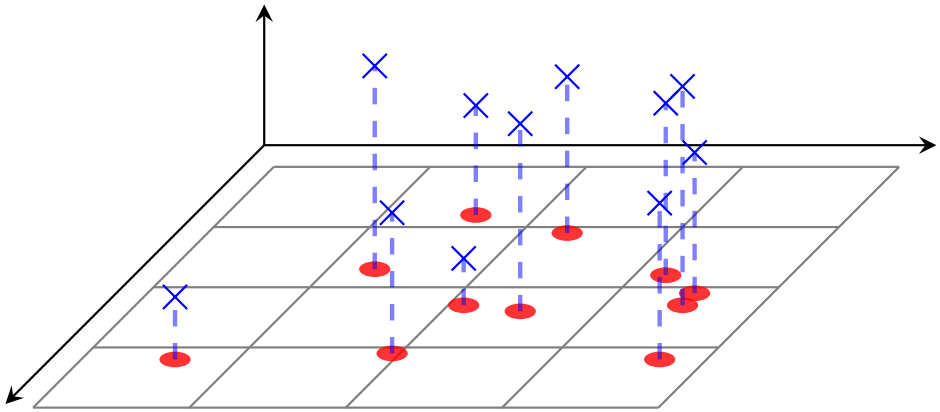


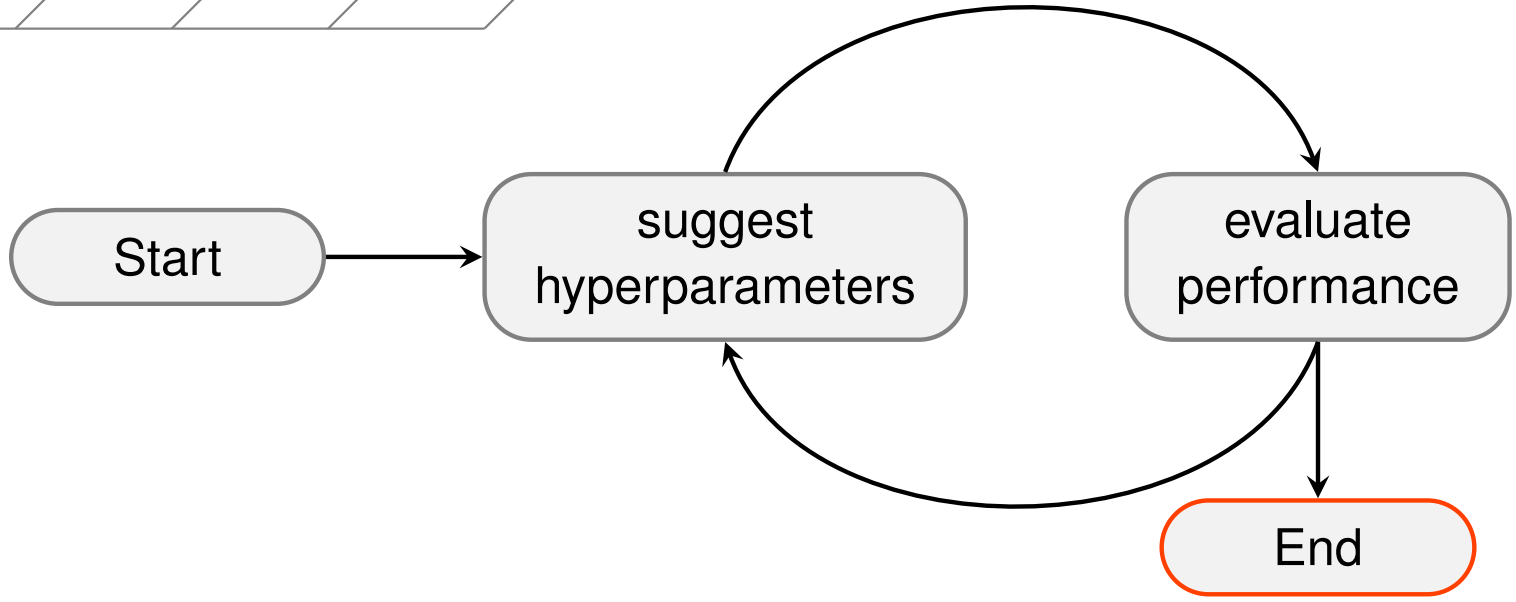
TUNING



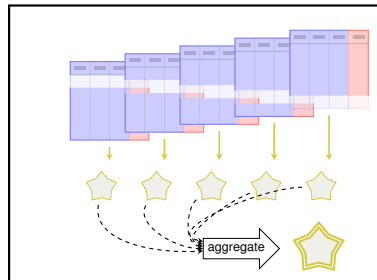


TUNING

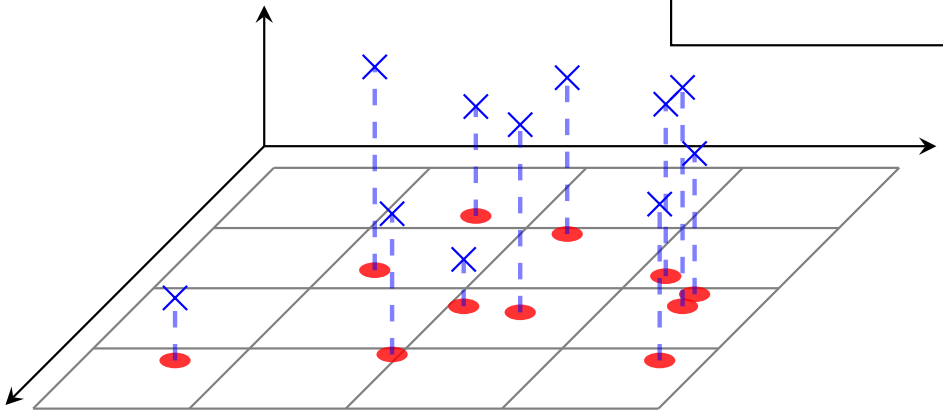


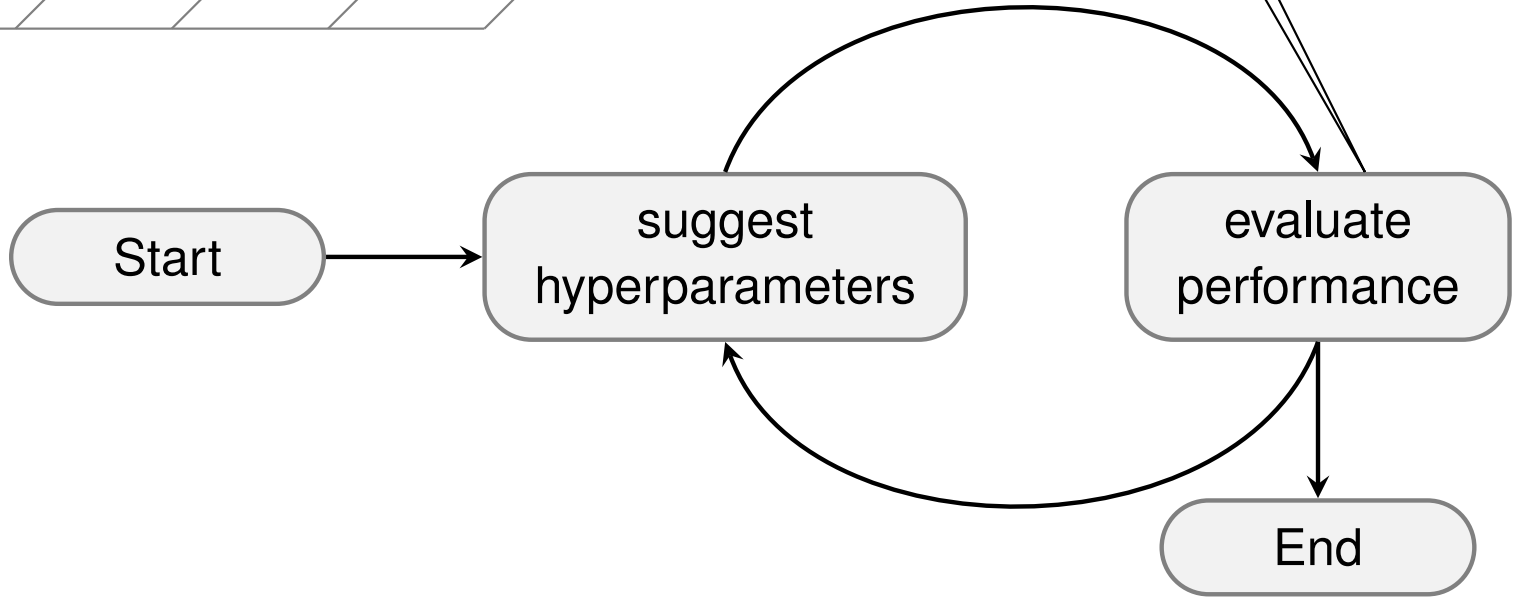


TUNING

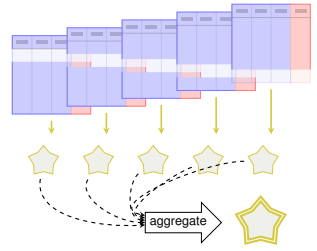


`Learner (lrn())`
`Task`
`Resampling (rsmp())`
`Measure (msr())`

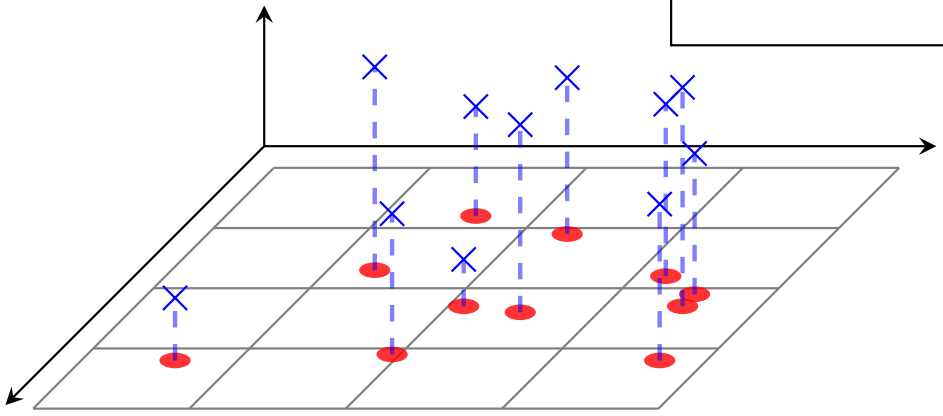




TUNING



`Learner (lrn())`
`Task`
`Resampling (rsmp())`
`Measure (msr())`



Start

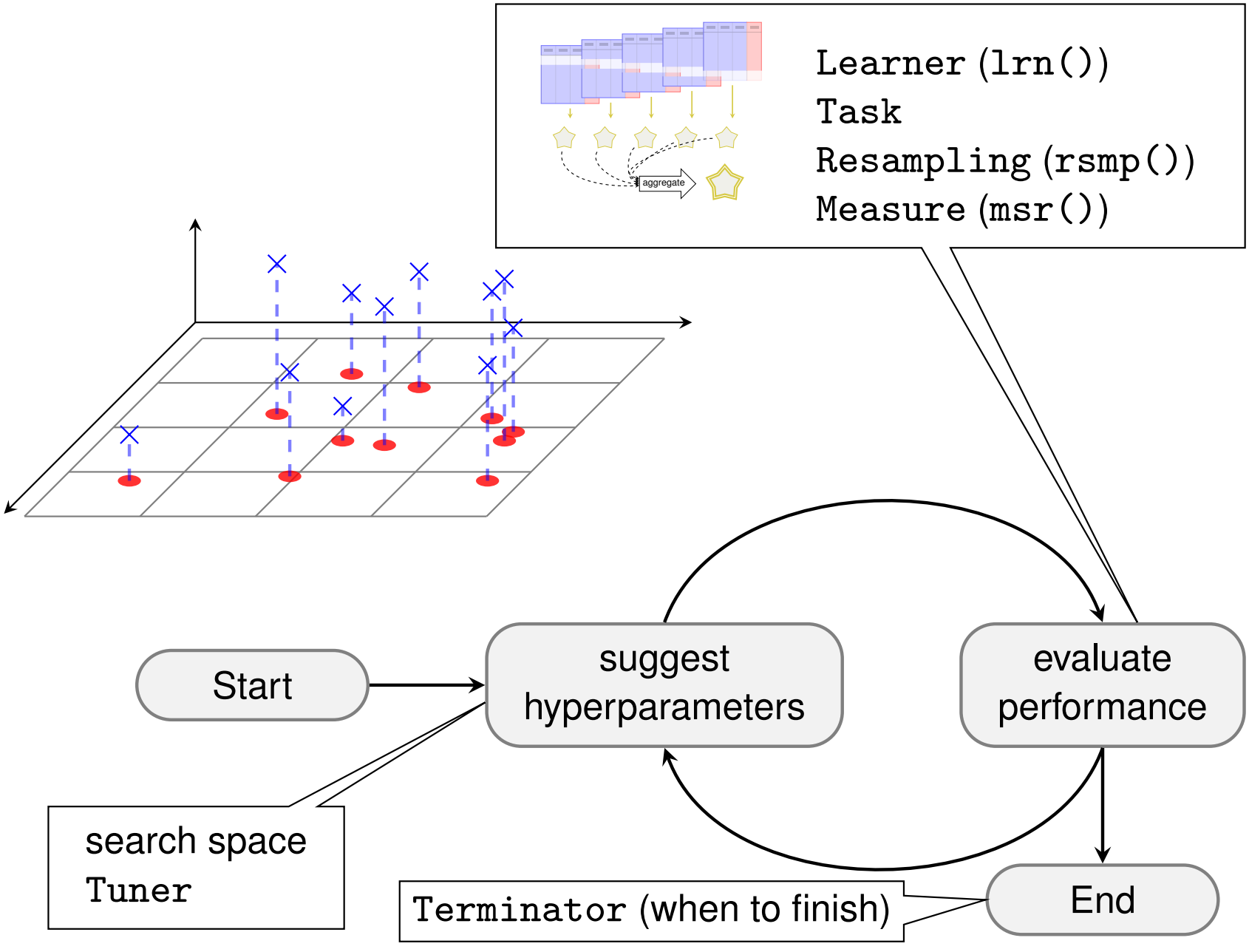
suggest hyperparameters

evaluate performance

End

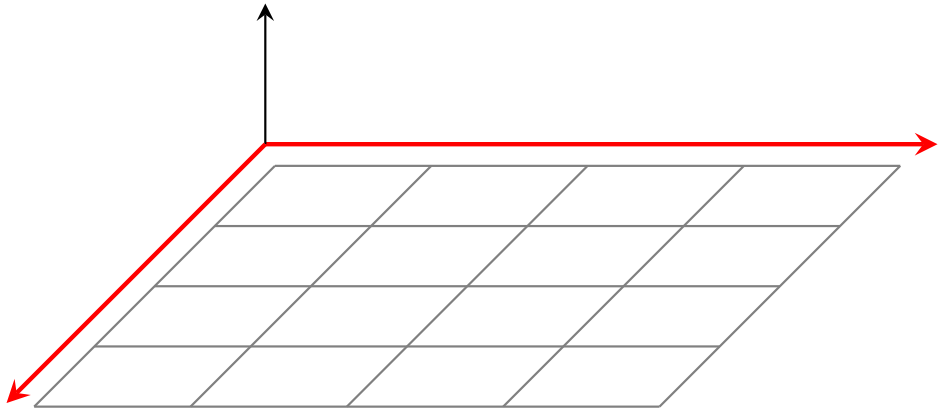
search space
`Tuner`

TUNING

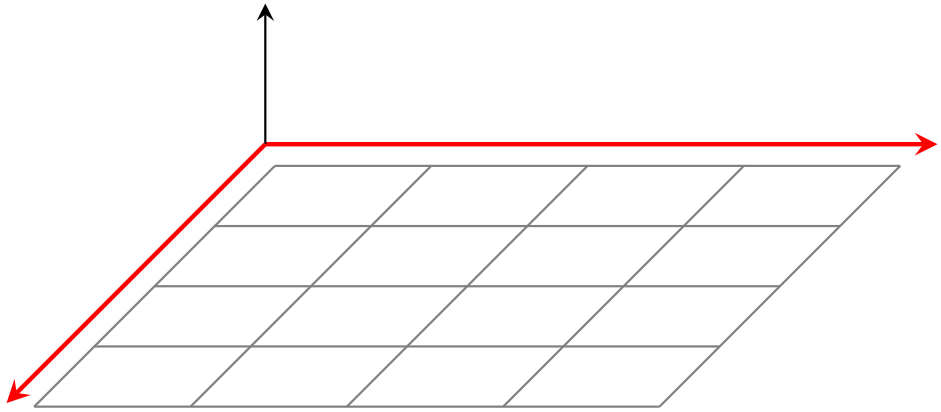

aggregate
Learner (lrn())
Task
Resampling (rsmp())
Measure (msr())
Start
suggest hyperparameters
evaluate performance
search space
Tuner
Terminator (when to finish)
End

