

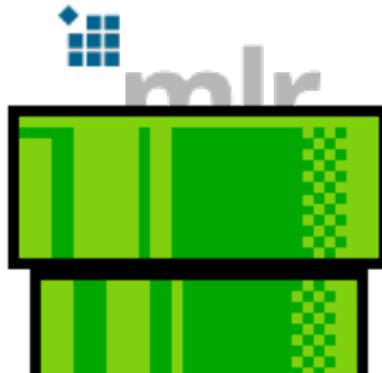
MLR3PIPELINES: MACHINE LEARNING PIPELINES AS GRAPHS

Martin Binder, Florian Pfisterer, Michel Lang, Bernd Bischl

Computational Statistics, LMU

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OpenML Hackathon Dagstuhl



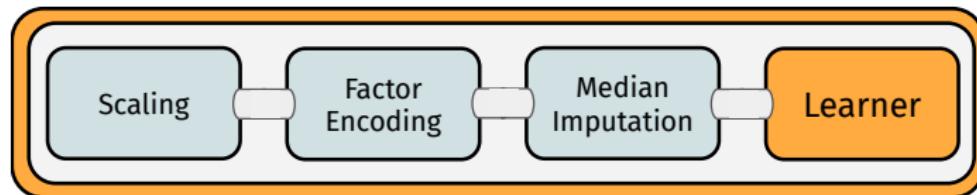
INTRO

MLR3PIPELINES

MACHINE LEARNING WORKFLOWS:

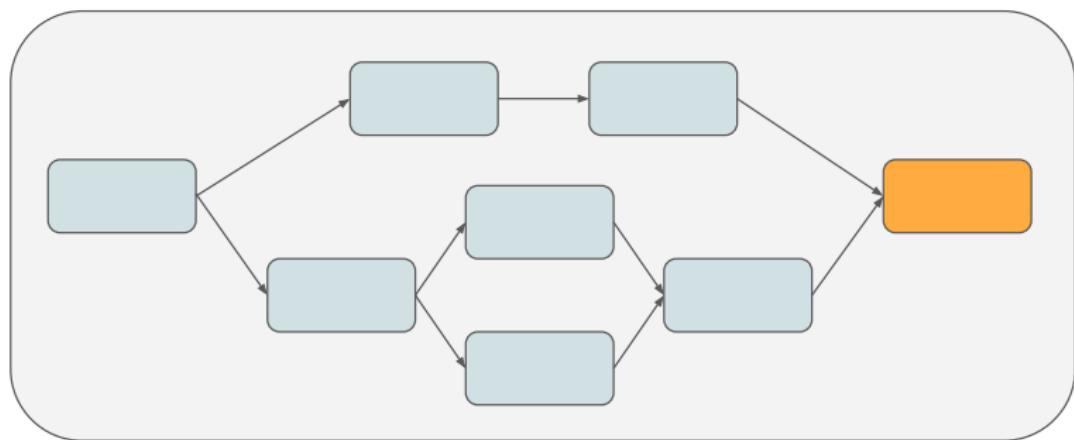
- **Preprocessing:** Feature extraction, feature selection, missing data imputation,...
- **Ensemble methods:** Model averaging, model stacking
- **mlr3:** modular model fitting

⇒ **mlr3pipelines:** modular ML workflows



MACHINE LEARNING WORKFLOWS

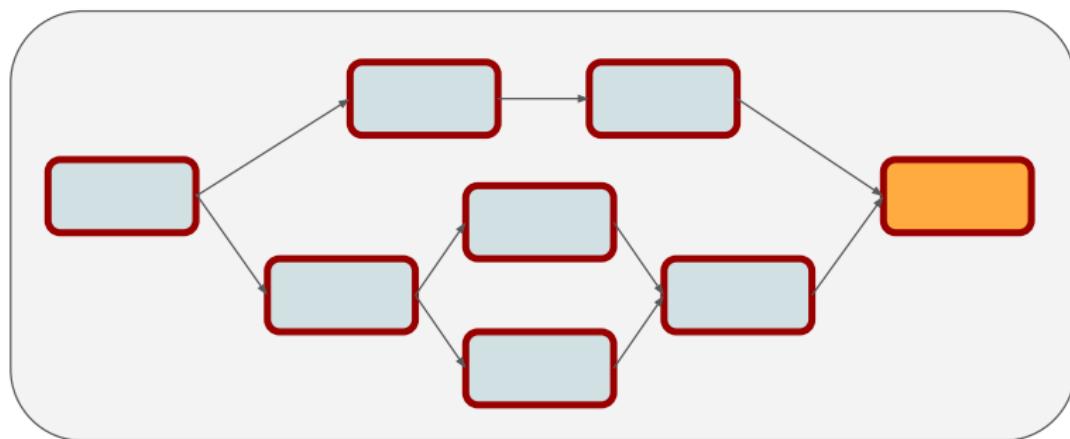
- what do they look like?



MACHINE LEARNING WORKFLOWS

– what do they look like?

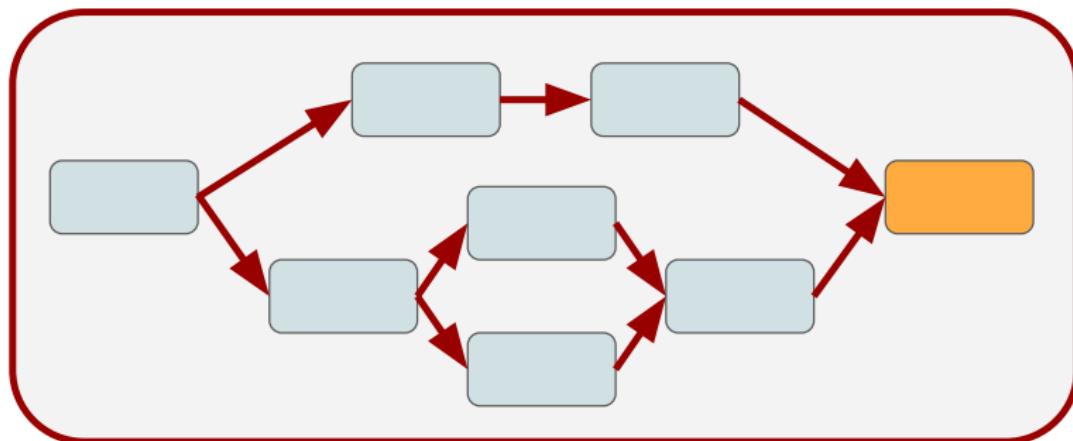
■ **Building blocks:** *what is happening? → PipeOp*



