LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

Machine Learning Pipelines in R

mlr3pipelines

Department of Statistics – LMU Munich

September 26, 2019

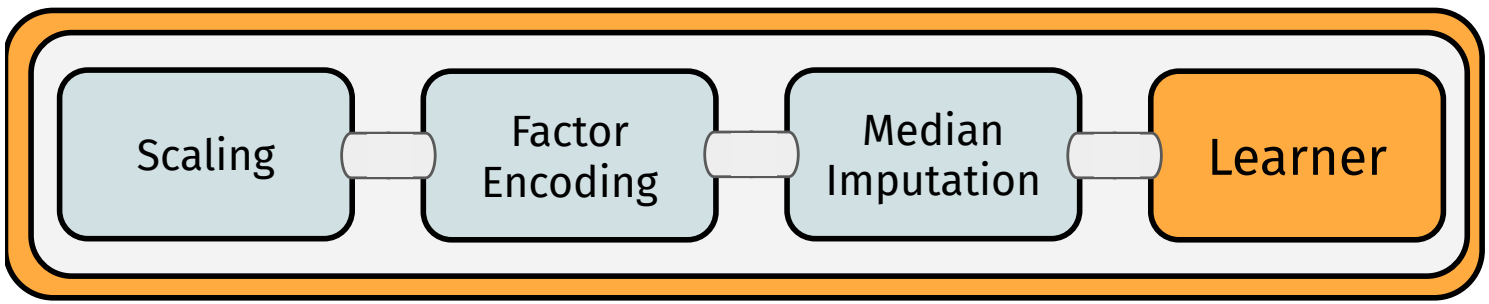
Intro

MLR3PIPELINES

Machine Learning Workflows:

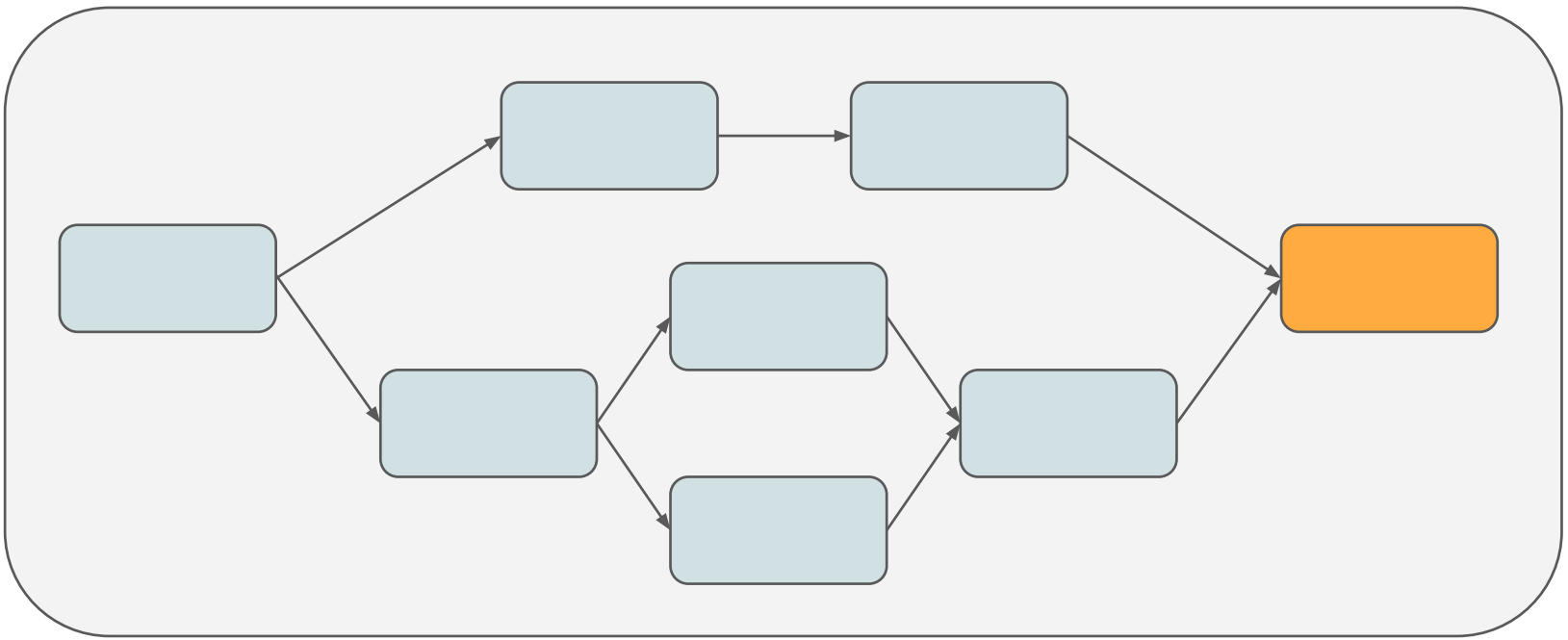
- **Preprocessing**: Feature extraction, feature selection, missing data imputation,...
- **Ensemble methods**: Model averaging, model stacking
- `mlr3`: modular model fitting