Tuning in mlr3

SEARCH SPACE

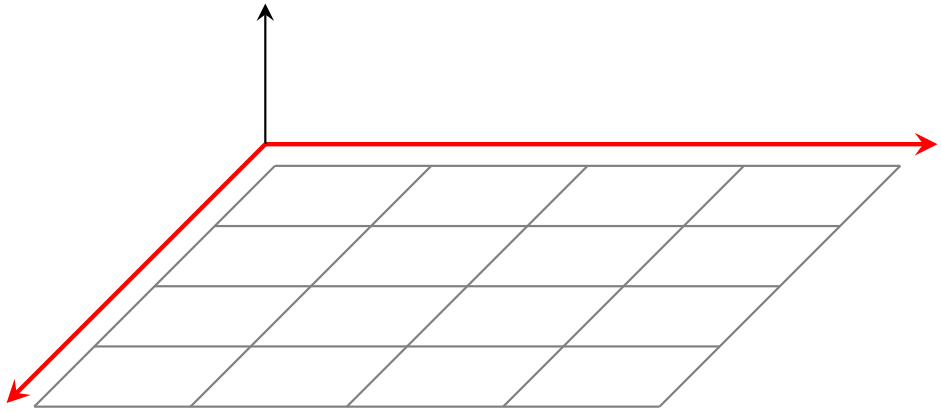


SEARCH SPACE



```
ps(param1 = ..., param2 = ..., ...)
```

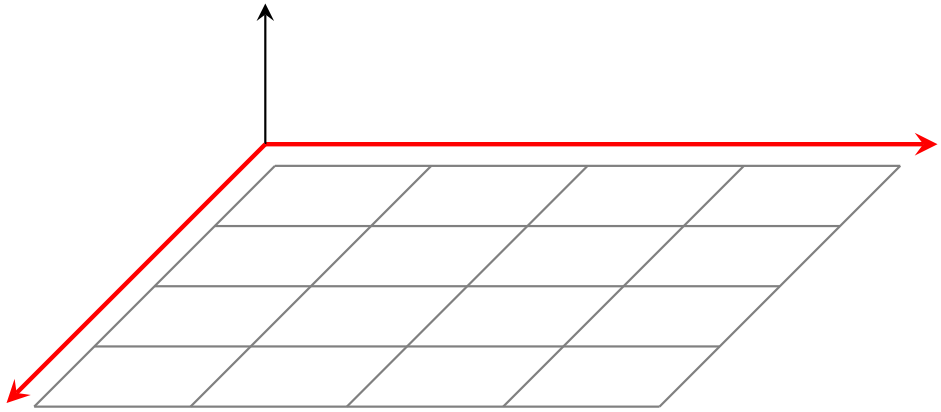
SEARCH SPACE



```
ps(param1 = ..., param2 = ..., ...)
```

Numerical parameter	`p_dbl(lower, upper)`
Integer parameter	`p_int(lower, upper)`
Discrete parameter	`p_fct(levels)`
Logical parameter	`p_lgl()`
Untyped parameter	`p_uty()`

SEARCH SPACE



```
ps(param1 = ..., param2 = ..., ...)
```

Numerical parameter	`p_dbl(lower, upper)`
Integer parameter	`p_int(lower, upper)`
Discrete parameter	`p_fct(levels)`
Logical parameter	`p_lgl()`
Untyped parameter	`p_uty()`

```
library("paradox")
searchspace_knn = ps(k = p_int(1, 20))
```

TERMINATION

- Tuning needs a *termination condition*: when to finish
- `Terminator` class
- `mlr_terminators` dictionary, `trm()` short form

```
as.data.table(mlr_terminators)
#>                  key
#> 1:        clock_time
#> 2:             combo
#> 3:             evals
#> 4:              none
#> 5:     perf_reached
#> 6:          run_time
#> 7:        stagnation
#> 8: stagnation_batch
```

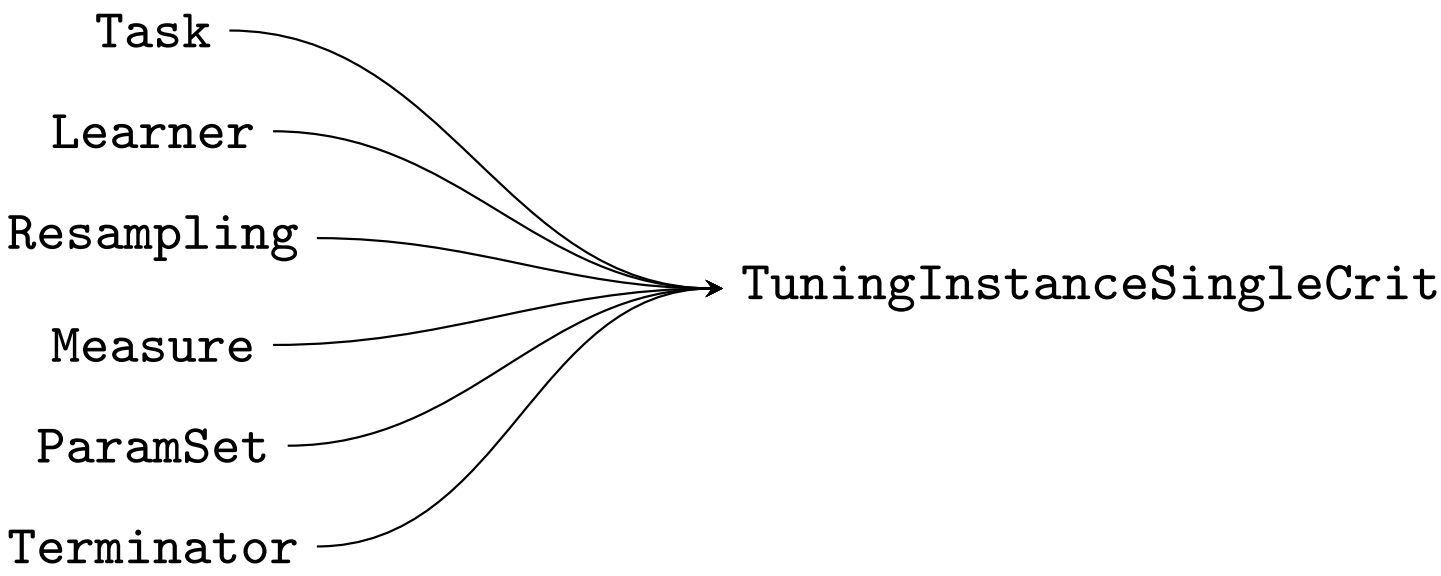
```
trm("evals", n_evals = 20)
#> <TerminatorEvals>
#> * Parameters: n_evals=20
```

TUNING METHOD

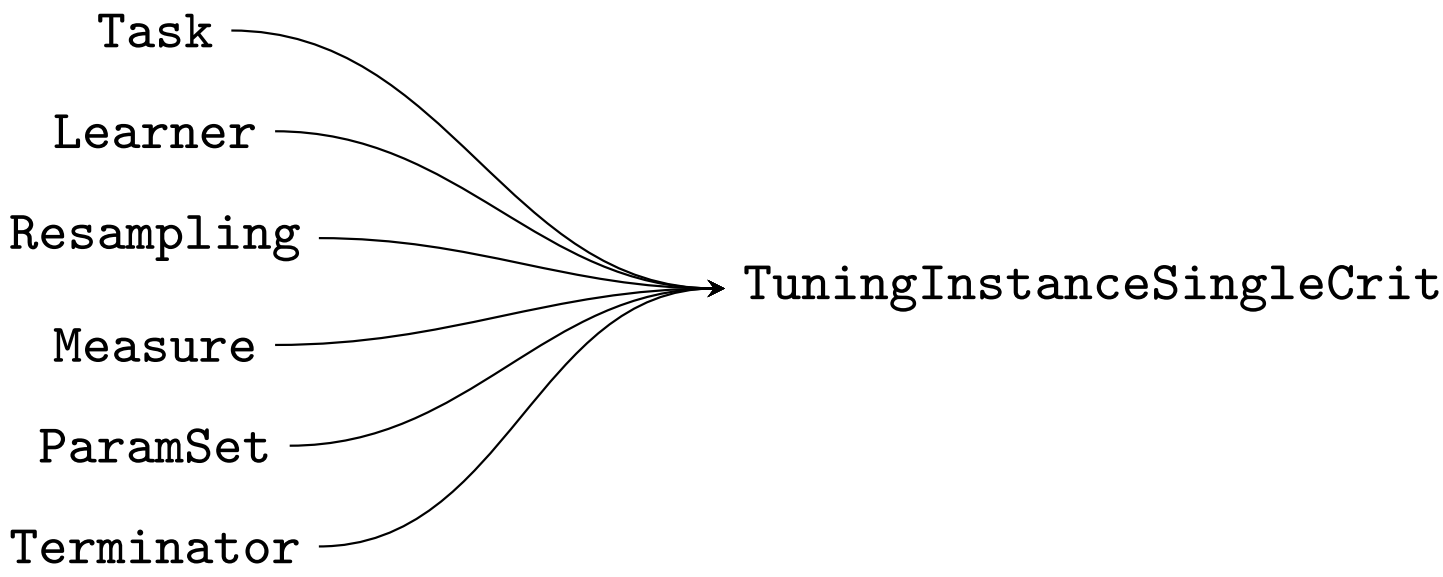
- load `Tuner` with `tnr()`, set parameters
- ```
  gsearch = tnr("grid_search", resolution = 3)

  print(gsearch)
  #> <TunerGridSearch>
  #> * Parameters: resolution=3, batch_size=1
  #> * Parameter classes: ParamLgl, ParamInt, ParamDbl, ParamFct
  #> * Properties: dependencies, single-crit, multi-crit
  #> * Packages: -
  ```
- common parameter `batch_size` for parallelization
  ```

CALLING THE TUNER



CALLING THE TUNER




```
inst = TuningInstanceSingleCrit$new(
  tsk("iris"), lrn("classif.kknn", kernel="rectangular"),
  rsmp("holdout"), msr("classif.ce"), trm("none"),
  searchspace_knn
)
```

CALLING THE TUNER

```
gsearch$optimize(inst)

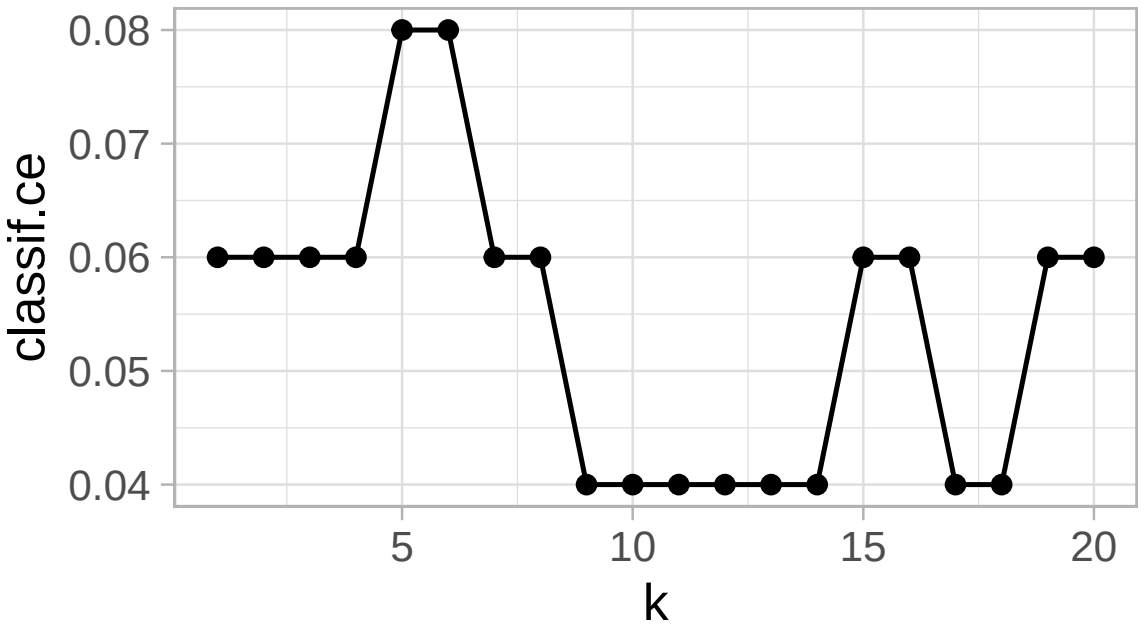
#> INFO  [15:07:32.603] Starting to optimize 1 parameter(s) with '<OptimizerGrid
#> INFO  [15:07:32.642] Evaluating 1 configuration(s)
#> INFO  [15:07:33.800] Result of batch 1:
#> INFO  [15:07:33.801]   k classif.ce                                    uhash
#> INFO  [15:07:33.801]  10       0.04 cc2a0cc9-b233-4aa7-abce-6d2f39d8ddba
#> INFO  [15:07:33.803] Evaluating 1 configuration(s)
#> INFO  [15:07:34.016] Result of batch 2:
#> INFO  [15:07:34.018]  k classif.ce                                   uhash
#> INFO  [15:07:34.018]  1       0.06 4c6e7c20-8b21-4999-bd71-129126c7a918
#> INFO  [15:07:34.020] Evaluating 1 configuration(s)
#> INFO  [15:07:34.116] Result of batch 3:
#> INFO  [15:07:34.118]   k classif.ce                                    uhash
#> INFO  [15:07:34.118]  20       0.08 b3f6a62c-d6fd-4eb9-94ca-db66118f5fed
#> INFO  [15:07:34.124] Finished optimizing after 3 evaluation(s)
#> INFO  [15:07:34.125] Result:
#> INFO  [15:07:34.127]   k learner_param_vals  x_domain classif.ce
#> INFO  [15:07:34.127]  10          <list[2]> <list[1]>       0.04
#>     k learner_param_vals  x_domain classif.ce
#> 1: 10          <list[2]> <list[1]>       0.04
```

TUNING RESULTS

```
gsearch = tnr("grid_search", resolution = 20)
inst = TuningInstanceSingleCrit$new(
  tsk("iris"), lrn("classif.kknn", kernel="rectangular"),
  rsmp("holdout"), msr("classif.ce"), trm("none"),
  searchspace_knn)
gsearch$optimize(inst)