MACHINE LEARNING WORKFLOWS

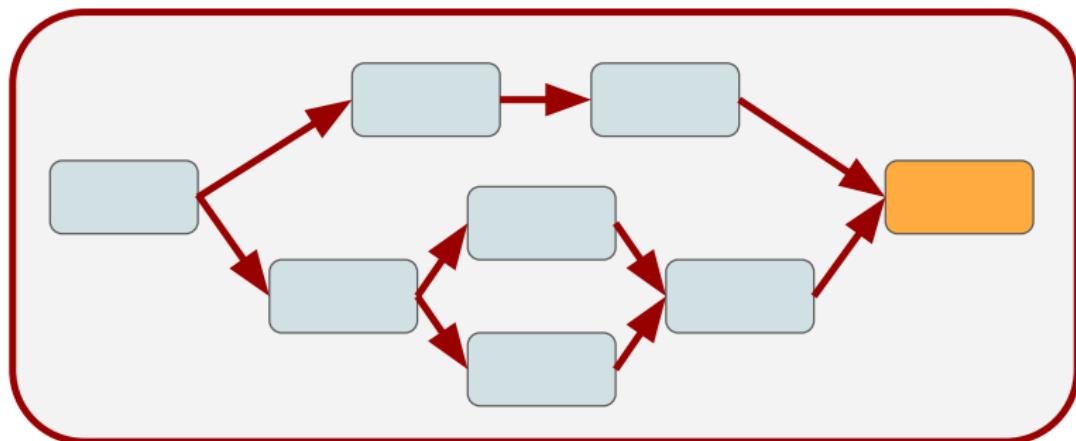
– what do they look like?

- **Building blocks:** *what is happening?* → PipeOp
- **Structure:** *In what sequence is it happening?* → Graph



MACHINE LEARNING WORKFLOWS

- what do they look like?
 - **Building blocks:** *what is happening?* → PipeOp
 - **Structure:** In what *sequence* is it happening? → Graph
- ⇒ Graph: PipeOps as **nodes** with **edges** (data flow) between them



PIPEOPS

THE BUILDING BLOCKS

PIPEOP: SINGLE UNIT OF DATA OPERATION

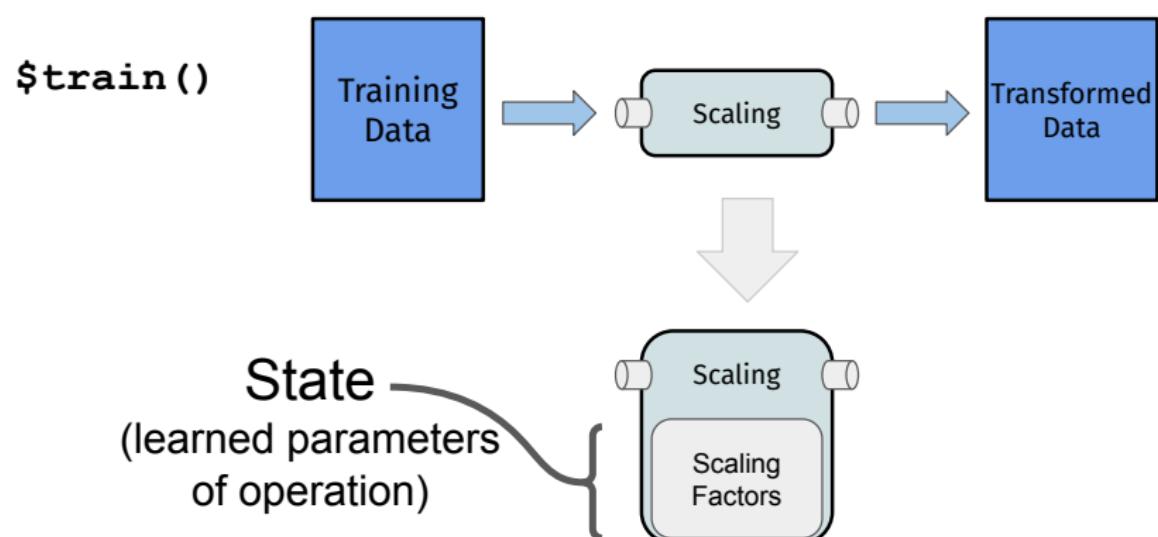
- `pip = po("scale")` to construct



THE BUILDING BLOCKS

PIPEOP: SINGLE UNIT OF DATA OPERATION

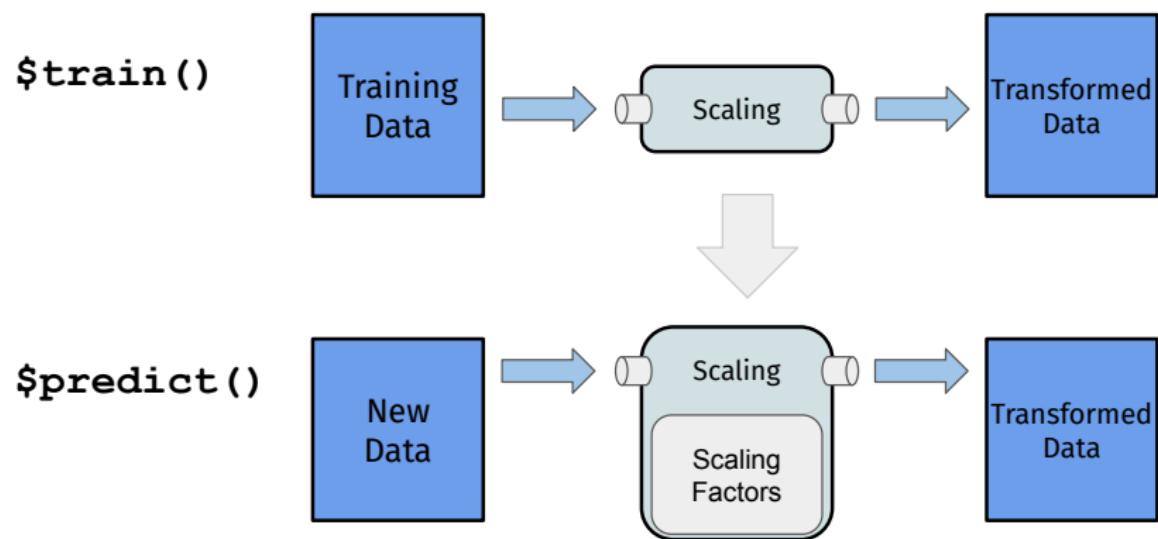
- `pip = po("scale")` to construct
- `pip$train()`: process data and create `pip$state`