$\Rightarrow$ `mlr3pipelines`: modular ML workflows



MACHINE LEARNING WORKFLOWS

– what do they look like?



MACHINE LEARNING WORKFLOWS

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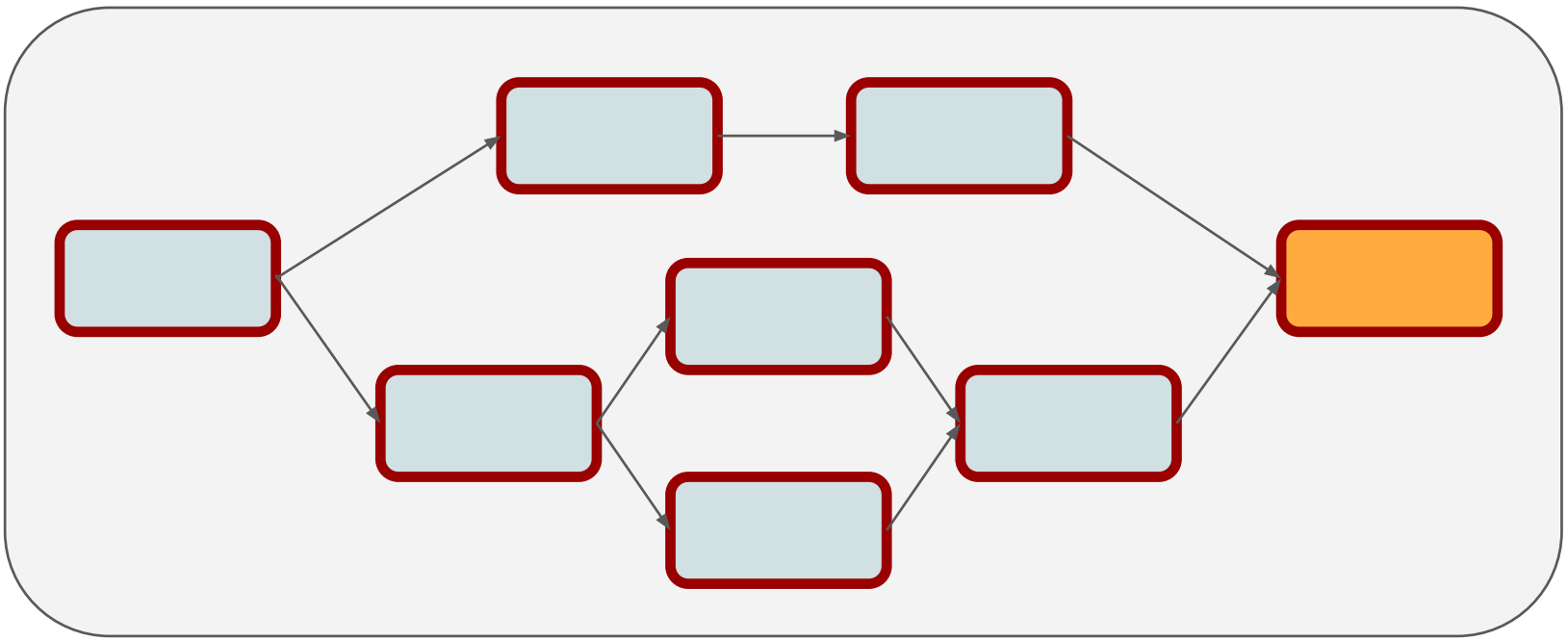
- **Building blocks**: *what* is happening? $\rightarrow$ `PipeOp`