#>     k learner_param_vals  x_domain classif.ce
#> 1: 11          <list[2]> <list[1]>       0.04

ggplot(inst$archive$data(), aes(x = k, y = classif.ce)) +
  geom_line() + geom_point()
```



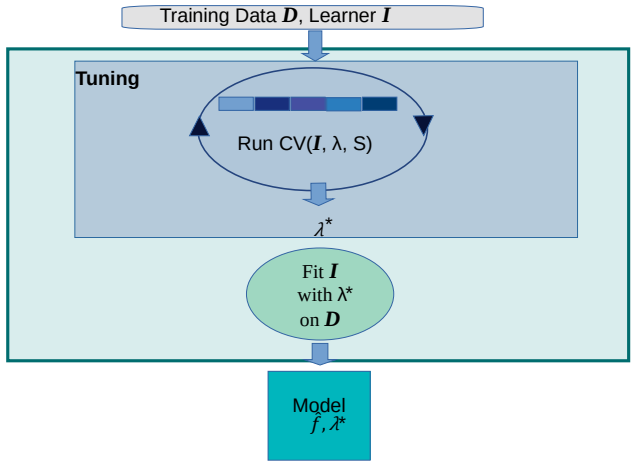
Nested Resampling

NESTED RESAMPLING

- Need to perform nested resampling to estimate tuned learner performance

$\Rightarrow$ Treat tuning as if it were a `Learner`!

  - Training:
    1. Tune model using (inner) resampling
    2. Train final model with best parameters on all (i.e. outer resampling) data
  - Predicting: Just use final model



NESTED RESAMPLING

```
optlrn = AutoTuner$new(lrn("classif.kknn", kernel="rectangular"),
  rsmp("holdout"), msr("classif.ce"), trm("none"),
  tnr("grid_search", resolution = 10), searchspace_knn)
```

```
optlrn$train(tsk("iris"))
```

```
optlrn$model$learner

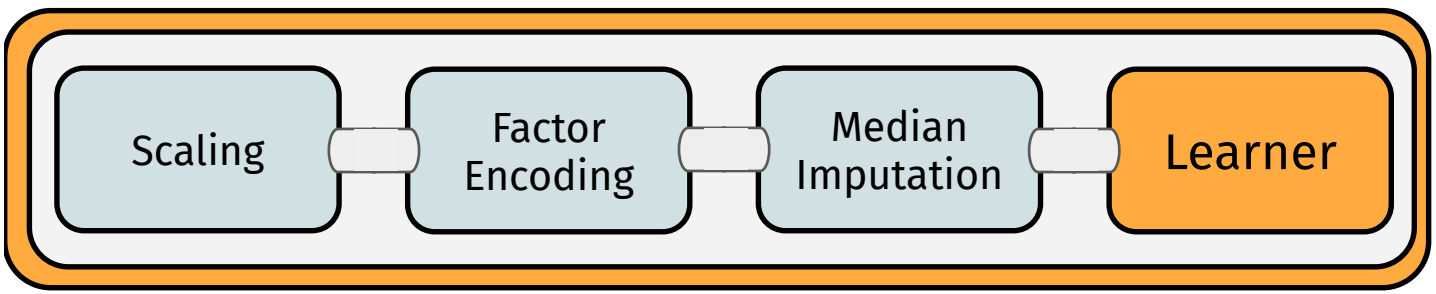
#> <LearnerClassifKKNN:classif.kknn>
#> * Model: list
#> * Parameters: kernel=rectangular, k=18
#> * Packages: kknn
#> * Predict Type: response
#> * Feature types: logical, integer, numeric, factor, ordered
#> * Properties: multiclass, twoclass
```

MLR3PIPELINES

Machine Learning Workflows:

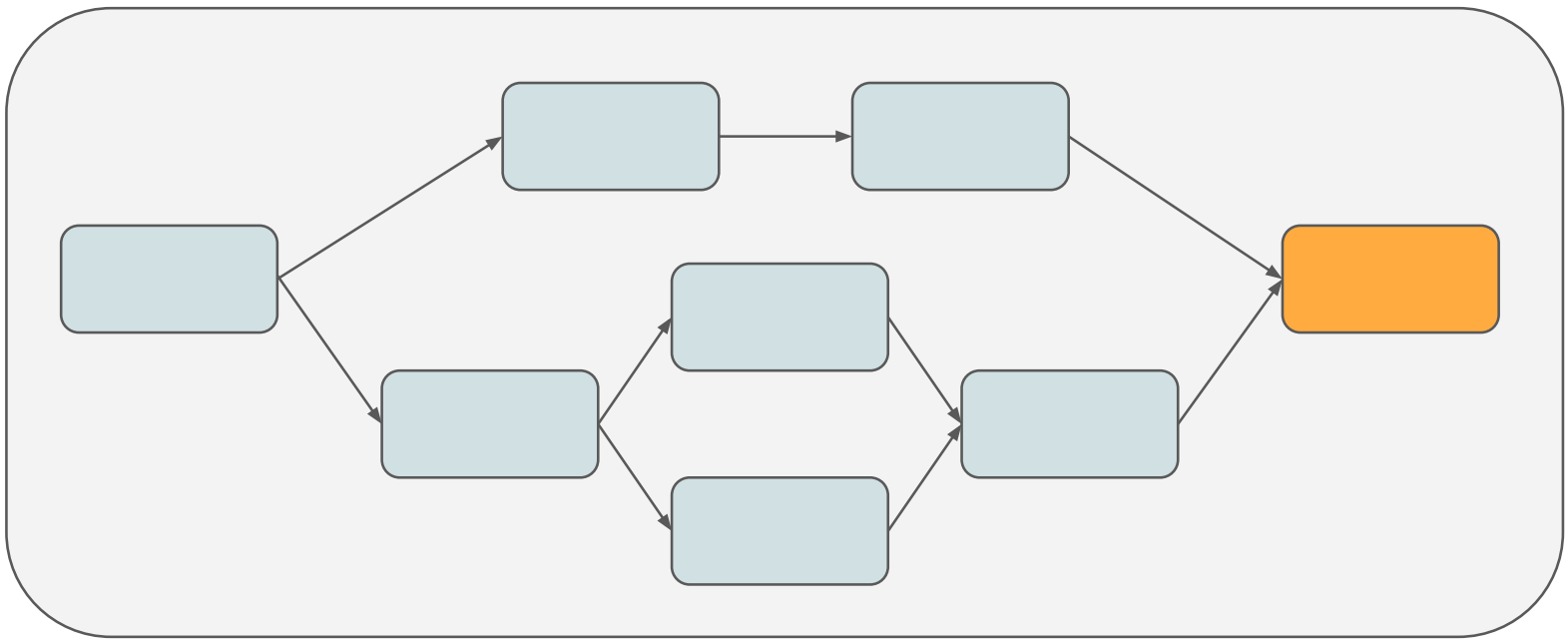
- **Preprocessing**: Feature extraction, feature selection, missing data imputation,...
- **Ensemble methods**: Model averaging, model stacking
- `mlr3`: modular model fitting

$\Rightarrow$ `mlr3pipelines`: modular ML workflows



MACHINE LEARNING WORKFLOWS

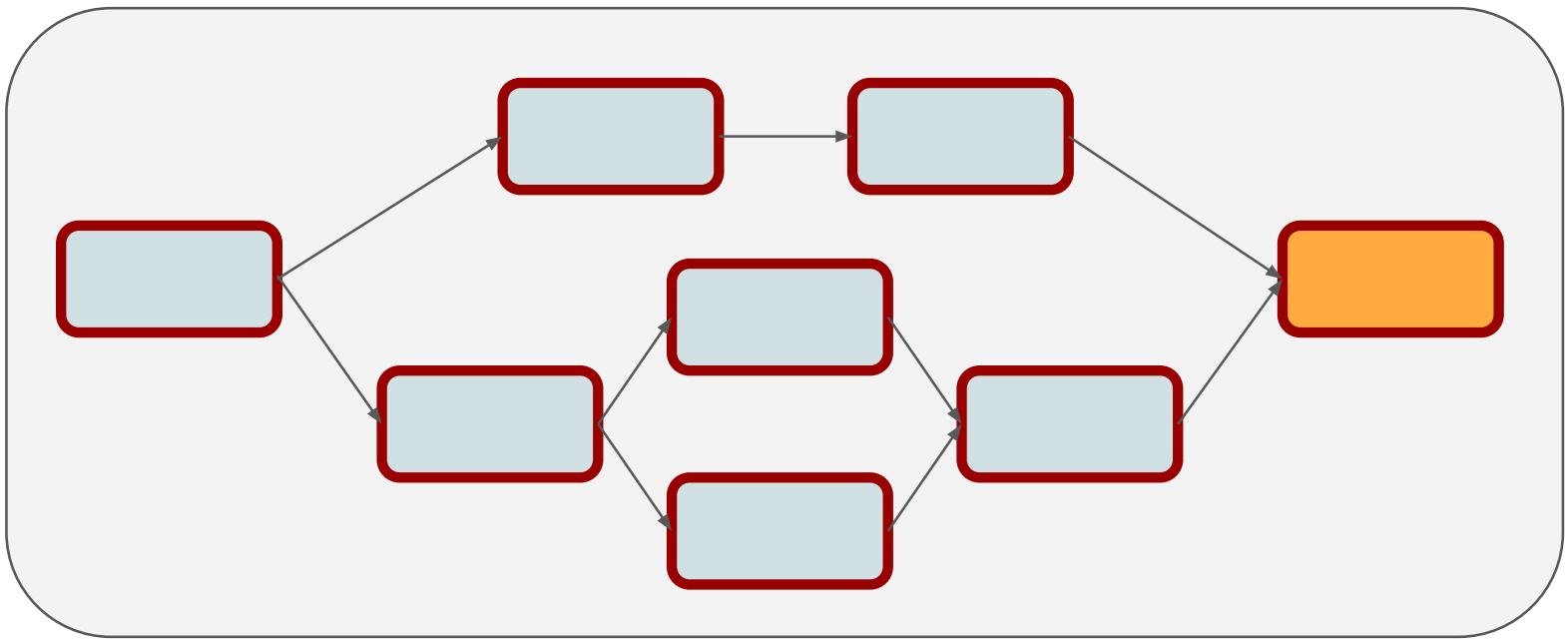
– what do they look like?



MACHINE LEARNING WORKFLOWS

– what do they look like?

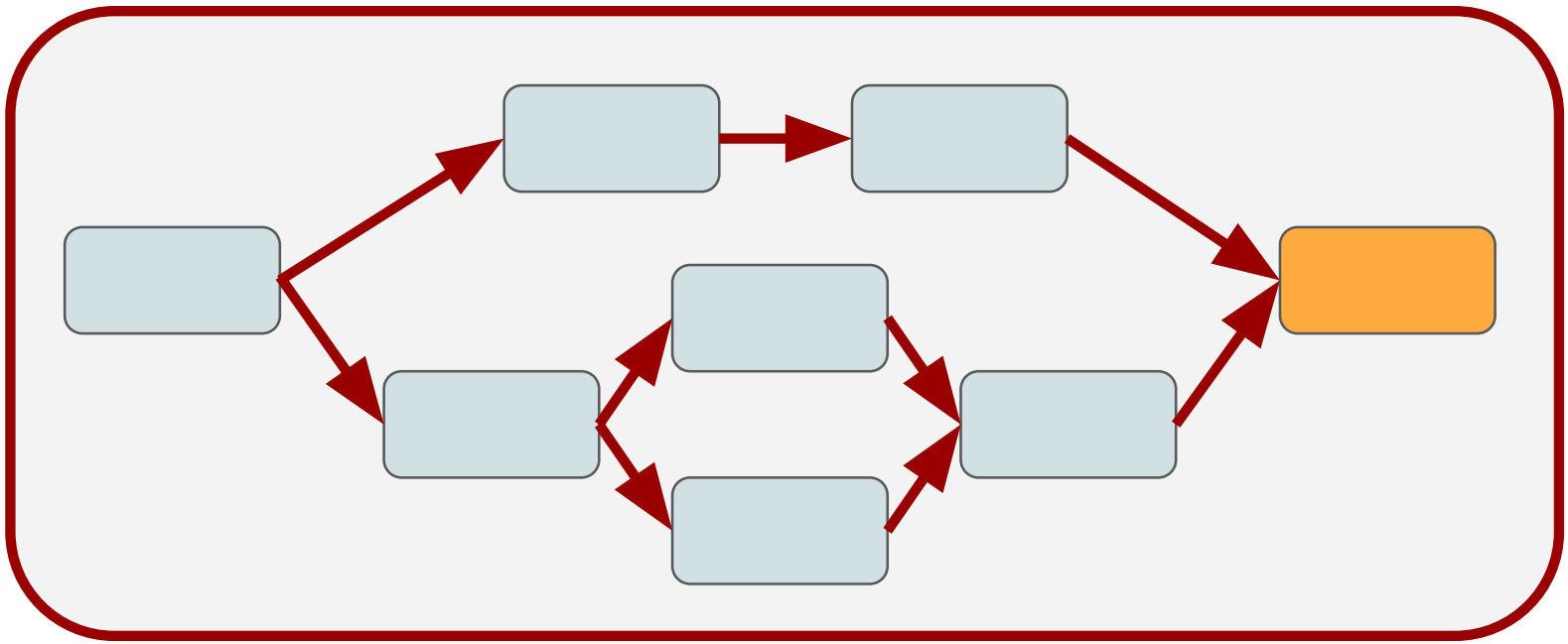
- **Building blocks**: *what* is happening? $\rightarrow$ `PipeOp`



MACHINE LEARNING WORKFLOWS

– what do they look like?

- **Building blocks**: *what* is happening? $\rightarrow$ `PipeOp`
- **Structure**: in what *sequence* is it happening? $\rightarrow$ `Graph`

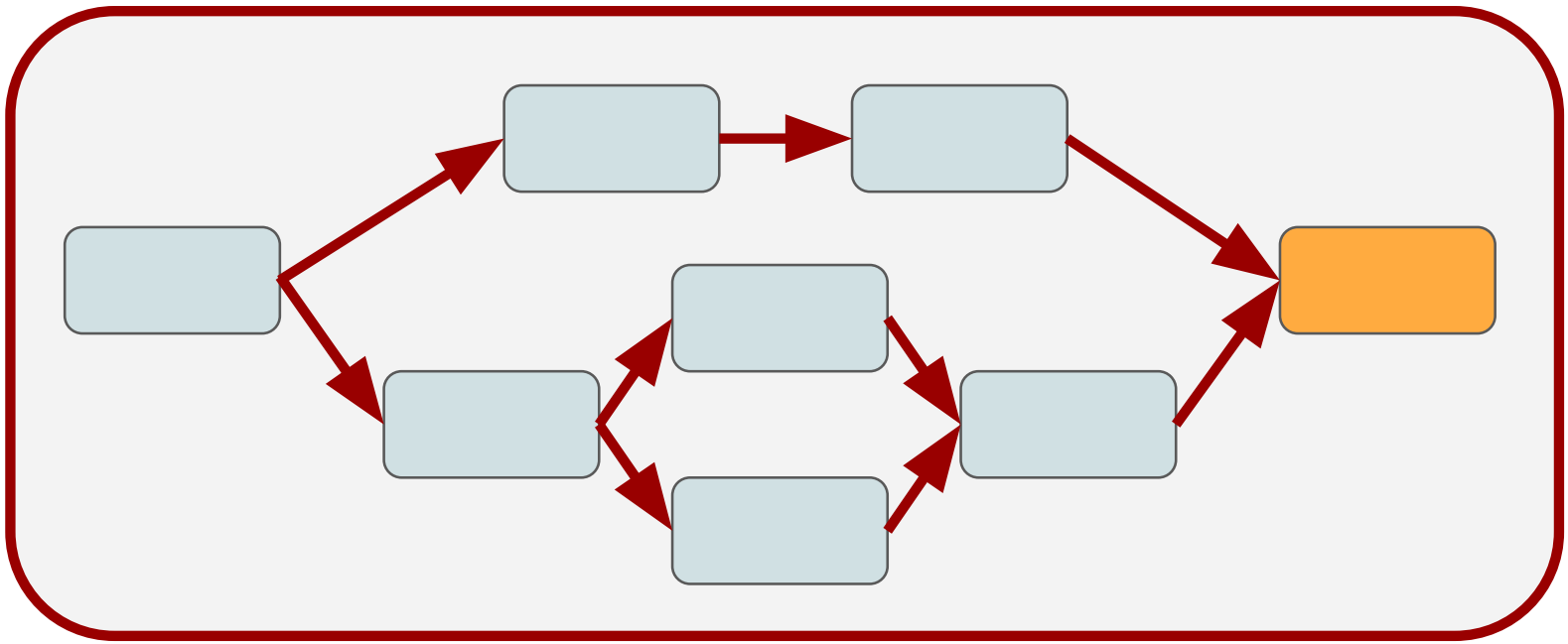


MACHINE LEARNING WORKFLOWS

– what do they look like?

- **Building blocks**: *what* is happening? $\rightarrow$ `PipeOp`
- **Structure**: in what *sequence* is it happening? $\rightarrow$ `Graph`

$\Rightarrow$ `Graph`: `PipeOps` as **nodes** with **edges** (data flow) between them

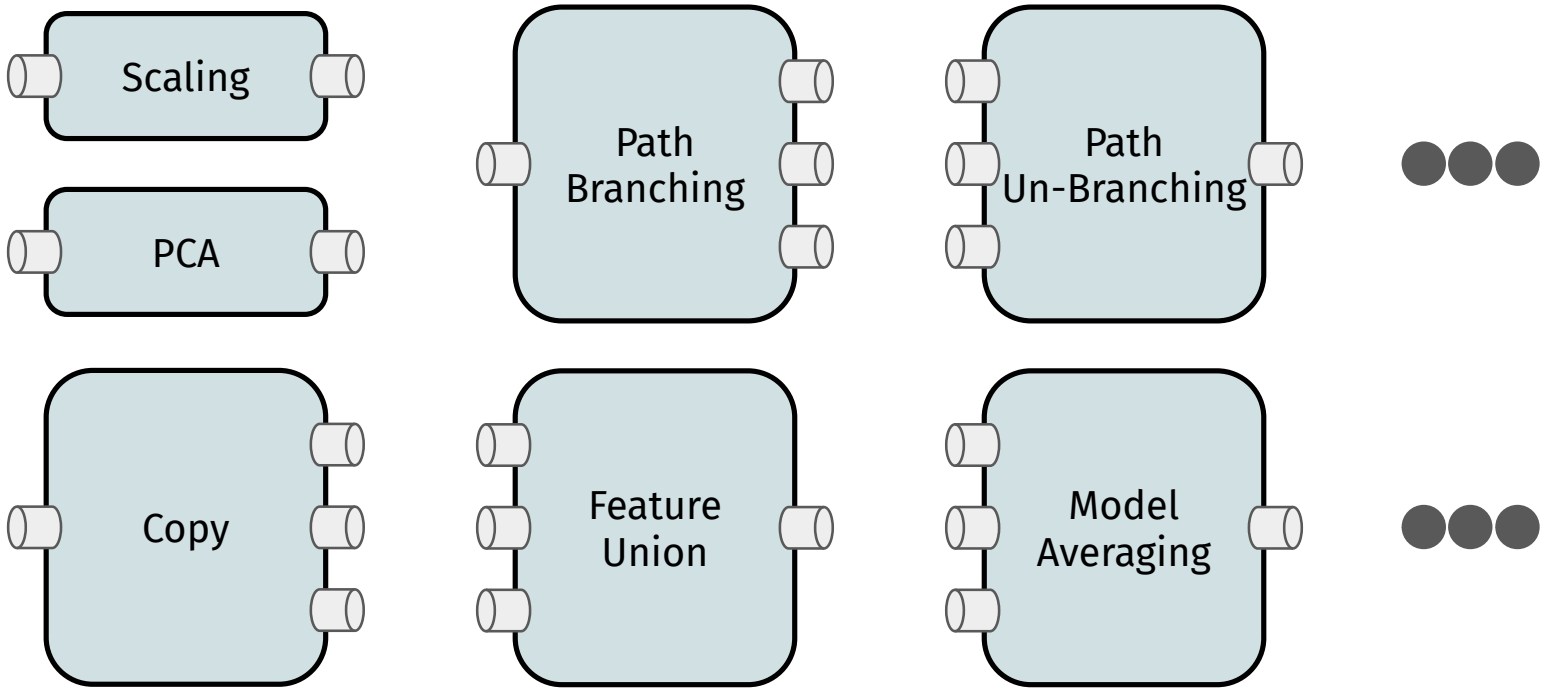


PipeOps

THE BUILDING BLOCKS

PipeOp: Single Unit of Data Operation

- `pip = po("scale")` to construct
- `pip$train()`: process data and create `pip$state`
- `pip$predict()`: process data depending on the `pip$state`
- Multiple inputs or multiple outputs



PIPEOPS SO FAR

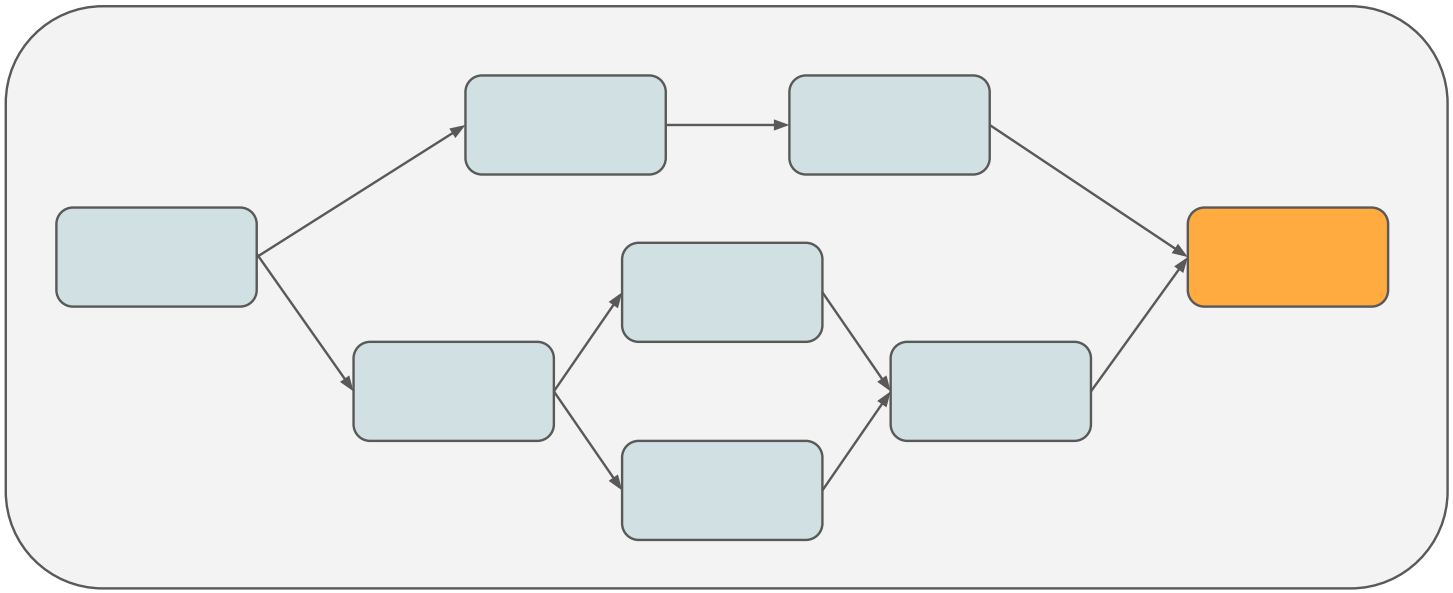
```
as.data.table(mlr_pipeops)
```