THE BUILDING BLOCKS

PIPEOP: SINGLE UNIT OF DATA OPERATION

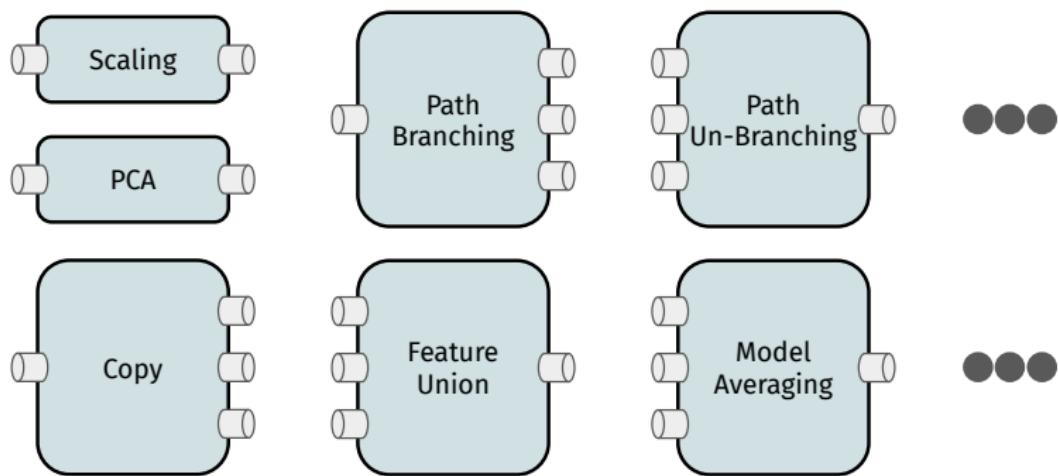
- `pip = po("scale")` to construct
- `pip$train()`: process data and create `pip$state`
- `pip$predict()`: process data depending on the `pip$state`



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



THE BUILDING BLOCKS

```
po = po("scale")

trained = po$train(list(task))

trained[[1]]$head(3)

##      Species Petal.Length Petal.Width Sepal.Length Sepal.Width
## 1:  setosa    -1.335752   -1.311052   -0.8976739   1.0156020
## 2:  setosa    -1.335752   -1.311052   -1.1392005  -0.1315388
## 3:  setosa    -1.392399   -1.311052   -1.3807271   0.3273175
```

THE BUILDING BLOCKS

```
po = po("scale")

trained = po$train(list(task))

trained[[1]]$head(3)

##      Species Petal.Length Petal.Width Sepal.Length Sepal.Width
## 1:  setosa    -1.335752   -1.311052   -0.8976739   1.0156020
## 2:  setosa    -1.335752   -1.311052   -1.1392005  -0.1315388
## 3:  setosa    -1.392399   -1.311052   -1.3807271   0.3273175
```

```
head(po$state, 2)

## $center
## Petal.Length  Petal.Width Sepal.Length  Sepal.Width
##      3.758000     1.199333     5.843333     3.057333
##
## $scale
## Petal.Length  Petal.Width Sepal.Length  Sepal.Width
##      1.7652982    0.7622377    0.8280661    0.4358663
```