MACHINE LEARNING WORKFLOWS

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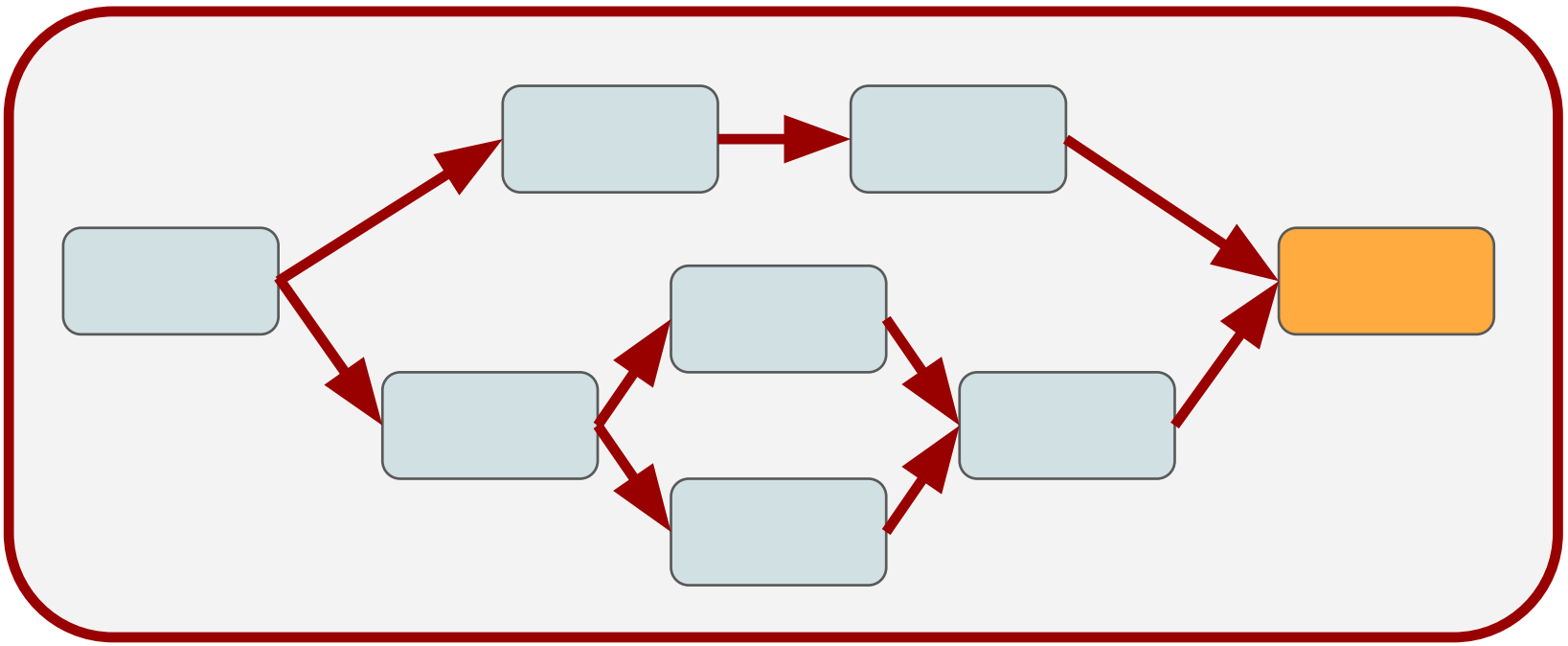
- **Building blocks**: *what* is happening? → `PipeOp`
- **Structure**: In what *sequence* is it happening? → `Graph`