```
#>                key      packages                                 tags ...
#> 1           boxcox bestNormalize                  data transform      
#> 2           branch                                          meta      
#> 3            chunk                                          meta      
#> 4   classbalancing                imbalanced data, data transform      
#> 5       classifavg         stats                           ensemble    
#> 6     classweights                imbalanced data, data transform      
#> 7         colapply                                 data transform      
#> 8  collapsefactors                                 data transform      
#> 9         colroles                                 data transform      
#> 10            copy                                          meta      
#> 11    datefeatures                                 data transform      
#> 12          encode         stats            encode, data transform      
#> 13    encodeimpact                          encode, data transform      
#> 14      encodelmer  lme4, nloptr            encode, data transform      
#> 15    featureunion                                    ensemble    
#> 16          filter               feature selection, data transform      
#> 17      fixfactors                       robustify, data transform      
#> [...]
```

Graph Operations

THE STRUCTURE

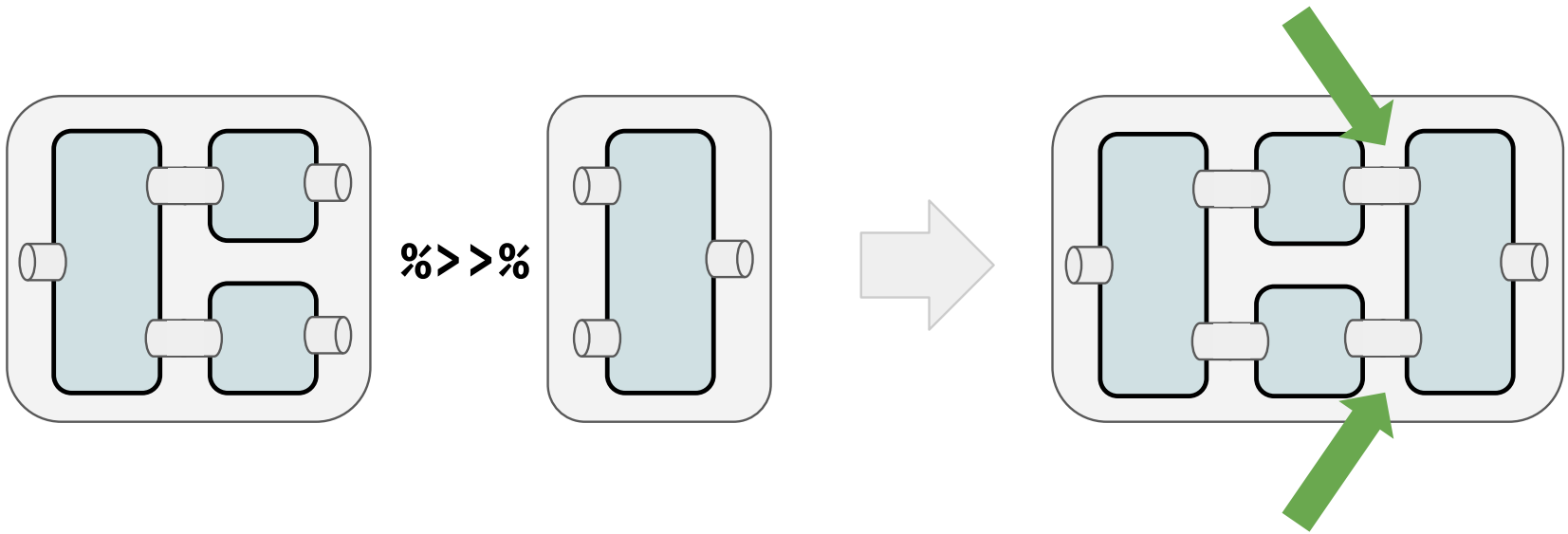
Graph Operations



THE STRUCTURE

Graph Operations

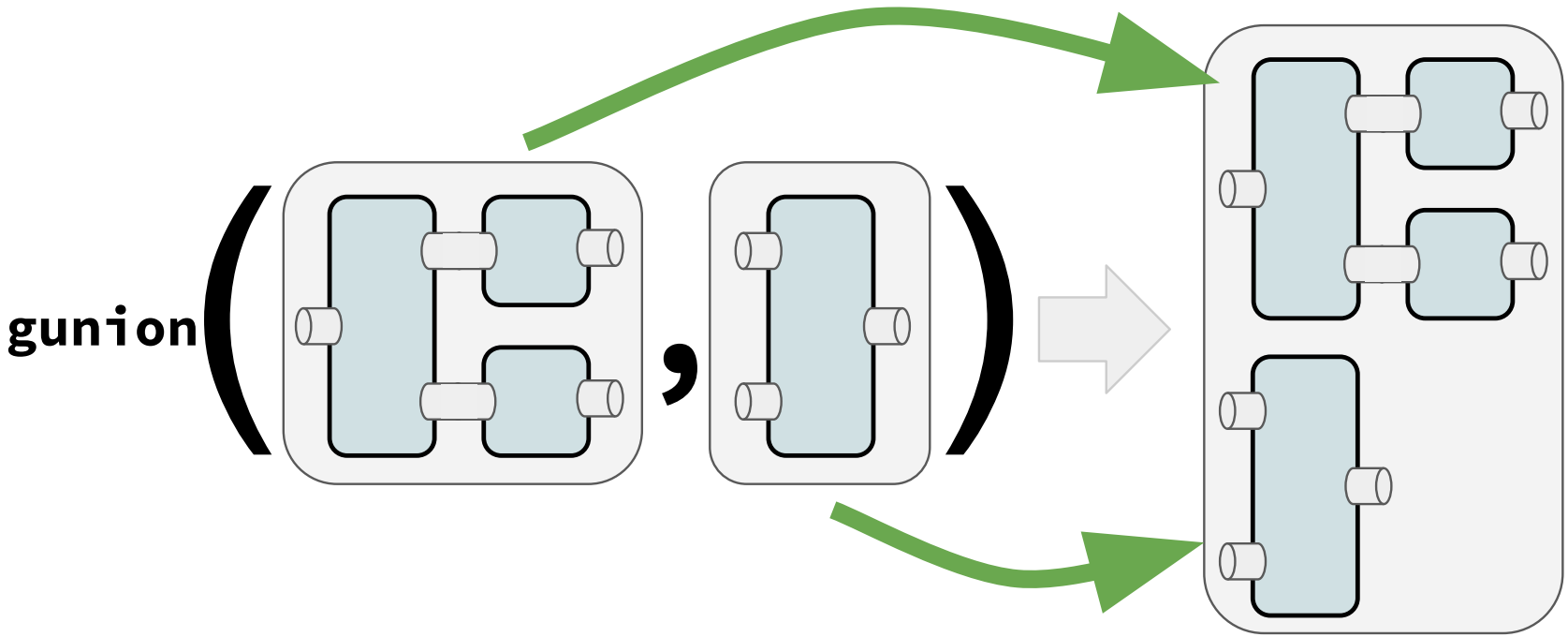
- The %>>%-operator concatenates `Graphs` and `PipeOps`



THE STRUCTURE

Graph Operations

- The `%>>%`-operator concatenates `Graphs` and `PipeOps`
- The `gunion()`-function unites `Graphs` and `PipeOps`



PIPELINES TUNING

```
glrn$param_set$values = list(
  branch.selection = to_tune(),
  anova.filter.frac = to_tune(0.1, 1),
  lrn_branch.selection = to_tune(),
  rf.mtry = to_tune(1, 20),
  xgb.nrounds = to_tune(1, 500),
  svm.cost = to_tune(p_dbl(-12, 4, trafo = function(x) 2^x)),
  svm.gamma = to_tune(p_dbl(-12, -1, trafo = function(x) 2^x)),
  xgb.verbose = 0, svm.type = "C-classification", svm.kernel = "radial"
)