THE BUILDING BLOCKS

```
po = po("scale")

trained = po$train(list(task))

trained[[1]]$head(3)

##      Species Petal.Length Petal.Width Sepal.Length Sepal.Width
## 1:  setosa    -1.335752   -1.311052   -0.8976739   1.0156020
## 2:  setosa    -1.335752   -1.311052   -1.1392005  -0.1315388
## 3:  setosa    -1.392399   -1.311052   -1.3807271   0.3273175

smalltask = task$clone()$filter(1:3)
po$predict(list(smalltask))[[1]]$data()

##      Species Petal.Length Petal.Width Sepal.Length Sepal.Width
## 1:  setosa    -1.335752   -1.311052   -0.8976739   1.0156020
## 2:  setosa    -1.335752   -1.311052   -1.1392005  -0.1315388
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```

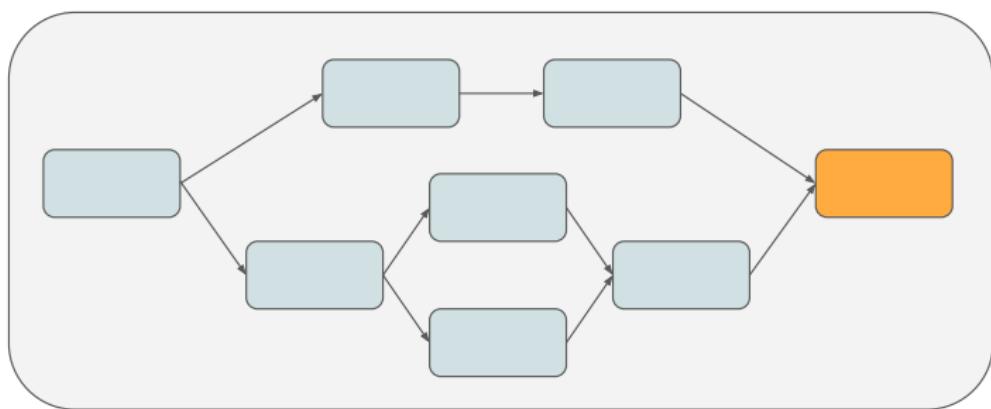
PIPEOPS SO FAR AND PLANNED

- Simple data preprocessing operations (scaling, Box Cox, Yeo Johnson, PCA, ICA)
- Missing value imputation (sampling, median, as new level)
- Feature selection (by name, by type, using filter methods)
- Categorical data encoding (one-hot, treatment, impact)
- Sampling (subsampling for speed, sampling for class balance)
- Ensemble methods on Predictions (weighted average, possibly learned weights)
- Branching (simultaneous branching, alternative branching)
- Combination of data: `featureunion`
- Text processing (*planned*)
- Time series and spatio-temporal data (*planned*)
- Multi-output and ordinal targets (*planned*)
- Outlier detection (*planned*)
- Hurdle models (*planned*)

GRAPH OPERATIONS

THE STRUCTURE

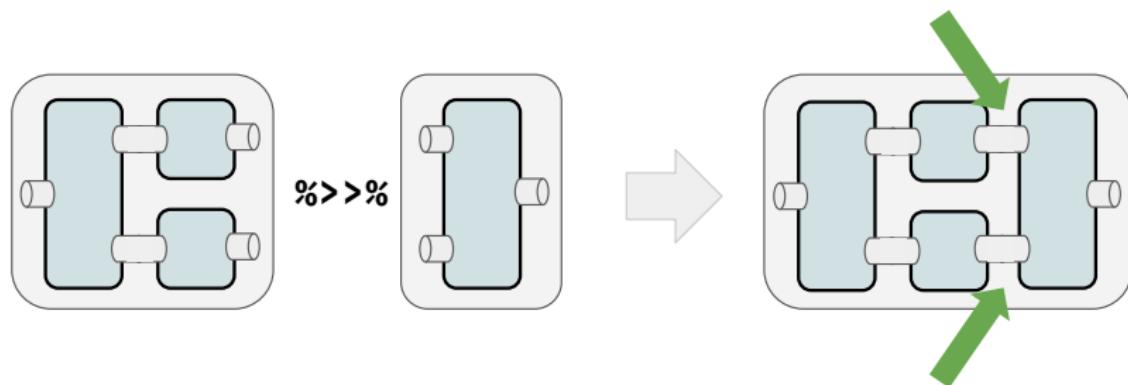
GRAPH OPERATIONS



THE STRUCTURE

GRAPH OPERATIONS

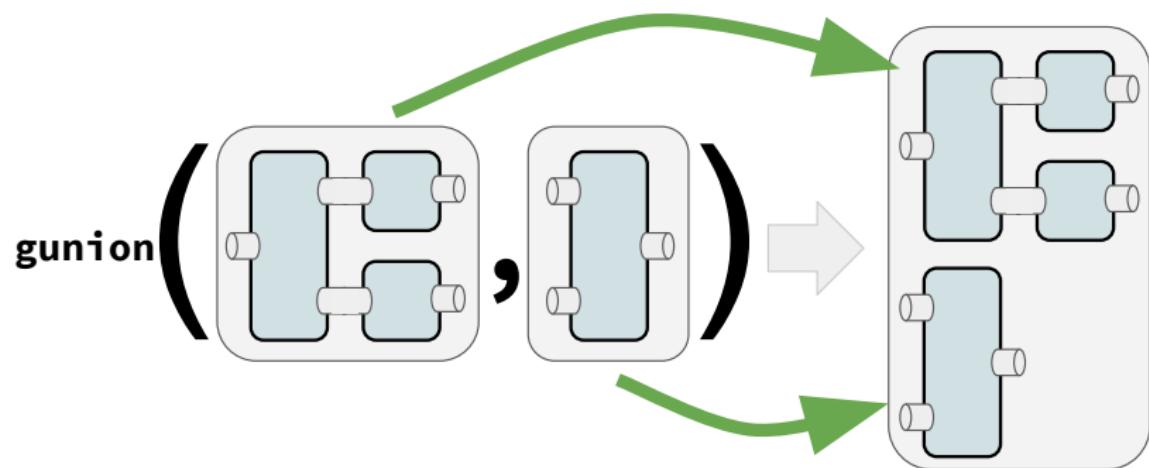
- The `%>>%`-operator concatenates Graphs and PipeOps



THE STRUCTURE

GRAPH OPERATIONS

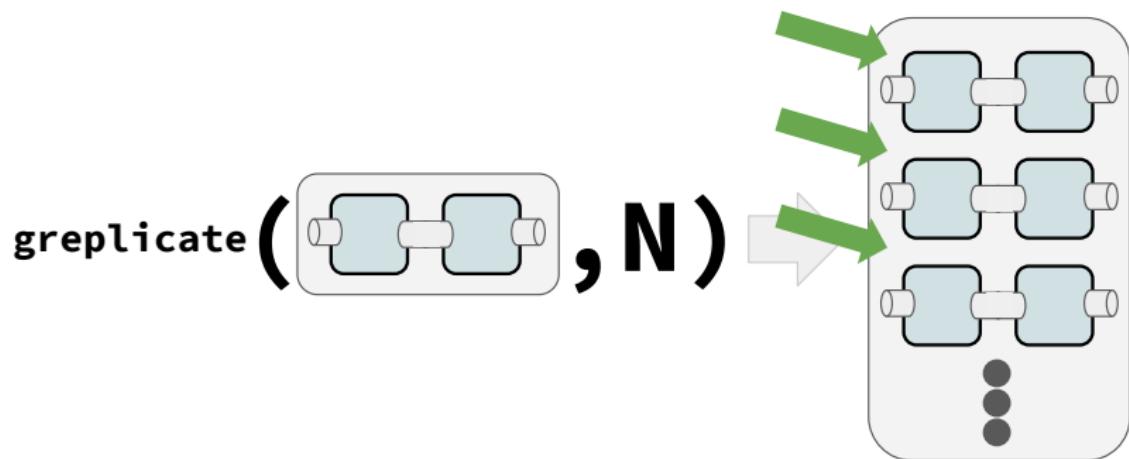
- The `%>>%`-operator concatenates Graphs and PipeOps
- The `gunion()`-function unites Graphs and PipeOps



THE STRUCTURE

GRAPH OPERATIONS

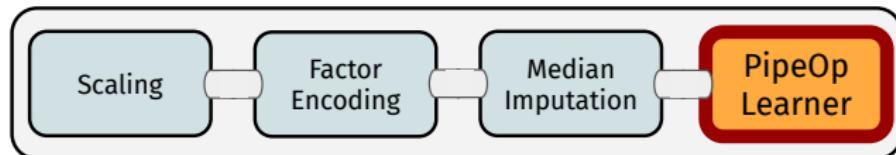
- The `%>>%`-operator concatenates Graphs and PipeOps
- The `gunion()`-function unites Graphs and PipeOps
- The `grePLICATE()`-function unites copies of Graphs and PipeOps



LEARNERS AND GRAPHS