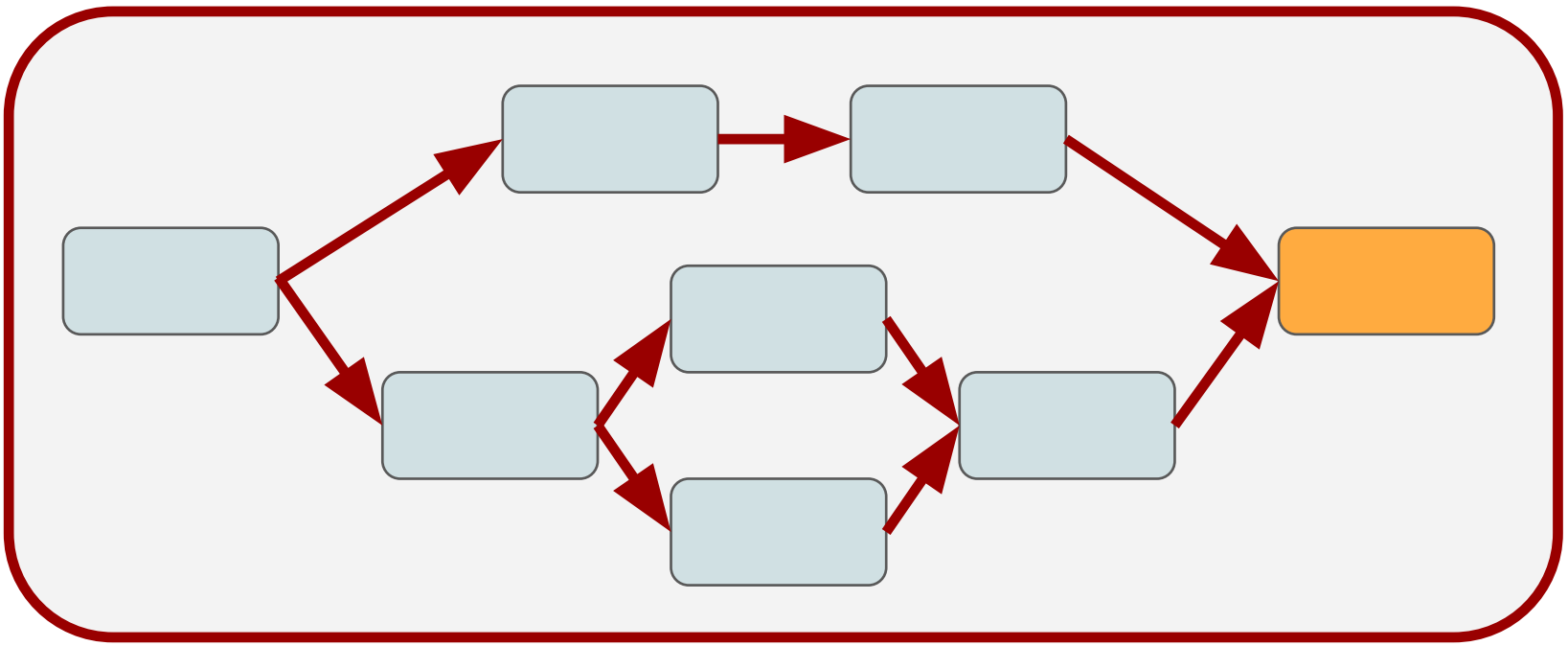


MACHINE LEARNING WORKFLOWS

– 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

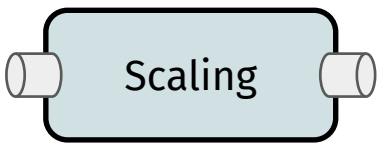


PipeOps

THE BUILDING BLOCKS

PipeOp: Single Unit of Data Operation