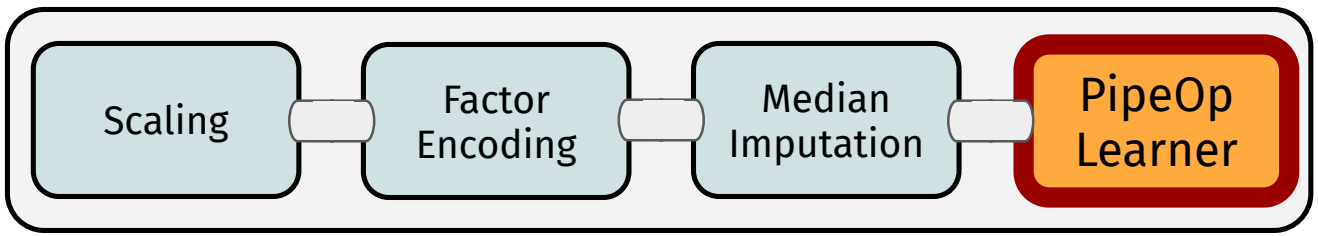
inst = TuningInstanceSingleCrit$new(tsk("sonar"), glrn,
  rsmp("cv", folds = 3), msr("classif.ce"), trm("evals", n_evals = 10))
tnr("random_search")$optimize(inst)
```

Linear Pipelines

LEARNERS AND GRAPHS

PipeOpLearner

- `Learner` as a `PipeOp`
- Fits a model, output is `Prediction`



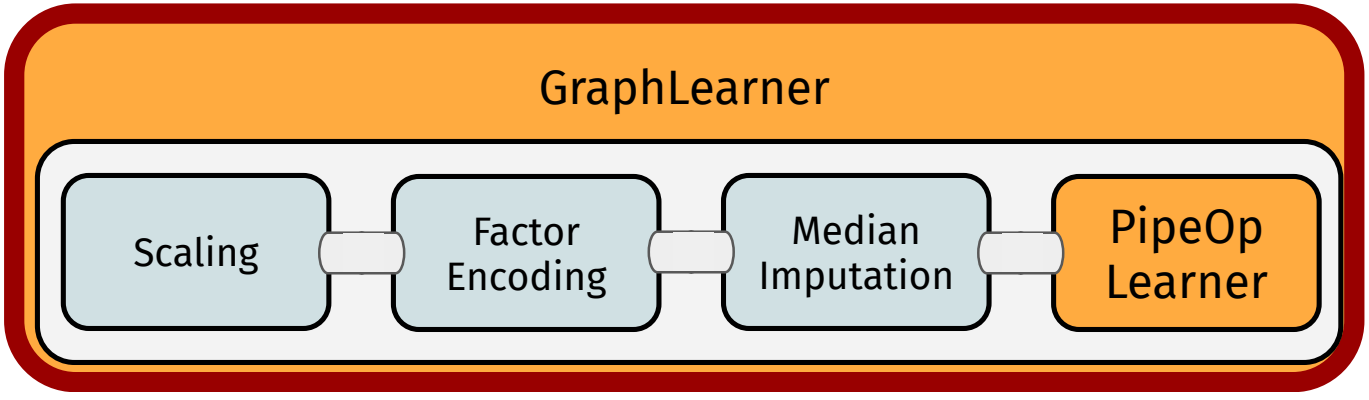
LEARNERS AND GRAPHS

PipeOpLearner

- `Learner` as a `PipeOp`
- Fits a model, output is `Prediction`

GraphLearner

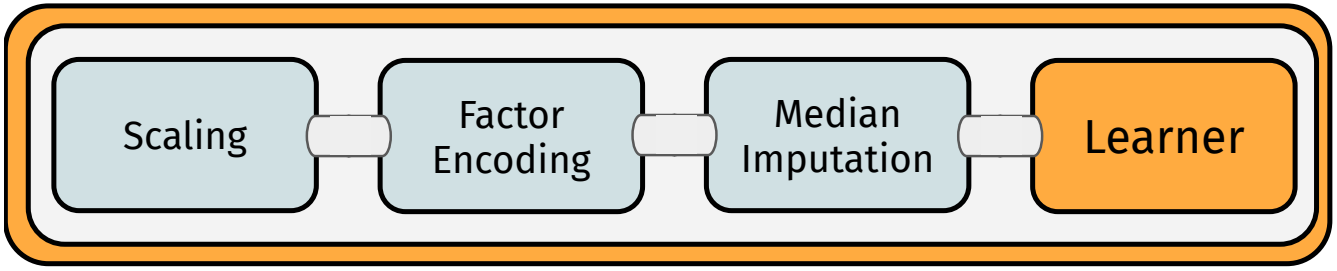
- `Graph` as a `Learner`
- All benefits of `mlr3`: **resampling**, **tuning**, **nested resampling**, ...



MLR3PIPELINES IN ACTION

Linear Preprocessing Pipeline

```
graph_pp = po("scale") %>>%
  po("encode") %>>%
  po("imputemedian") %>>%
  lrn("classif.rpart")
```

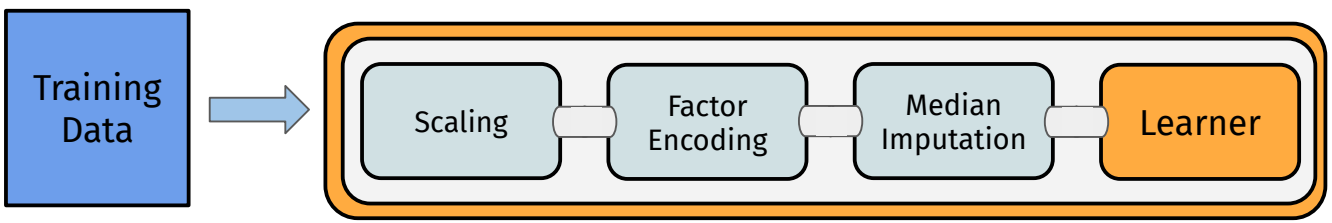


MLR3PIPELINES IN ACTION

Linear Preprocessing Pipeline

- `train()`ing: Data propagates and creates `$states`

```
glrn = GraphLearner$new(graph_pp)
glrn$train(task)
```

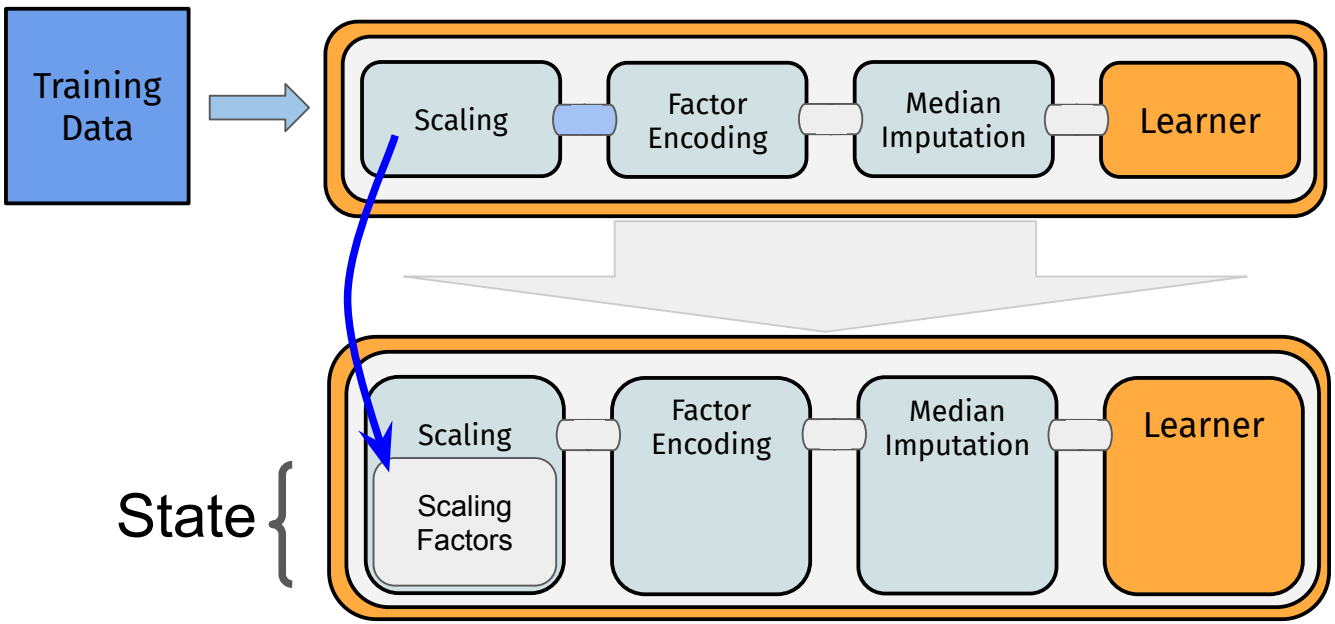


MLR3PIPELINES IN ACTION

Linear Preprocessing Pipeline

- `train()`ing: Data propagates and creates `$states`

```
glrn = GraphLearner$new(graph_pp)
glrn$train(task)
```

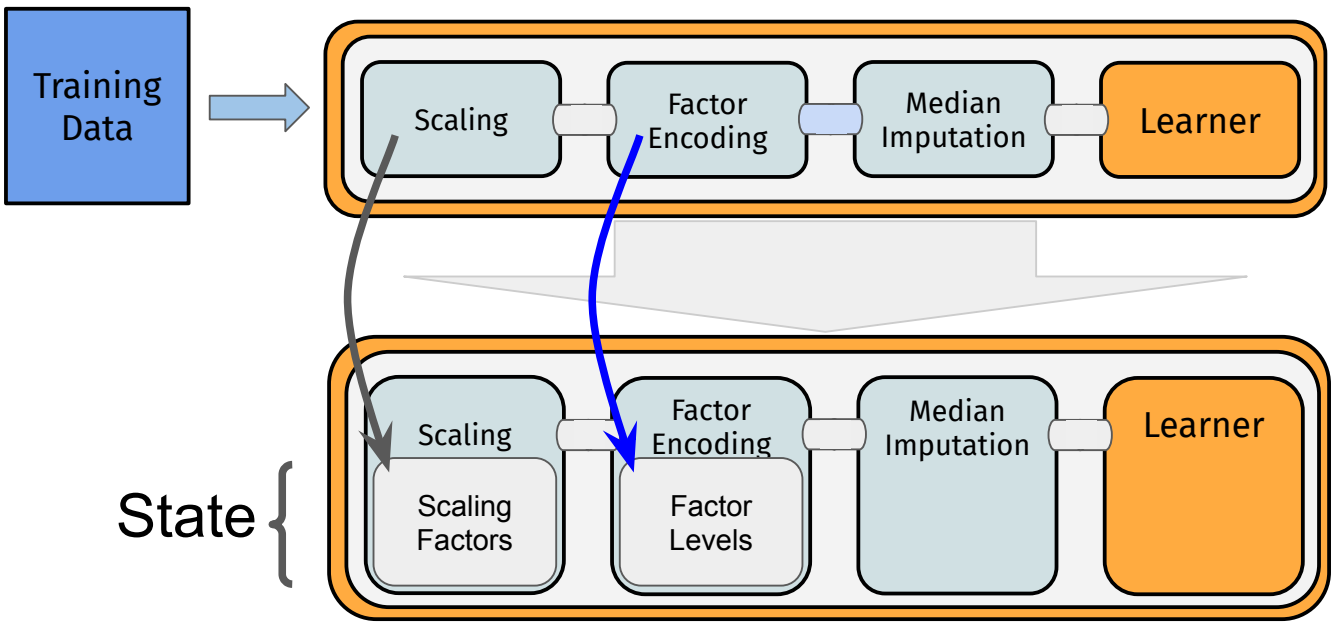


MLR3PIPELINES IN ACTION

Linear Preprocessing Pipeline

- `train()`ing: Data propagates and creates `$states`

```
glrn = GraphLearner$new(graph_pp)
glrn$train(task)
```

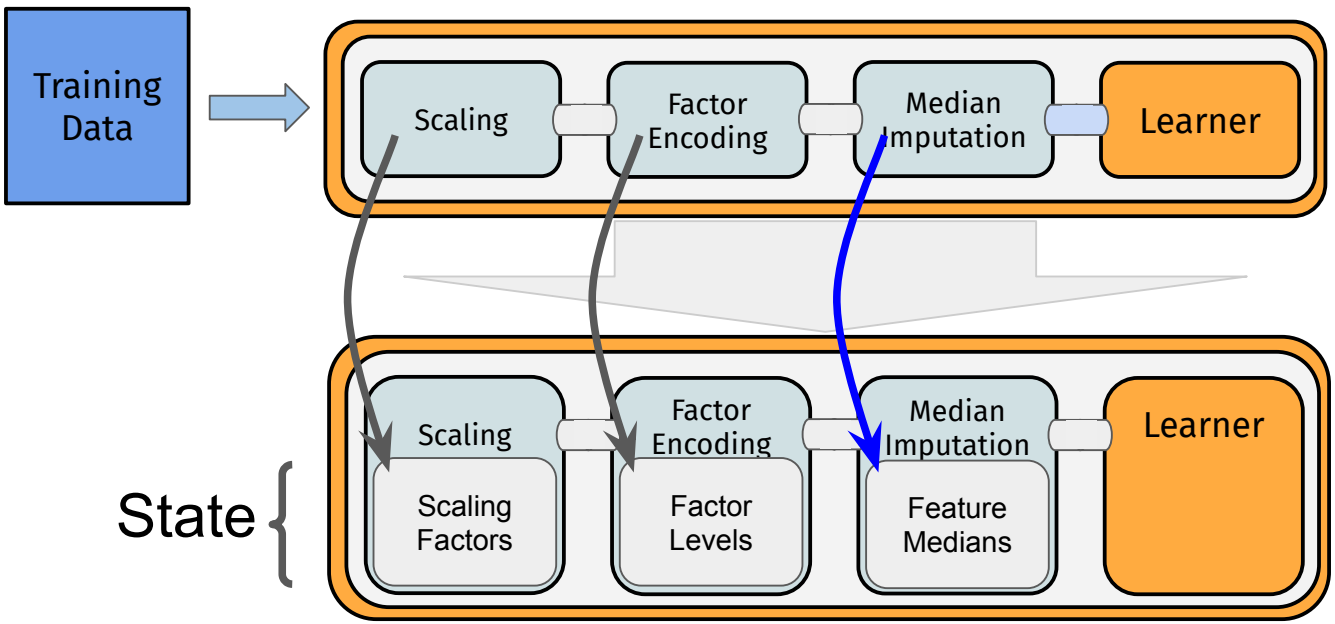


MLR3PIPELINES IN ACTION

Linear Preprocessing Pipeline

- `train()`ing: Data propagates and creates `$states`

```
glrn = GraphLearner$new(graph_pp)
glrn$train(task)
```

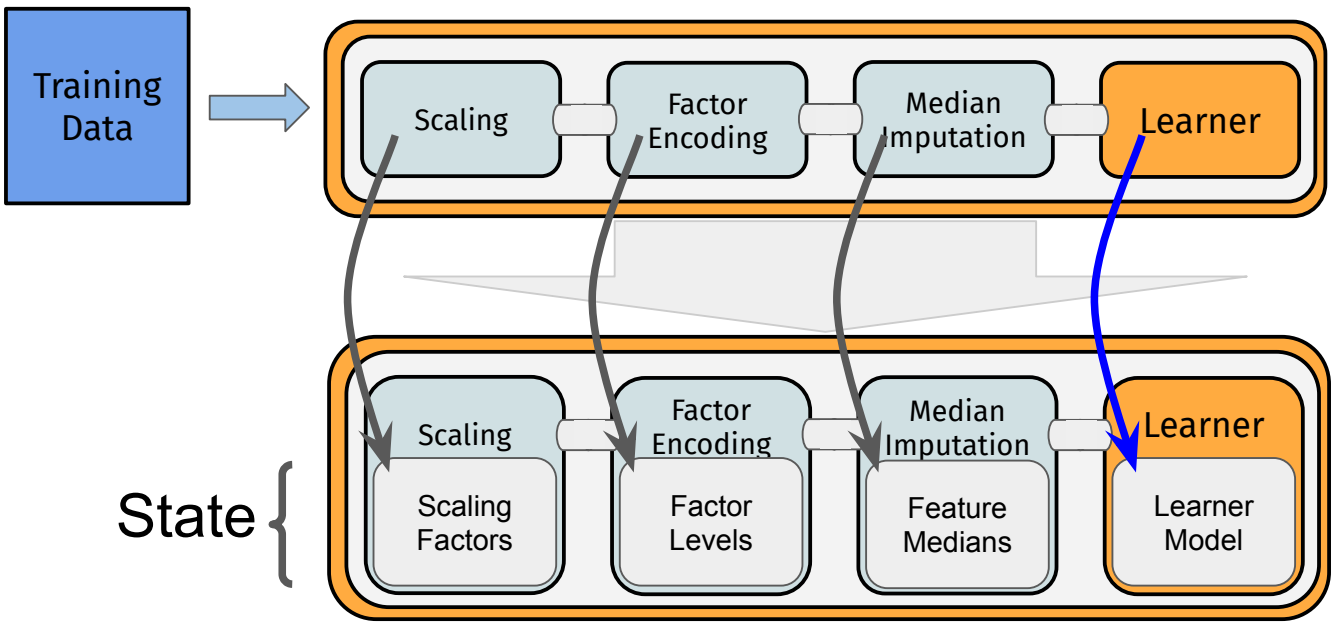


MLR3PIPELINES IN ACTION

Linear Preprocessing Pipeline

- `train()`ing: Data propagates and creates `$states`