PIPEOPLEARNER

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



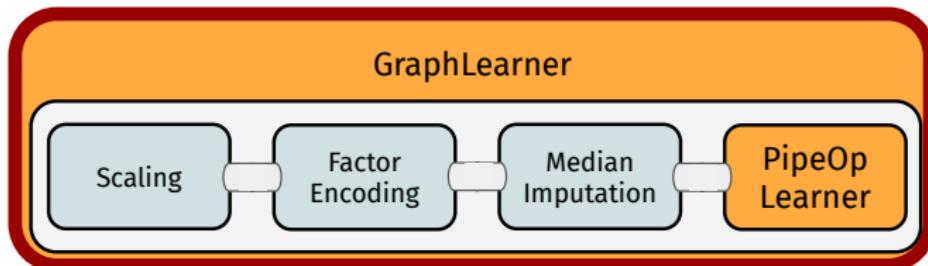
LEARNERS AND GRAPHS

PIPEOPLEARNER

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

GRAPHLEARNER

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

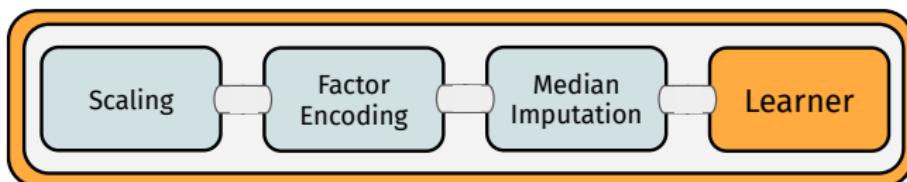


LINEAR PIPELINES

MLR3PIPELINES IN ACTION

LINEAR PREPROCESSING PIPELINE

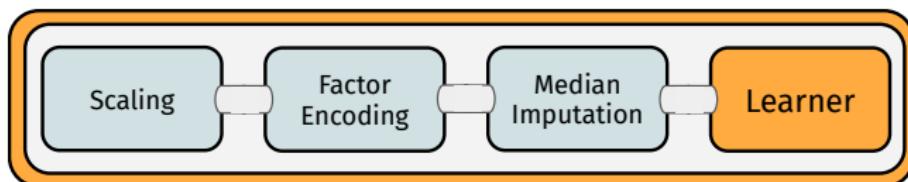
```
graph_pp = PipeOpScale$new() %>>%  
  PipeOpEncode$new() %>>%  
  PipeOpImputeMedian$new() %>>%  
  PipeOpLearner$new(  
    learner = lrn("classif.rpart"))
```



MLR3PIPELINES IN ACTION

LINEAR PREPROCESSING PIPELINE

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

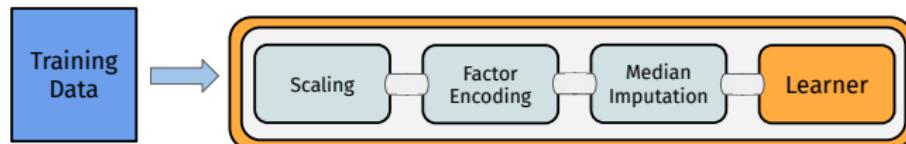


MLR3PIPELINES IN ACTION

LINEAR PREPROCESSING PIPELINE

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

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

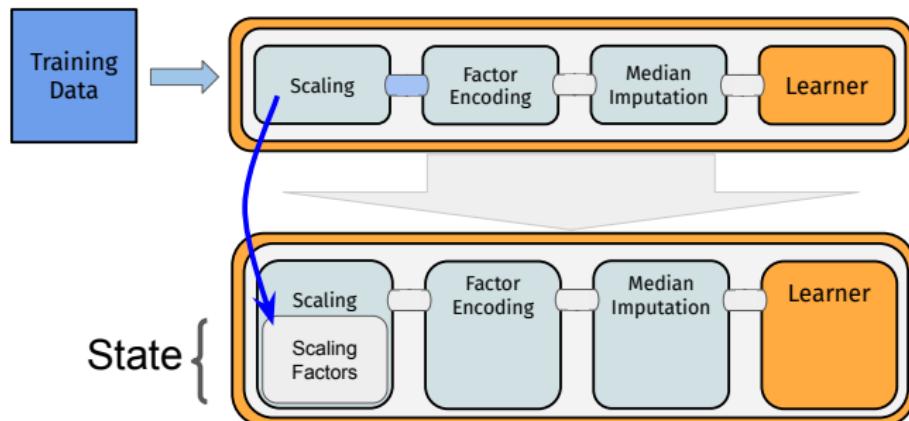


MLR3PIPELINES IN ACTION

LINEAR PREPROCESSING PIPELINE

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

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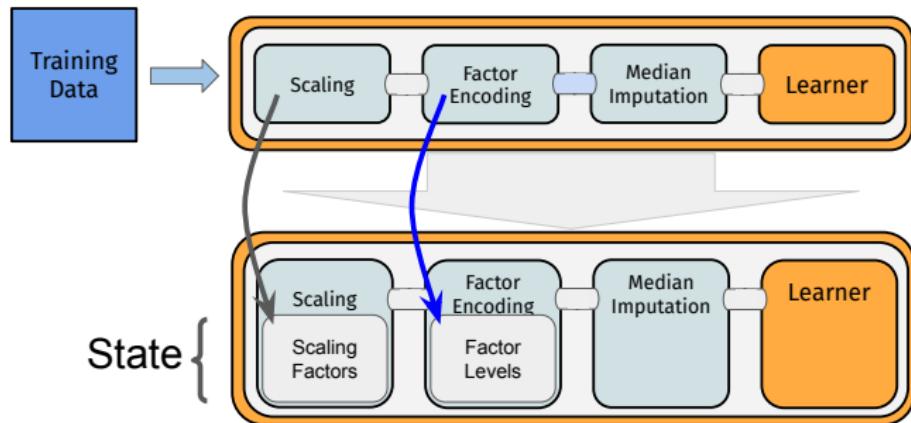


MLR3PIPELINES IN ACTION

LINEAR PREPROCESSING PIPELINE

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

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

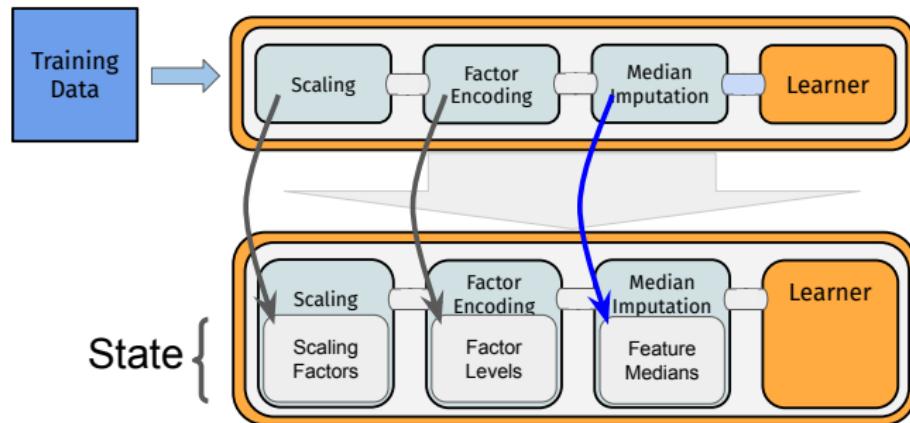


MLR3PIPELINES IN ACTION

LINEAR PREPROCESSING PIPELINE

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

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

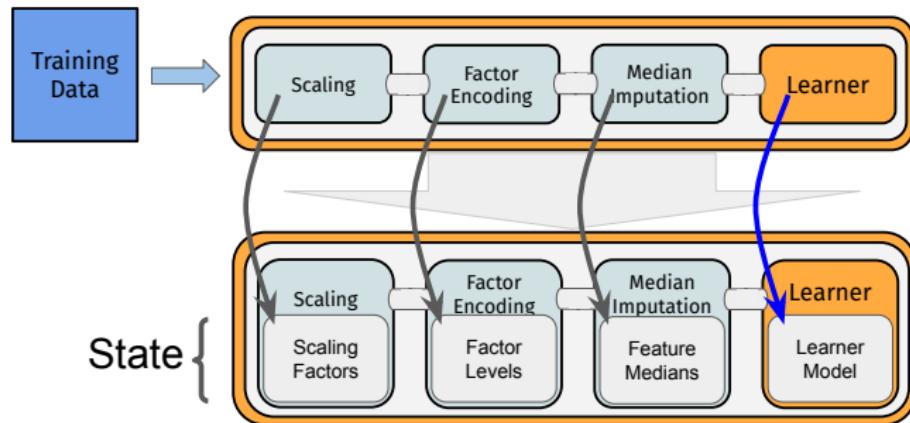


MLR3PIPELINES IN ACTION

LINEAR PREPROCESSING PIPELINE

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

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

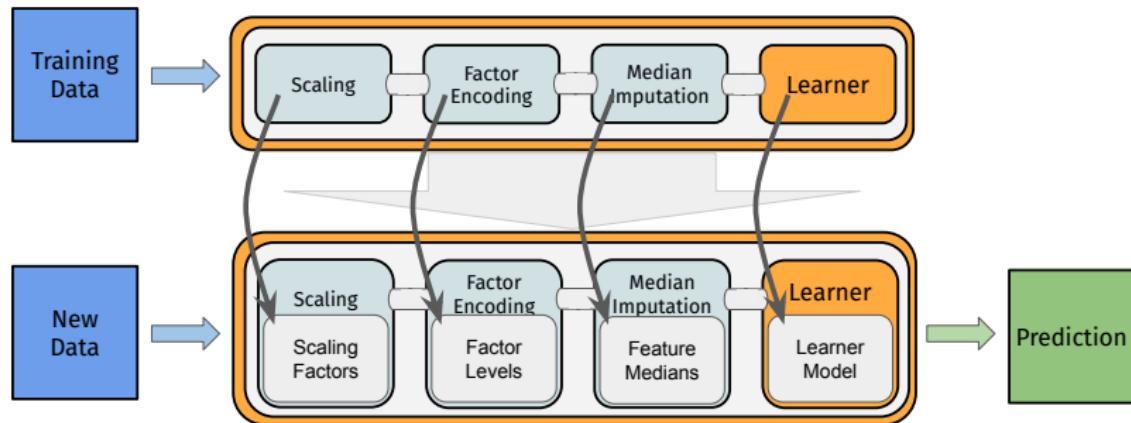


MLR3PIPELINES IN ACTION

LINEAR PREPROCESSING PIPELINE

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

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



MLR3PIPELINES IN ACTION

LINEAR PREPROCESSING PIPELINE `SCALE %>>% ENCODE %>>%
IMPUTE %>>% RPART`

- Setting / retrieving parameters: `$param_set`