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



THE BUILDING BLOCKS

PipeOp: Single Unit of Data Operation

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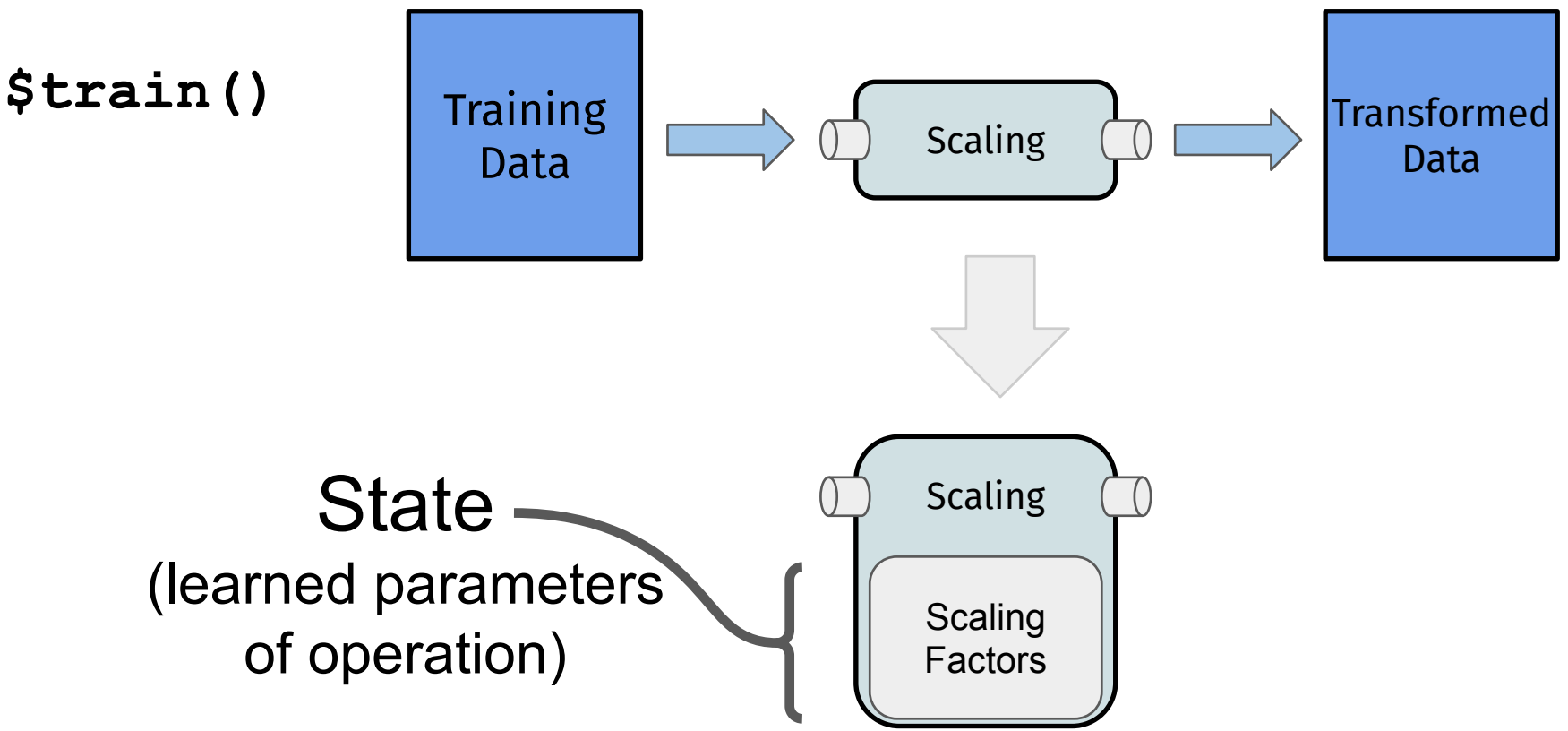
- `pip$train()`: process data and create `pip$state`