```
glrn = GraphLearner$new(graph_pp)
glrn$train(task)
```

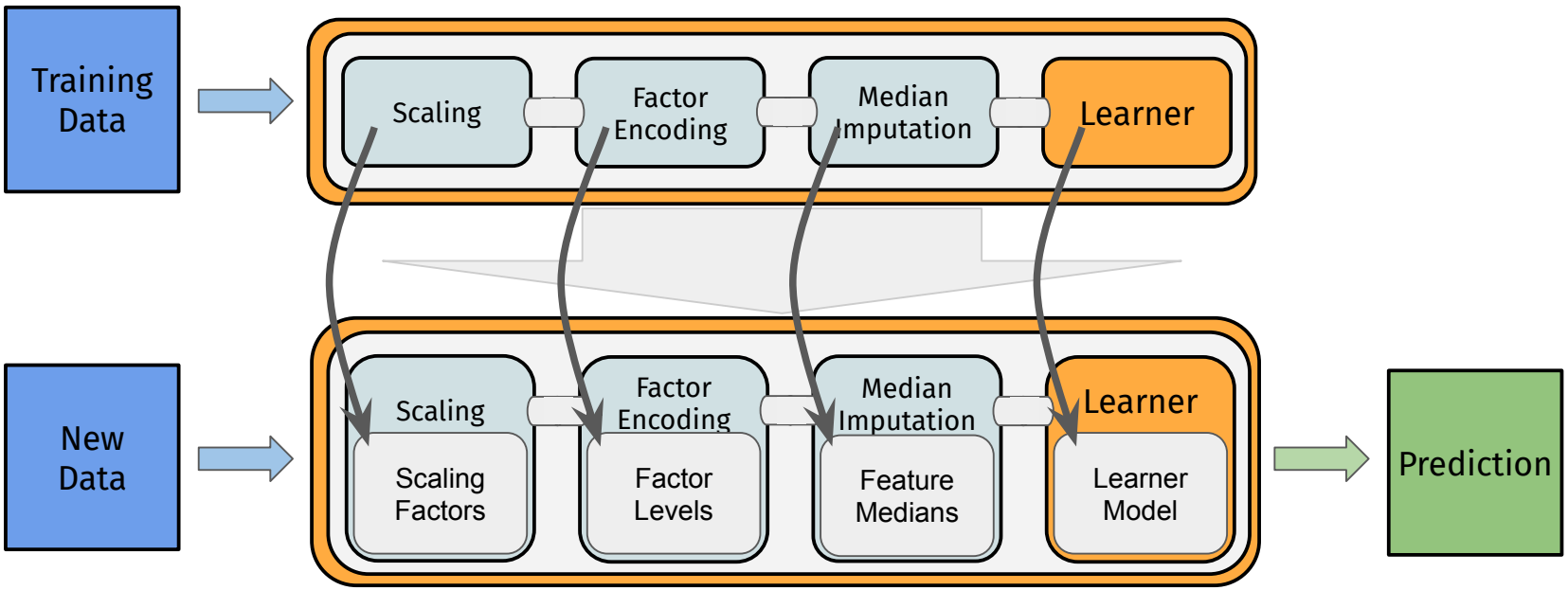


MLR3PIPELINES IN ACTION

Linear Preprocessing Pipeline

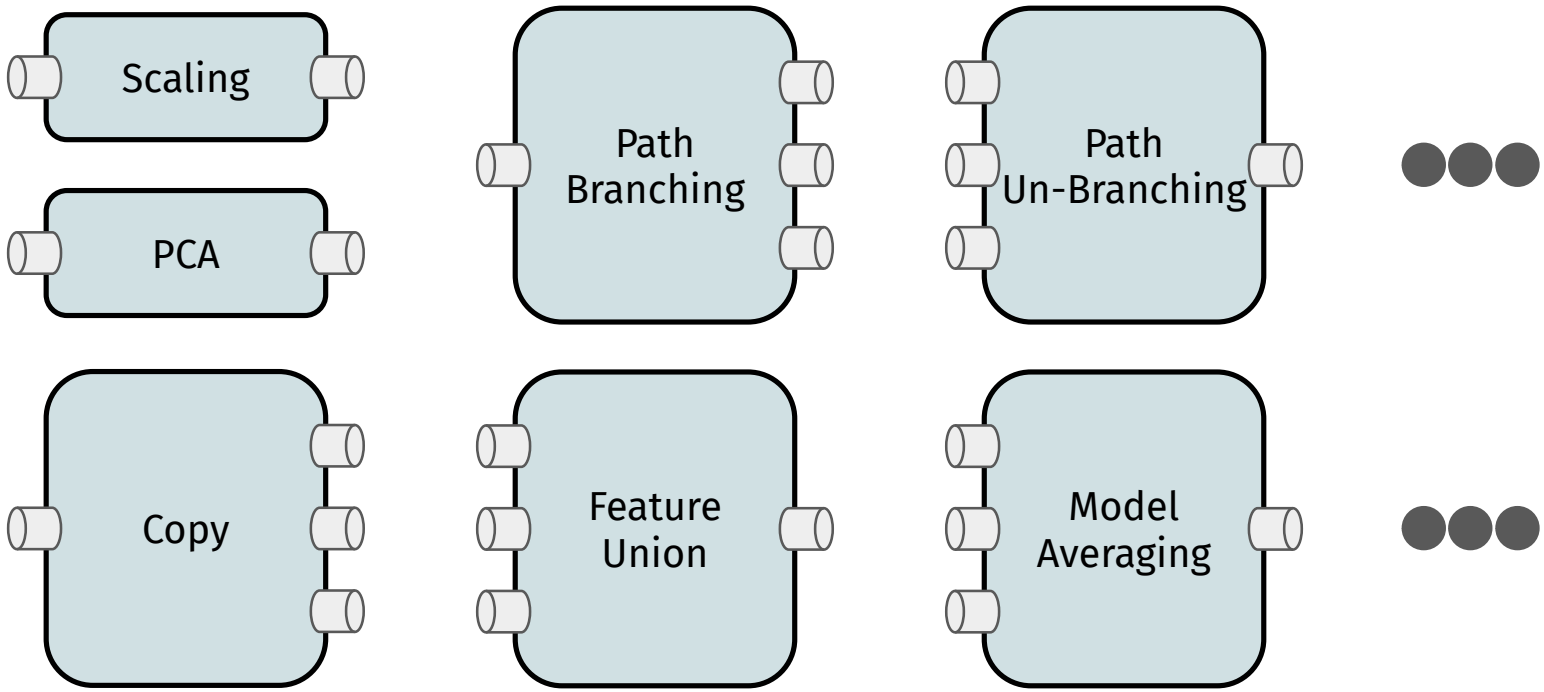
- `train()`ing: Data propagates and creates `$states`
- `predict()`tion: Data propagates, uses `$states`

```
glrn$predict(task)
```



Nonlinear Pipelines

PIPEOPS WITH MULTIPLE INPUTS / OUTPUTS

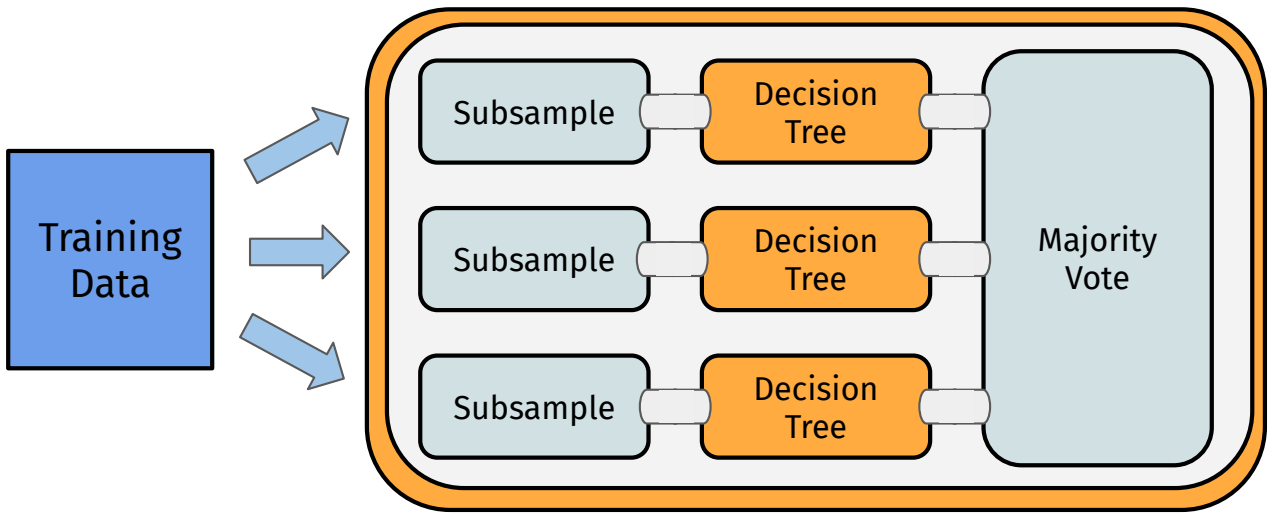


MLR3PIPELINES IN ACTION

Ensemble Method: Bagging

```
single_path = po("subsample") %>>% lrn("classif.rpart")

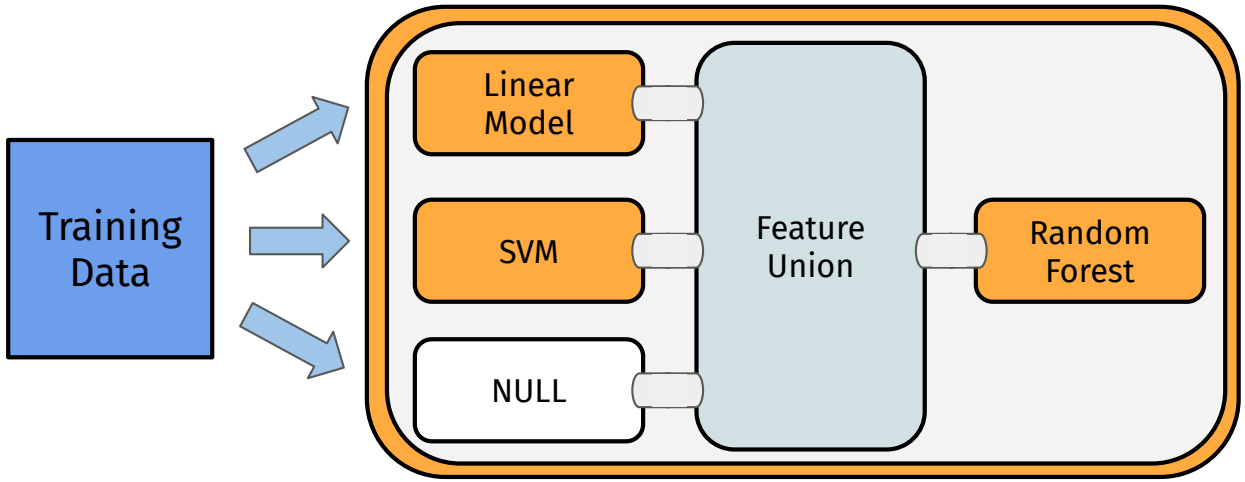
graph_bag = pipeline_greplicate(single_path, n = 3) %>>%
  po("classifavg")
```



MLR3PIPELINES IN ACTION

Ensemble Method: Stacking

```
graph_stack = gunion(list(
      po("learner_cv", learner = lrn("regr.lm")),
      po("learner_cv", learner = lrn("regr.svm")),
      po("nop"))) %>>%
  po("featureunion") %>>%
  lrn("regr.ranger")
```

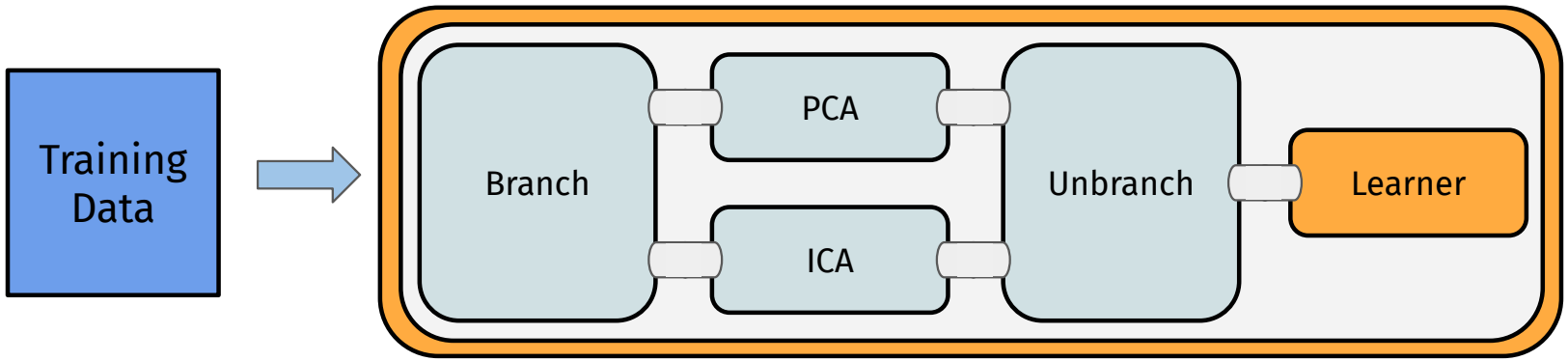


MLR3PIPELINES IN ACTION

Branching

```
graph_branch = ppl("branch", list(
  pca = po("pca"),
  ica = po("ica"))) %>>%
  lrn("classif.kknn")
```

Execute only one of several alternative paths

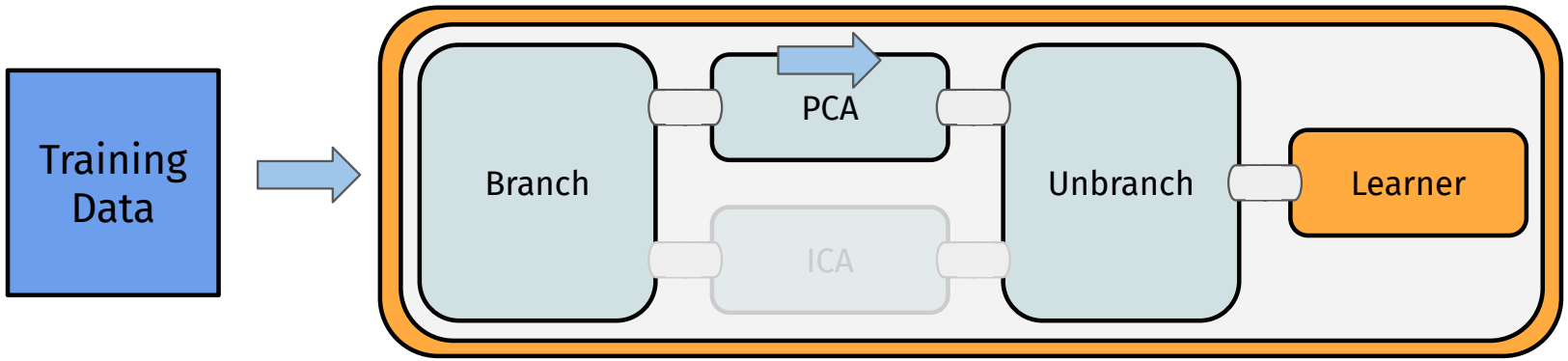


MLR3PIPELINES IN ACTION

Branching