```
graph_pp$pipeops$scale$param_set$values$center = FALSE
```

MLR3PIPELINES IN ACTION

LINEAR PREPROCESSING PIPELINE `SCALE %>>% ENCODE %>>%
IMPUTE %>>% RPART`

- Setting / retrieving parameters: `$param_set`

```
graph_pp$pipeops$scale$param_set$values$center = FALSE
```

- Retrieving state: `$state` of individual PipeOps (*after \$train()*)

```
graph_pp$pipeops$scale$state$scale  
## Petal.Length  Petal.Width Sepal.Length  Sepal.Width  
##        4.163367      1.424451      5.921098      3.098387
```

MLR3PIPELINES IN ACTION

LINEAR PREPROCESSING PIPELINE `SCALE %>>% ENCODE %>>%`

```
IMPUTE %>>% RPART
```

- Setting / retrieving parameters: `$param_set`

```
graph_pp$pipeops$scale$param_set$values$center = FALSE
```

- Retrieving state: `$state` of individual PipeOps (*after \$train()*)

```
graph_pp$pipeops$scale$state$scale
```

```
## Petal.Length  Petal.Width Sepal.Length  Sepal.Width  
##      4.163367      1.424451      5.921098      3.098387
```

- Retrieving intermediate results: `$.result` (set debug option before)

```
graph_pp$pipeops$scale$.result[[1]]$head(3)
```

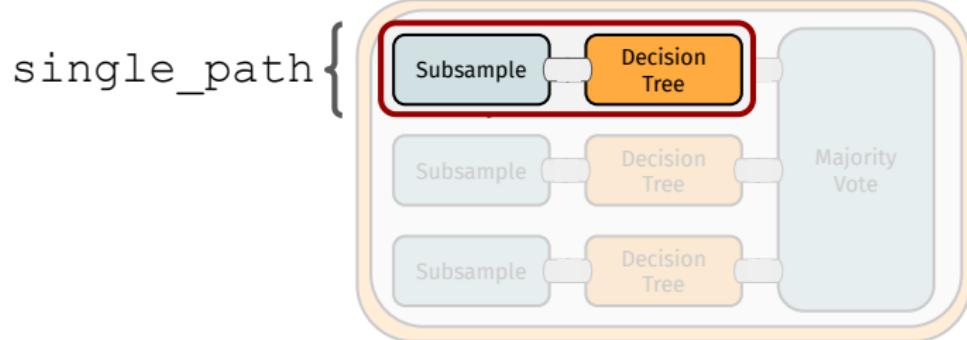
```
##      Species Petal.Length Petal.Width Sepal.Length Sepal.Width  
## 1:  setosa     0.3362663    0.140405    0.8613268   1.1296201  
## 2:  setosa     0.3362663    0.140405    0.8275493   0.9682458  
## 3:  setosa     0.3122473    0.140405    0.7937718   1.0327956
```

NONLINEAR PIPELINES

MLR3 PIPELINES IN ACTION

ENSEMBLE METHOD: BAGGING

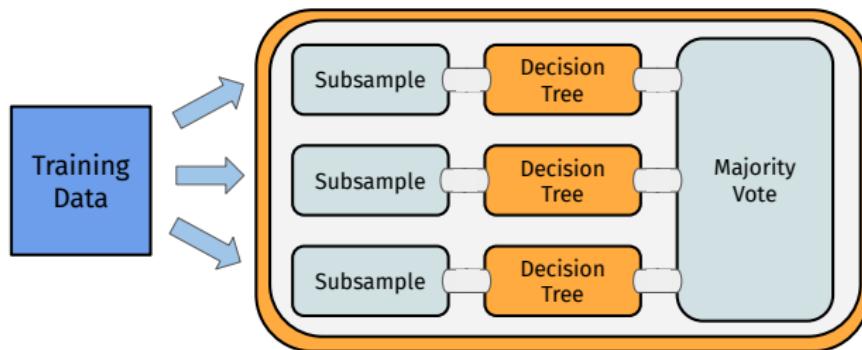
```
single_path = po("subsample") %>>% lrn("classif.rpart")
```



MLR3 PIPELINES IN ACTION

ENSEMBLE METHOD: BAGGING

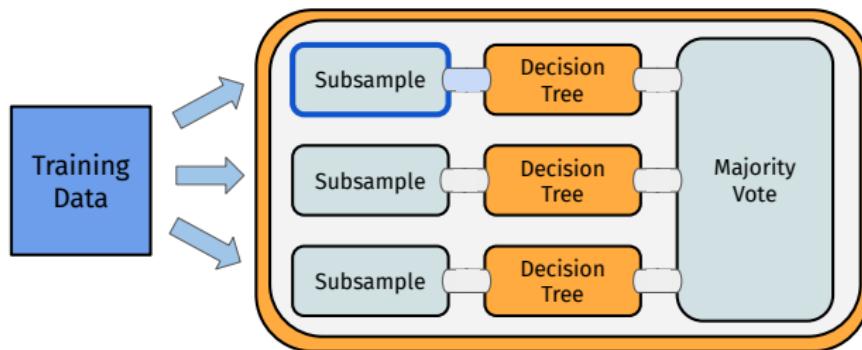
```
single_path = po("subsample") %>>% lrn("classif.rpart")  
  