THE BUILDING BLOCKS

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- `pip$train()`: process data and create `pip$state`
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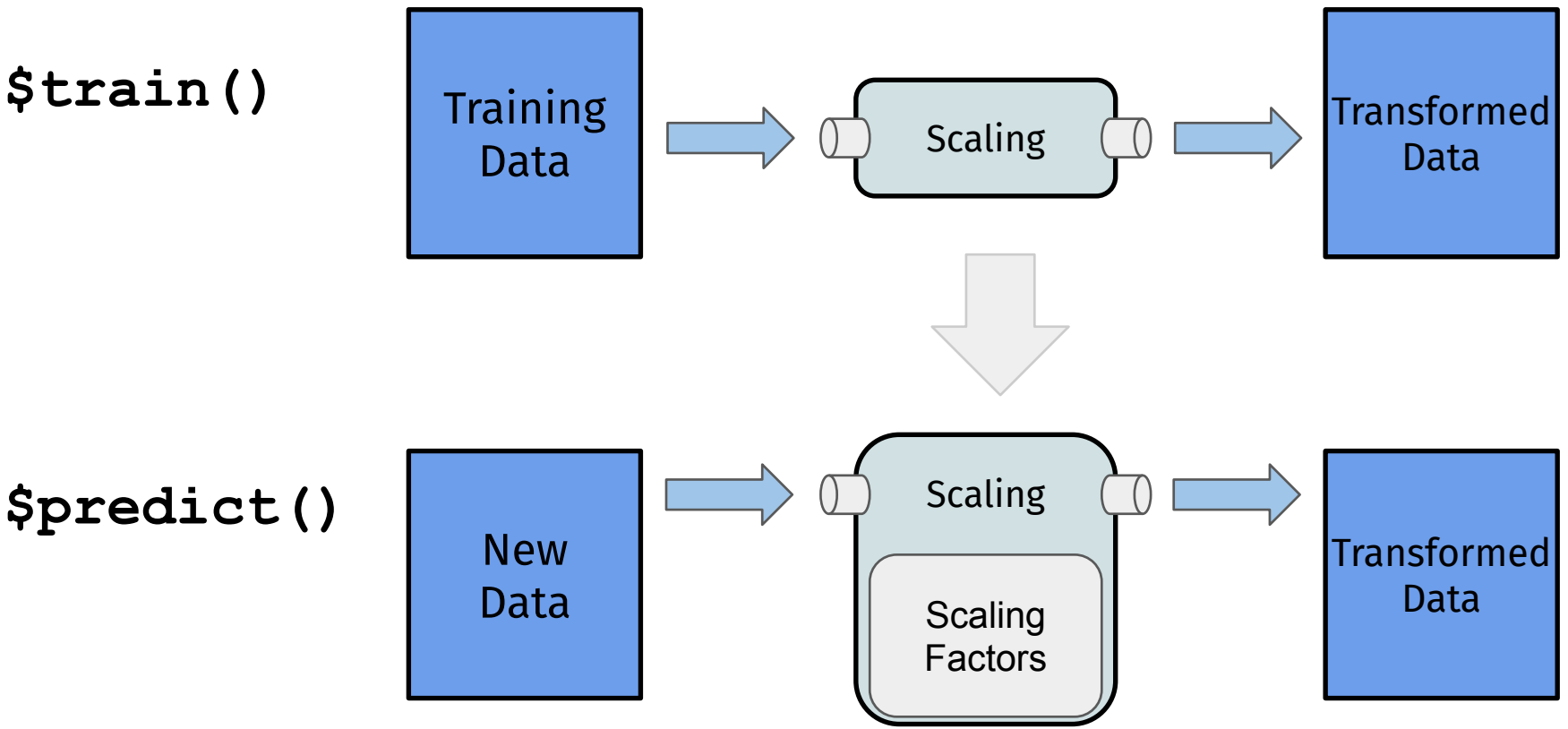
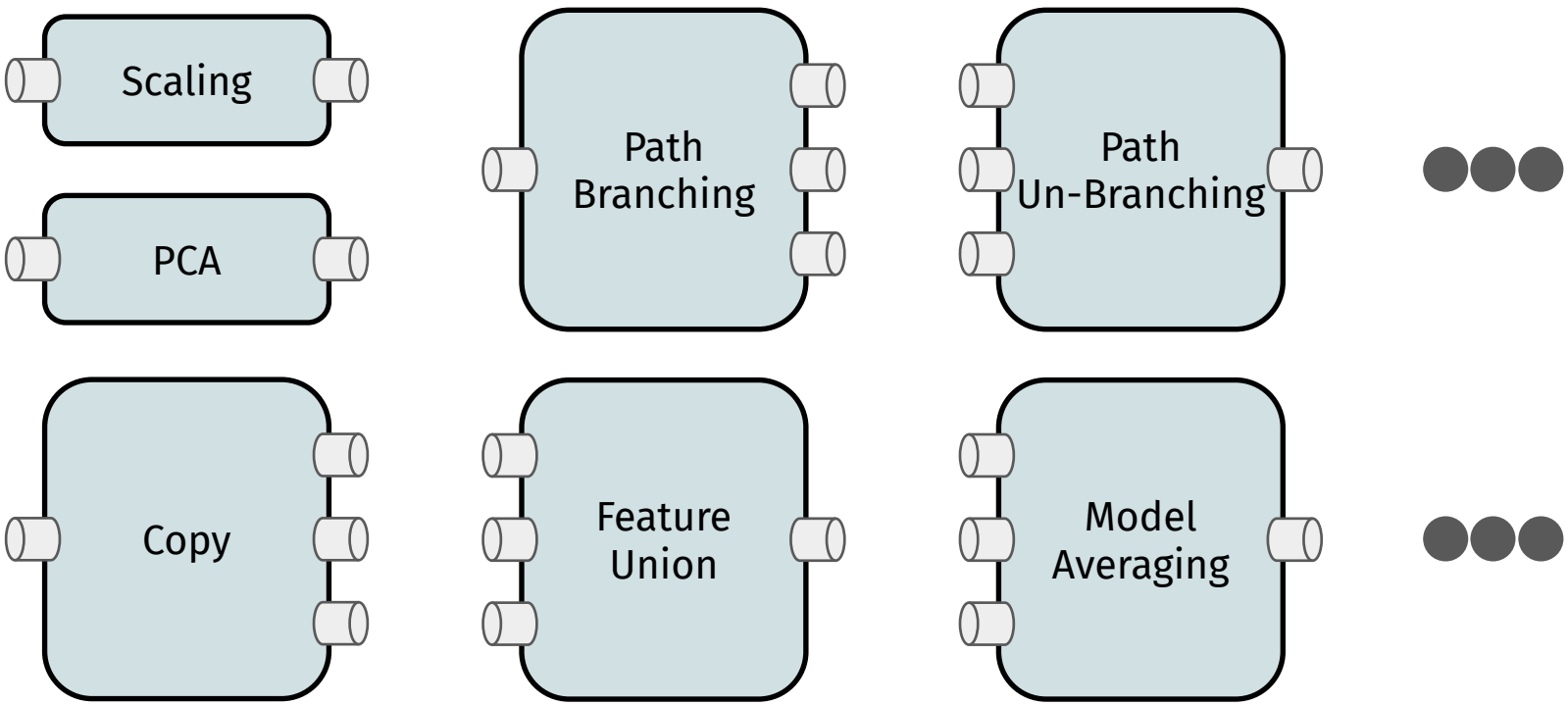