```
graph_branch = ppl("branch", list(
  pca = po("pca"),
  ica = po("ica"))) %>>%
  lrn("classif.kknn")
```

```
> graph_branch$pipeops$branch$
    param_set$values$selection = "pca"
```

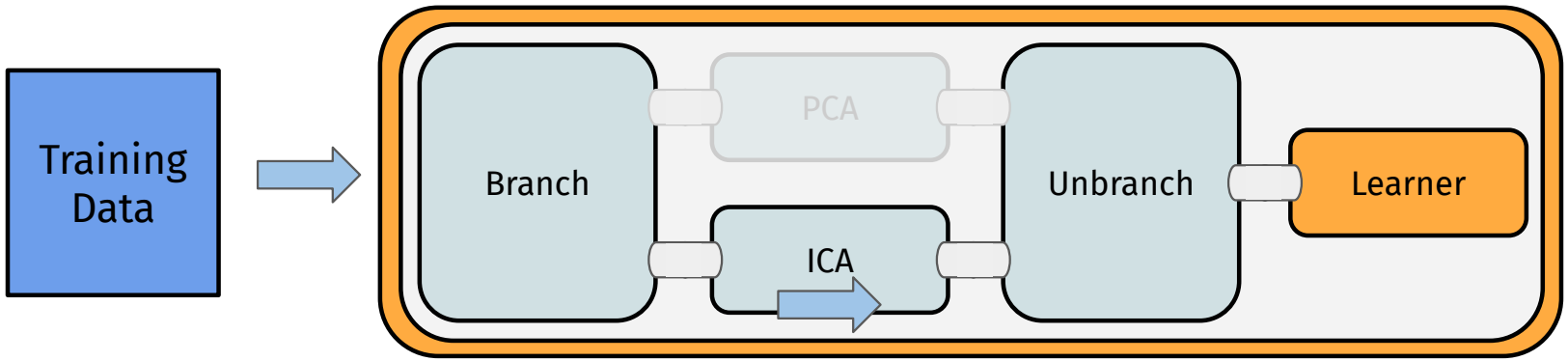


MLR3PIPELINES IN ACTION

Branching

```
graph_branch = ppl("branch", list(
  pca = po("pca"),
  ica = po("ica"))) %>>%
  lrn("classif.kknn")
```

```
> graph_branch$pipeops$branch$
    param_set$values$selection = "ica"
```



“PIPELINES” DICTIONARY & SHORT FORM

Many frequently used *patterns* for pipelines

- Making Learners robust to bad data
  (imputation + feature encoding + . . .)
- Bagging
- Branching

AutoML with mlr3pipelines

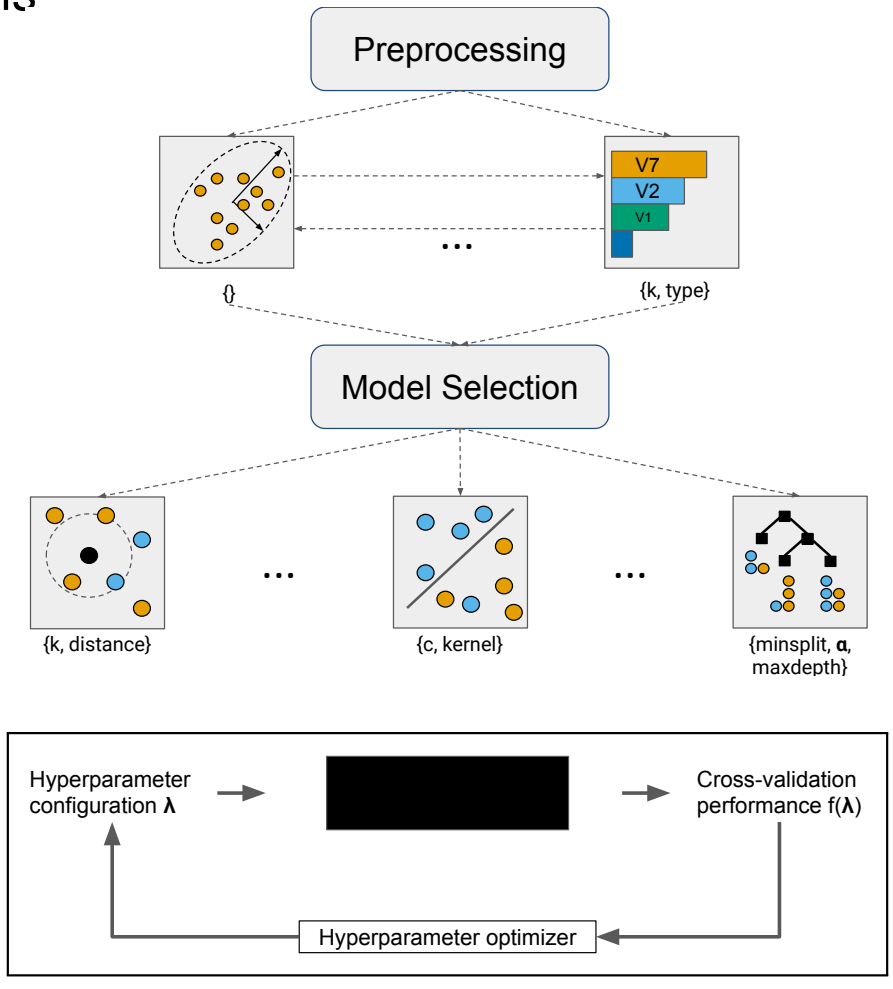
AUTOML <3 PIPELINES

- AutoML: Automatic Machine Learning
- Let the algorithm make decisions about
  1. *what learner* to use,
  2. *what preprocessing* to use, and
  3. *what hyperparameters* to use.

AUTOML WITH MLR3PIPELINES

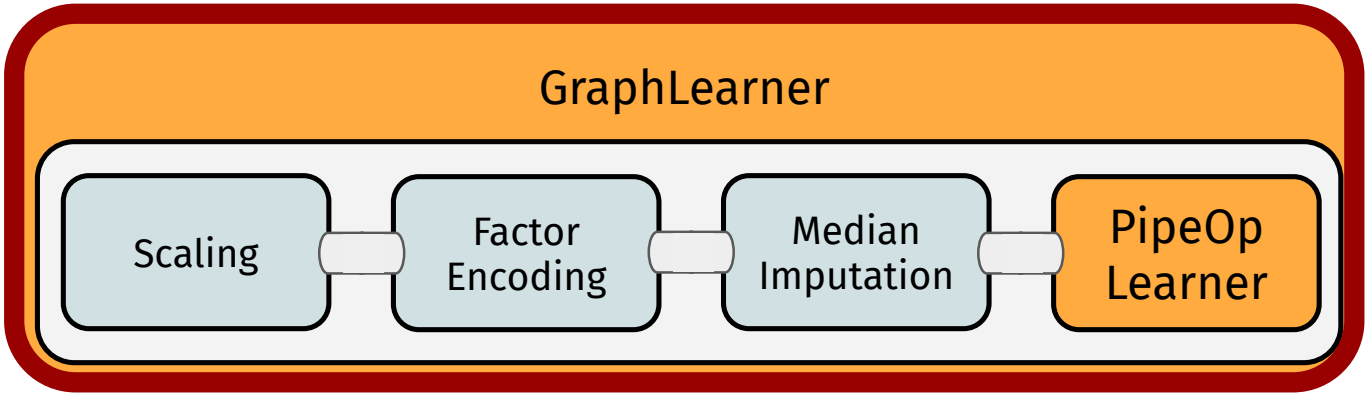
AutoML in a Nutshell

- Preprocessing steps
- ML Algorithms
- Tuner



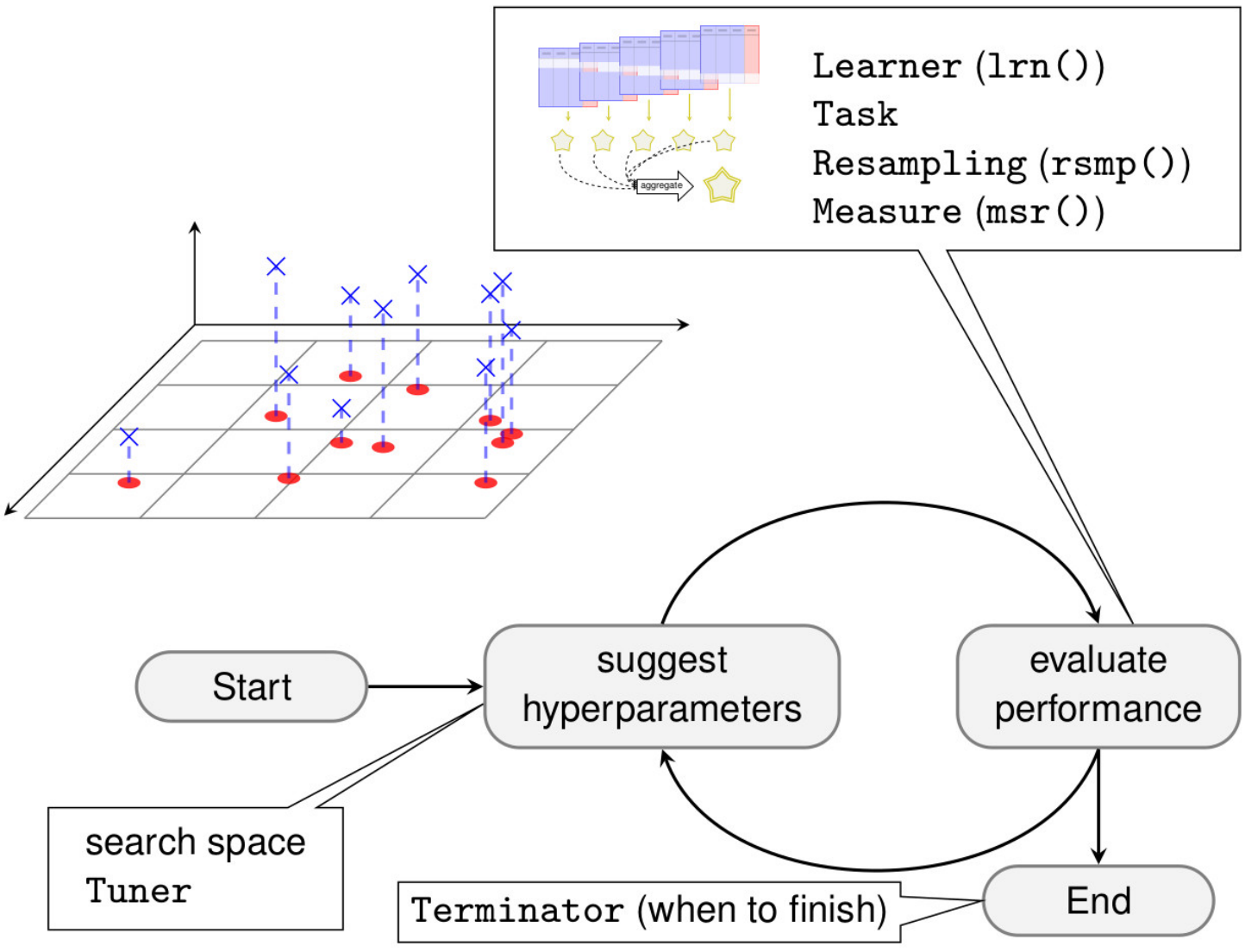
GRAPHLEARNER

- `Graph` as a `Learner`
- All benefits of `mlr3`: **resampling**, **tuning**, **nested resampling**, ...




```
graph_pp = po("scale") %>>% po("encode") %>>%
  po("imputemedian") %>>% lrn("classif.rpart")
glrn = GraphLearner$new(graph_pp)
glrn$train(task)
glrn$predict(task)
resample(task, glrn, rsmp("cv", folds = 3))
```

TUNING

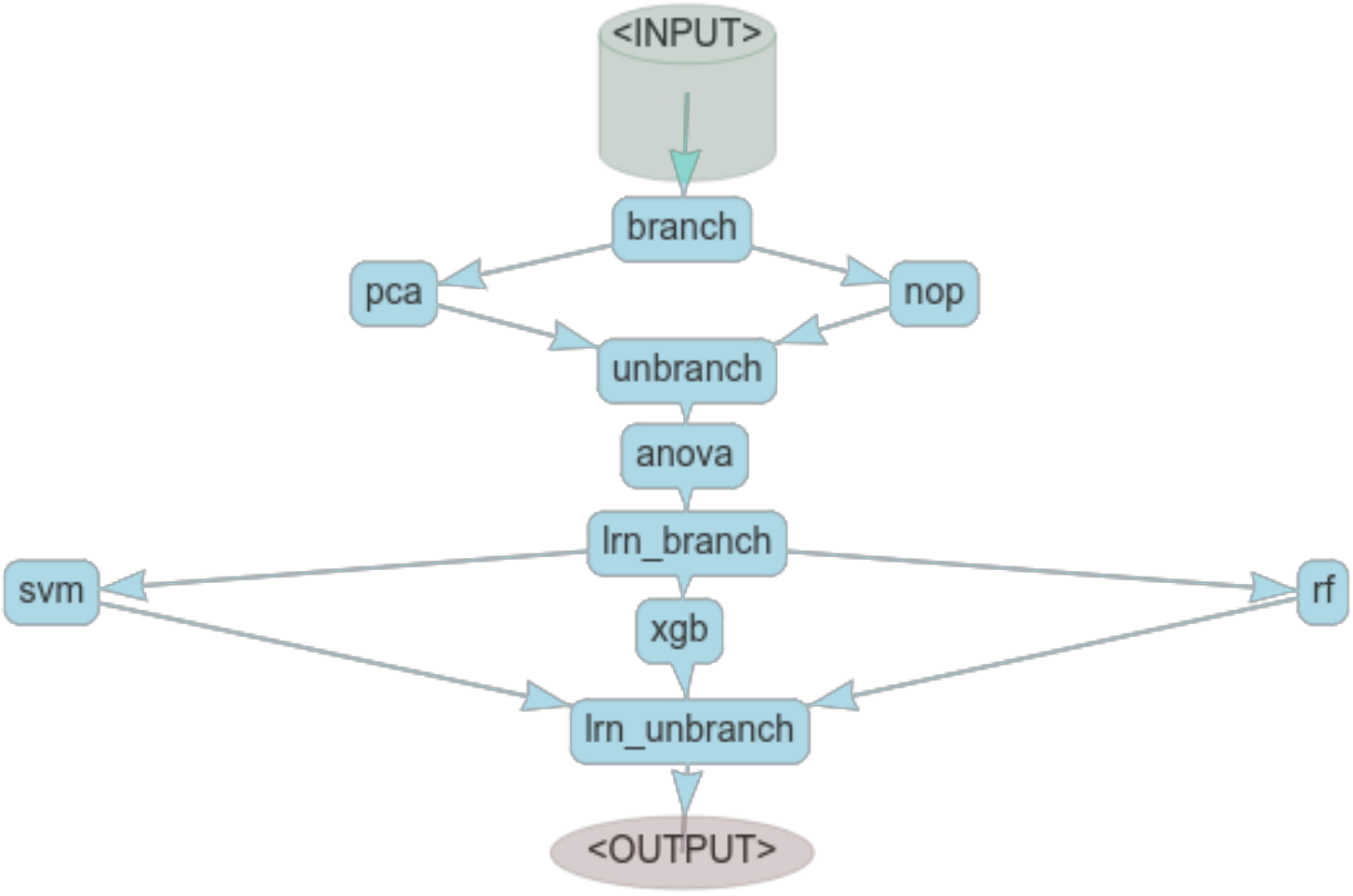

Learner (lrn())
Task
Resampling (rsmp())
Measure (msr())
aggregate
Start
suggest hyperparameters
evaluate performance
search space
Tuner
Terminator (when to finish)
End

PIPELINES TUNING

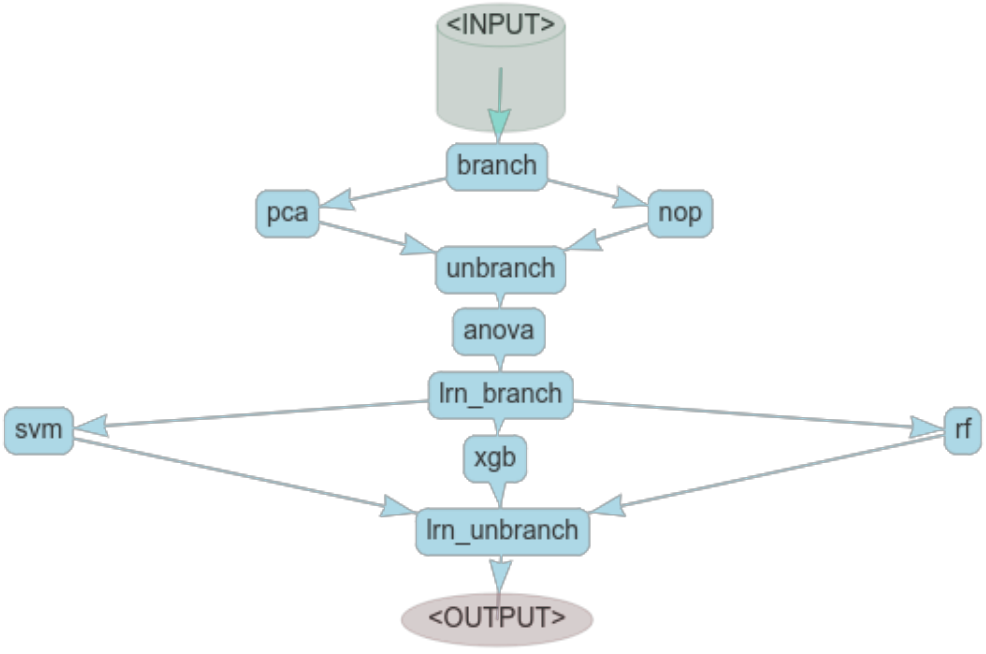
- Works **exactly** as in basic `mlr3` / `mlr3tuning`
- `PipeOps` have *hyperparameters* (using `paradox` pkg)
- `Graphs` have hyperparameters of all components *combined*
- $\Rightarrow$ Joint **tuning** and nested CV of complete graph