graph_bag = grepligate(single_path, n = 3) %>>%  
  po("classifavg")
```



MLR3 PIPELINES IN ACTION

ENSEMBLE METHOD: BAGGING

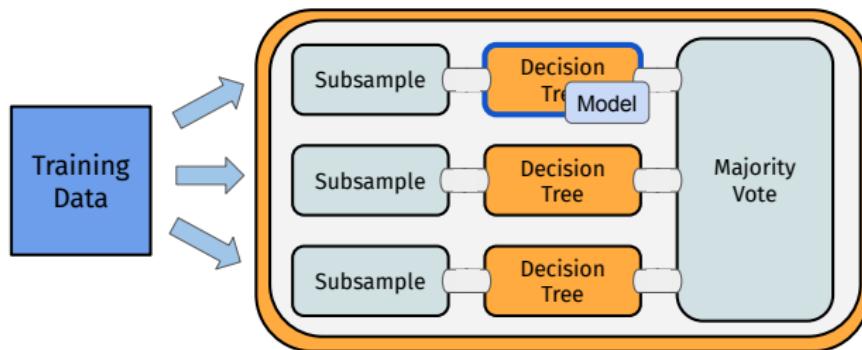
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MLR3 PIPELINES IN ACTION

ENSEMBLE METHOD: BAGGING

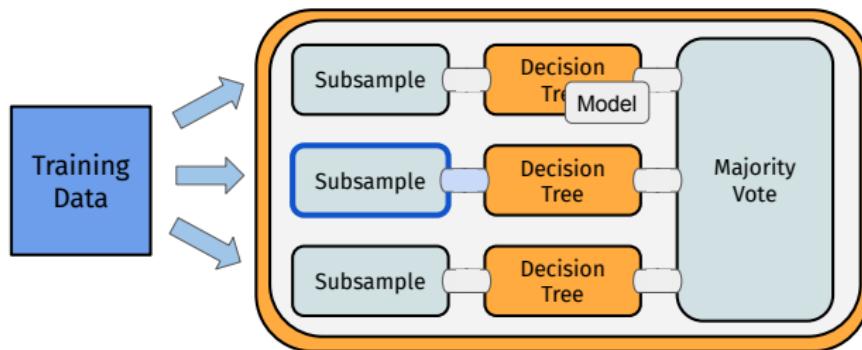
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single_path = po("subsample") %>>% lrn("classif.rpart")  
  
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```



MLR3 PIPELINES IN ACTION

ENSEMBLE METHOD: BAGGING

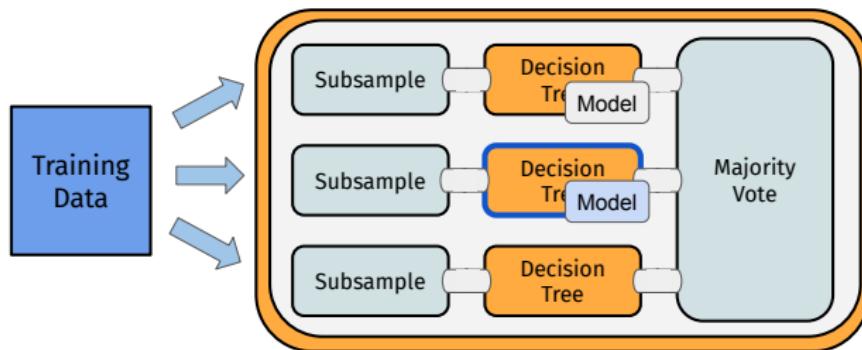
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```



MLR3 PIPELINES IN ACTION

ENSEMBLE METHOD: BAGGING

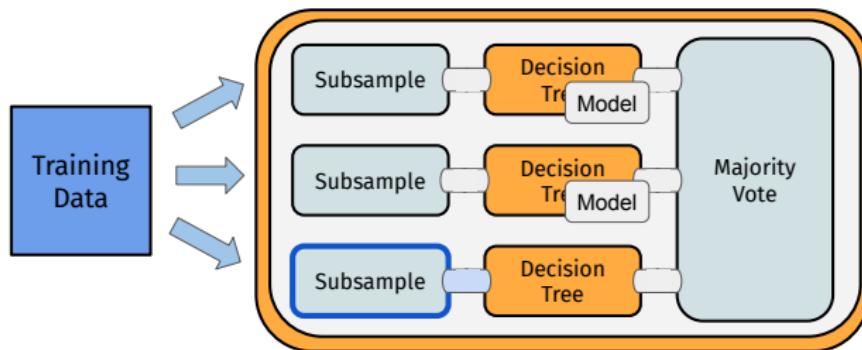
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single_path = po("subsample") %>>% lrn("classif.rpart")  
  
graph_bag = grepligate(single_path, n = 3) %>>%  
  po("classifavg")
```



MLR3 PIPELINES IN ACTION

ENSEMBLE METHOD: BAGGING

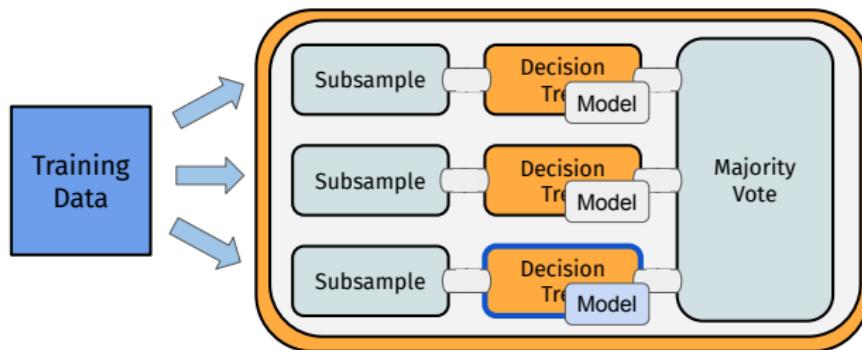
```
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graph_bag = grepligate(single_path, n = 3) %>>%  
  po("classifavg")
```