```
p1 = ppl("branch", list(
  "pca" = po("pca"),
  "nothing" = po("nop")
))
p2 = flt("anova")
p3 = ppl("branch", list(
  "svm" = lrn("classif.svm", id = "svm"),
  "xgb" = lrn("classif.xgboost", id = "xgb"),
  "rf" = lrn("classif.ranger",  id = "rf")
), prefix_branchops = "lrn_")
gr = p1 %>>% p2 %>>% p3
glrn = GraphLearner$new(gr)
```

PIPELINES TUNING



PIPELINES TUNING




```
glrn$param_set$values = list(
  branch.selection = to_tune(),
  anova.filter.frac = to_tune(0.1, 1),
  lrn_branch.selection = to_tune(),
  rf.mtry = to_tune(1, 20),
  xgb.nrounds = to_tune(1, 500),
  svm.cost = to_tune(p_dbl(-12, 4, trafo = function(x) 2^x)),
  svm.gamma = to_tune(p_dbl(-12, -1, trafo = function(x) 2^x)),
  xgb.verbose = 0, svm.type = "C-classification", svm.kernel = "radial"
)
```

PIPELINES TUNING

```
glrn$param_set$values = list(
  branch.selection = to_tune(),
  anova.filter.frac = to_tune(0.1, 1),
  lrn_branch.selection = to_tune(),
  rf.mtry = to_tune(1, 20),
  xgb.nrounds = to_tune(1, 500),
  svm.cost = to_tune(p_dbl(-12, 4, trafo = function(x) 2^x)),
  svm.gamma = to_tune(p_dbl(-12, -1, trafo = function(x) 2^x)),
  xgb.verbose = 0, svm.type = "C-classification", svm.kernel = "radial"
)

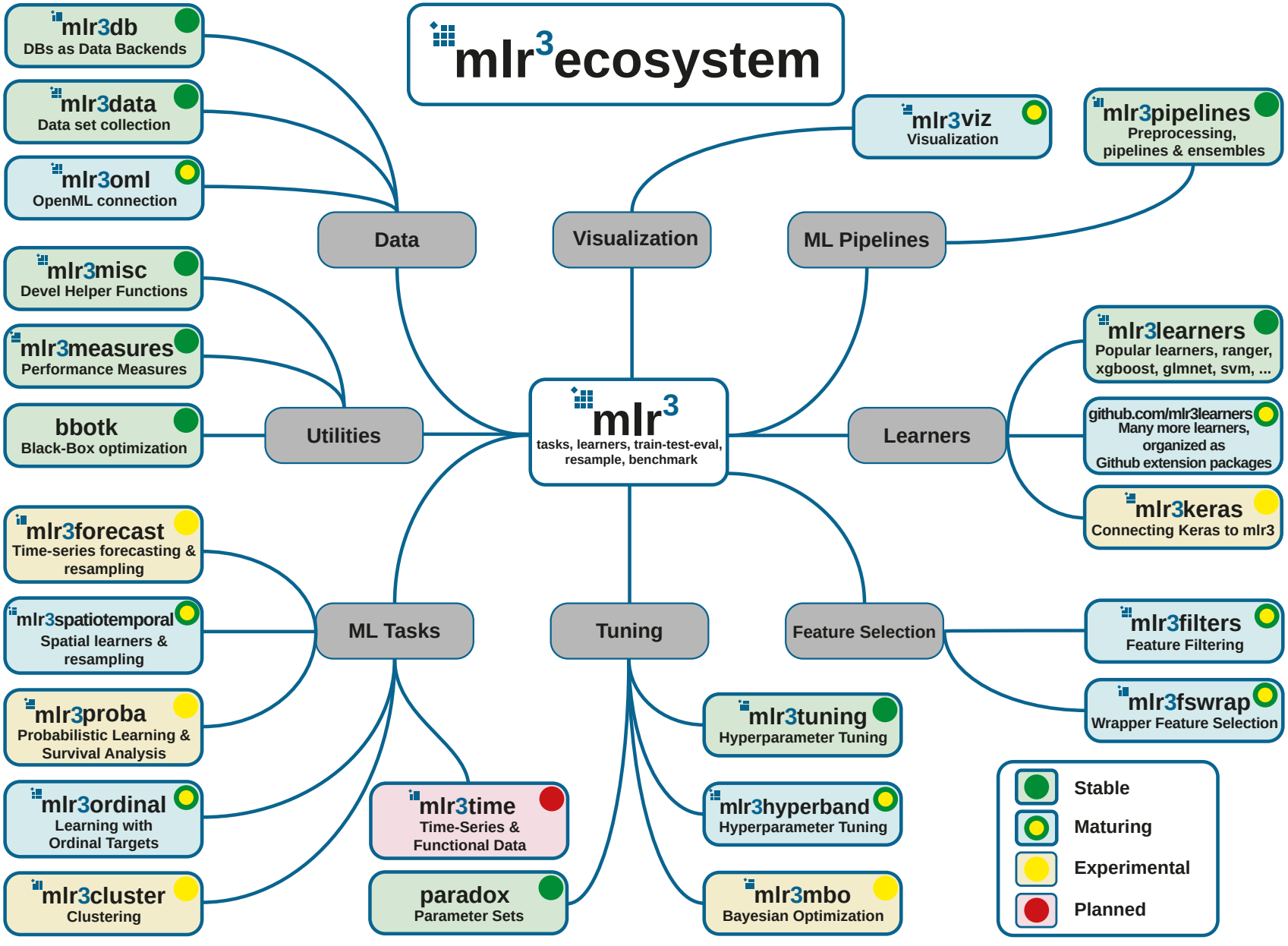
inst = TuningInstanceSingleCrit$new(tsk("sonar"), glrn,
  rsmp("cv", folds = 3), msr("classif.ce"), trm("evals", n_evals = 10))
tnr("random_search")$optimize(inst)
```

OUTLOOK

What is to come?

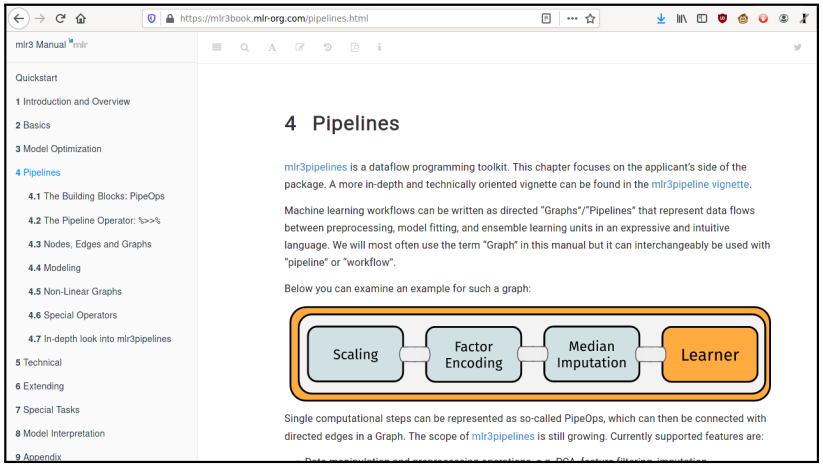
- `mlr3pipelines`: caching, parallelization
- Better **tuners**: Bayesian Optimization, Hyperband
- Survival and Forecasting (via `mlr3proba`, `mlr3forecast`)
- Deep Learning (via `mlr3keras`)

Thanks! Please ask questions!


mlr3ecosystem
mlr3db
DBs as Data Backends
mlr3data
Data set collection
mlr3oml
OpenML connection
mlr3misc
Devel Helper Functions
mlr3measures
Performance Measures
bbotk
Black-Box optimization
mlr3forecast
Time-series forecasting & resampling
mlr3spatiotemporal
Spatial learners & resampling
mlr3proba
Probabilistic Learning & Survival Analysis
mlr3ordinal
Learning with Ordinal Targets
mlr3cluster
Clustering
Data
Utilities
ML Tasks
Visualization
ML Pipelines
Tuning
Learners
Feature Selection
mlr3
tasks, learners, train-test-eval, resample, benchmark
mlr3viz
Visualization
mlr3pipelines
Preprocessing, pipelines & ensembles
mlr3learners
Popular learners, ranger, xgboost, glmnet, svm, ...
github.com/mlr3learners
Many more learners, organized as Github extension packages
mlr3keras
Connecting Keras to mlr3
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

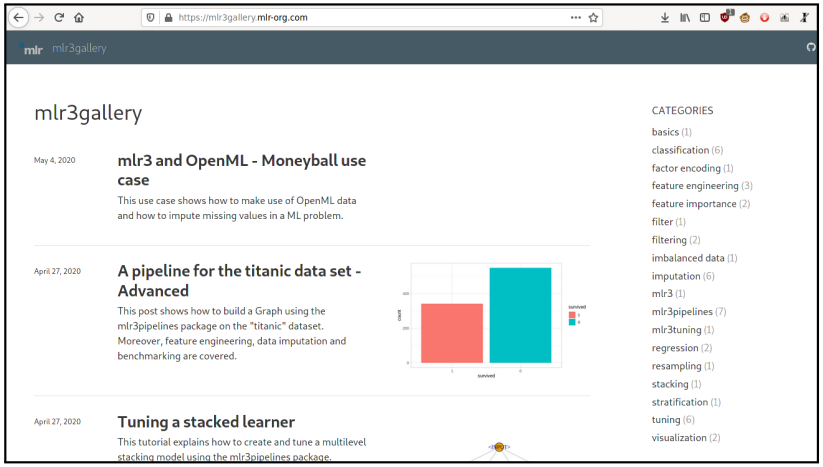
MLR3(PIPELINES) RESOURCES

mlr3 book



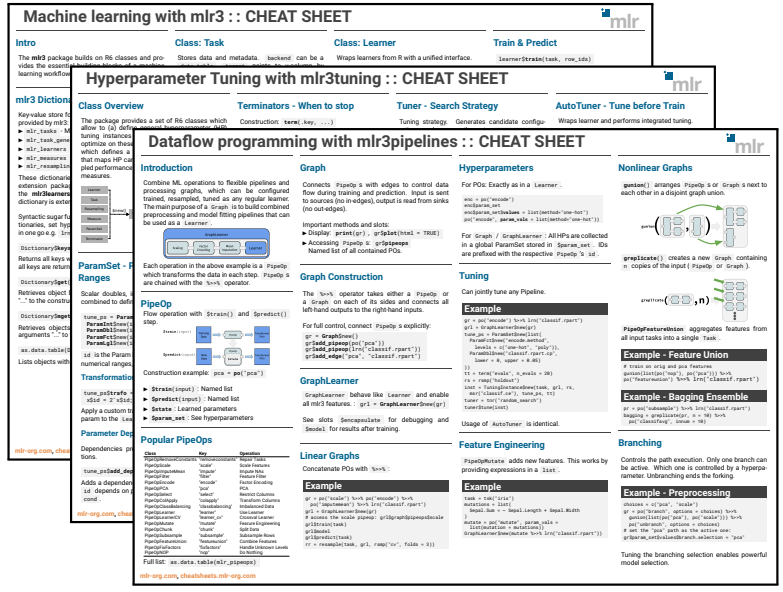
https://mlr3book.mlr-org.com/

mlr3 Use Case "Gallery"



https://mlr3gallery.mlr-org.com/

"cheat sheets"



https://cheatsheets.mlr-org.com/

Outro

MLR3PIPELINES

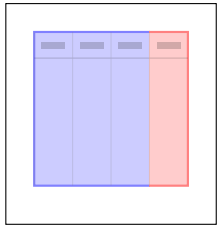
`mlr3pipelines` overview:

- Construct a `PipeOp` using `po()`
- Use `Graph` operators to connect them
  - %>>%—chain operations
  - `gunion()`—put operations in parallel
  - `pipeline_greplicate()`—put many copies of an operation in parallel
- Train/predict with the `PipeOp` or `Graph` using `$train()`/`$predict()`
- Inspect the trained state through `$state`
- Encapsulate the `Graph` in a `GraphLearner` for resampling, benchmarking, and tuning

OVERVIEW

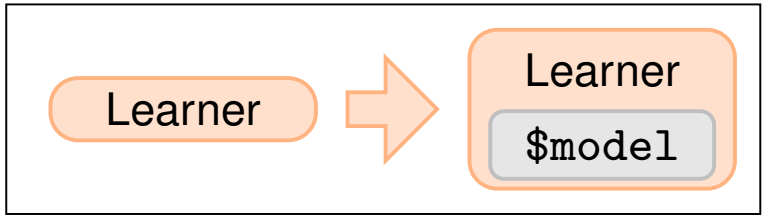
Ingredients:

Data



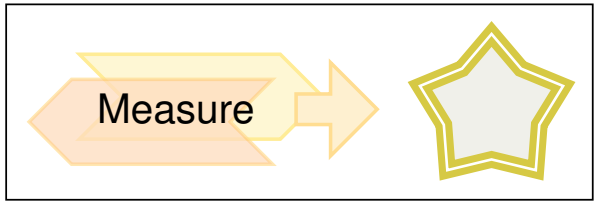
`TaskClassif`,
`TaskRegr`,
`tsk()`

Learning Algorithms



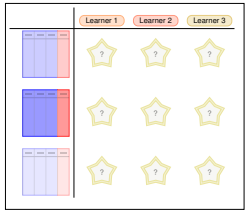
`lrn()` ⇒ `Learner`,
`$train()`,
`$predict()` ⇒ `Prediction`

Performance Evaluation



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

Performance Comparison



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

RECAP

```
inst = TuningInstanceSingleCrit$new(
  tsk("iris"), lrn("classif.kknn", kernel="rectangular"),
  rsmp("holdout"), msr("classif.ce"), trm("evals", n_evals = 2),
  ps(k = p_int(1, 20))
)

gsearch = tnr("grid_search", resolution = 3)

gsearch$optimize(inst)

#>    k learner_param_vals  x_domain classif.ce
#> 1: 1          <list[2]> <list[1]>       0.04
```