MLR3 PIPELINES IN ACTION

ENSEMBLE METHOD: BAGGING

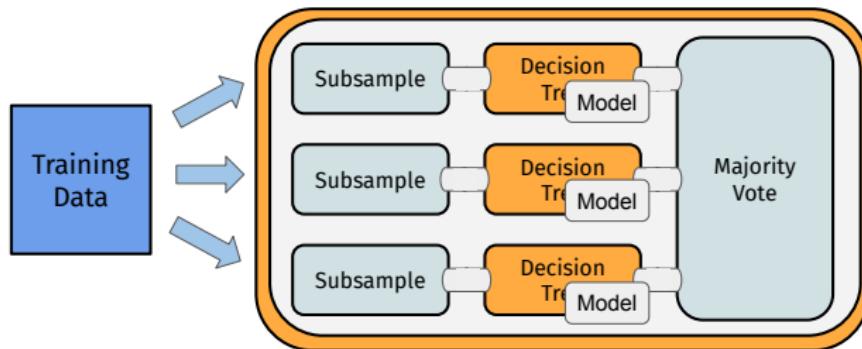
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graph_bag = grepligate(single_path, n = 3) %>>%  
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```



MLR3 PIPELINES IN ACTION

ENSEMBLE METHOD: BAGGING

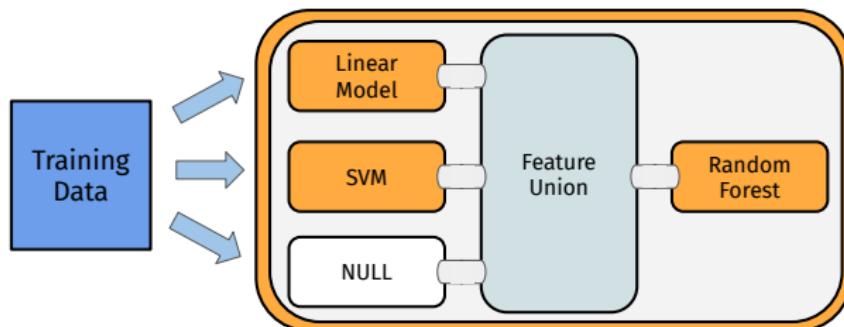
```
single_path = po("subsample") %>>% lrn("classif.rpart")  
  
graph_bag = grepligate(single_path, n = 3) %>>%  
  po("classifavg")
```



MLR3 PIPELINES 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")
```

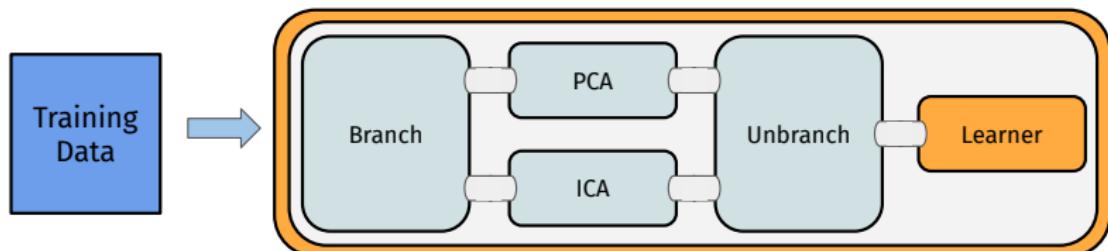


MLR3 PIPELINES IN ACTION

BRANCHING

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

Execute only one of several alternative paths

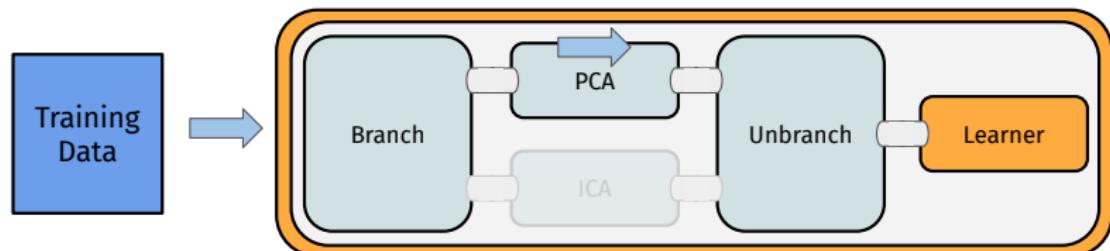


MLR3 PIPELINES IN ACTION

BRANCHING

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

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

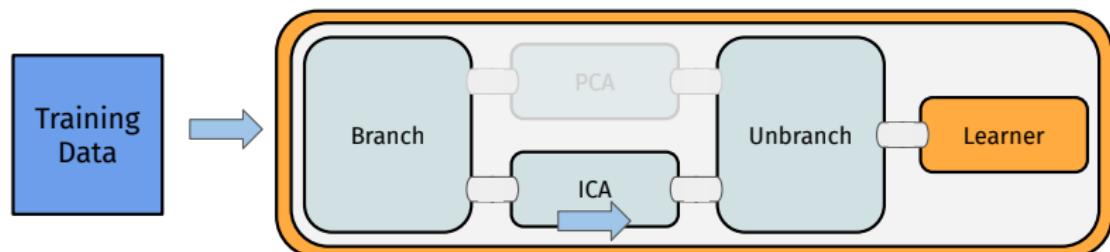


MLR3PIPELINES IN ACTION

BRANCHING

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

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



HYPERPARAMETERS AND TUNING

HYPERPARAMETERS AND TUNING

- PipeOps have *hyperparameters* (using `paradox` pkg)
- Graphs have hyperparameters of all components *combined*
- ⇒ simultaneous **Tuning** of Learner and preprocessing
(`mlr3tuning` package)

```
library("paradox") ; library("mlr3tuning")
glrn = po("scale") %>>% lrn("classif.rpart")
ps = ParamSet$new(list(
  ParamLgl$new("scale.scale"),
  ParamInt$new("classif.rpart.minsplit", 1, 20)
))
inst = TuningInstance$new(task, glrn,
  rsmp("cv"), msr("classif.ce"), ps,
  term("evals", n_evals = 10))

tnr("random_search")$tune(inst)

inst$result
```

OUTRO

MLR3PIPELINES

`mlr3pipelines` overview:

- Construct a PipeOp using `po()`
- Use Graph operators to connect them
 - ▶ `%>>%`—chain operations
 - ▶ `gunion()`—put operations in parallel
 - ▶ `greuplicate()`—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