THE BUILDING BLOCKS

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
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```

```
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

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```

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

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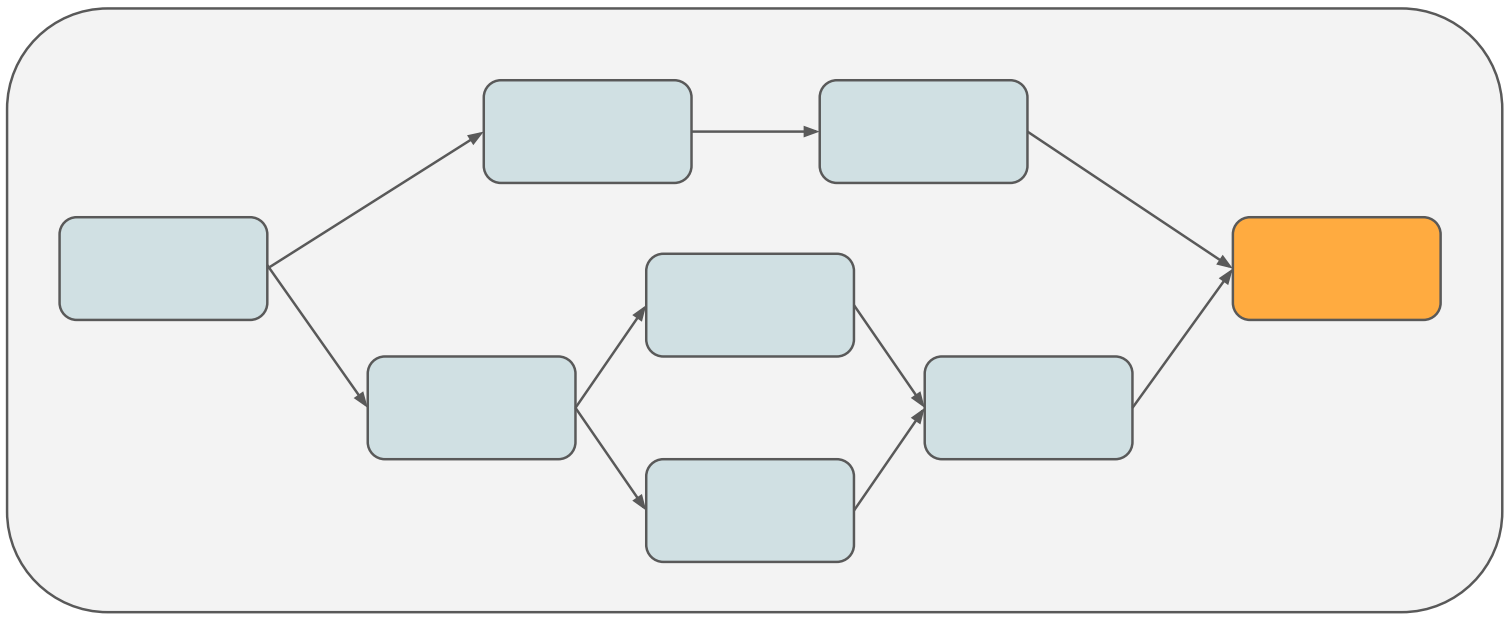
Graph Operations

THE STRUCTURE

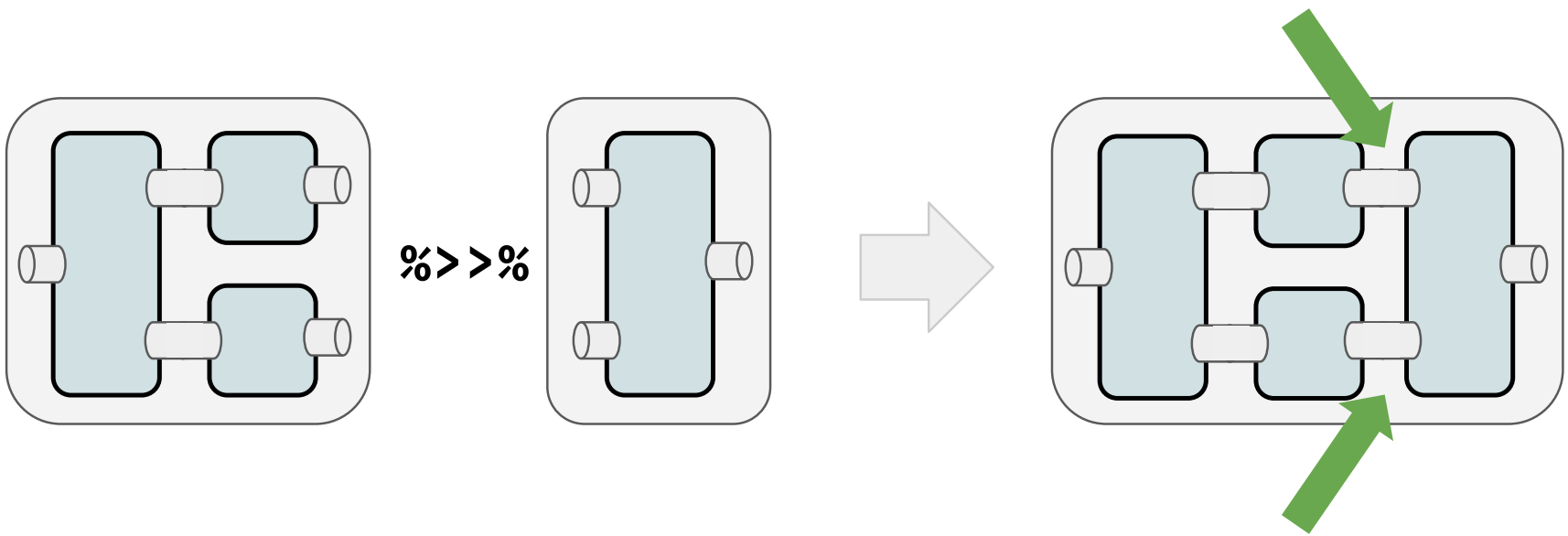
Graph Operations



THE STRUCTURE

Graph Operations

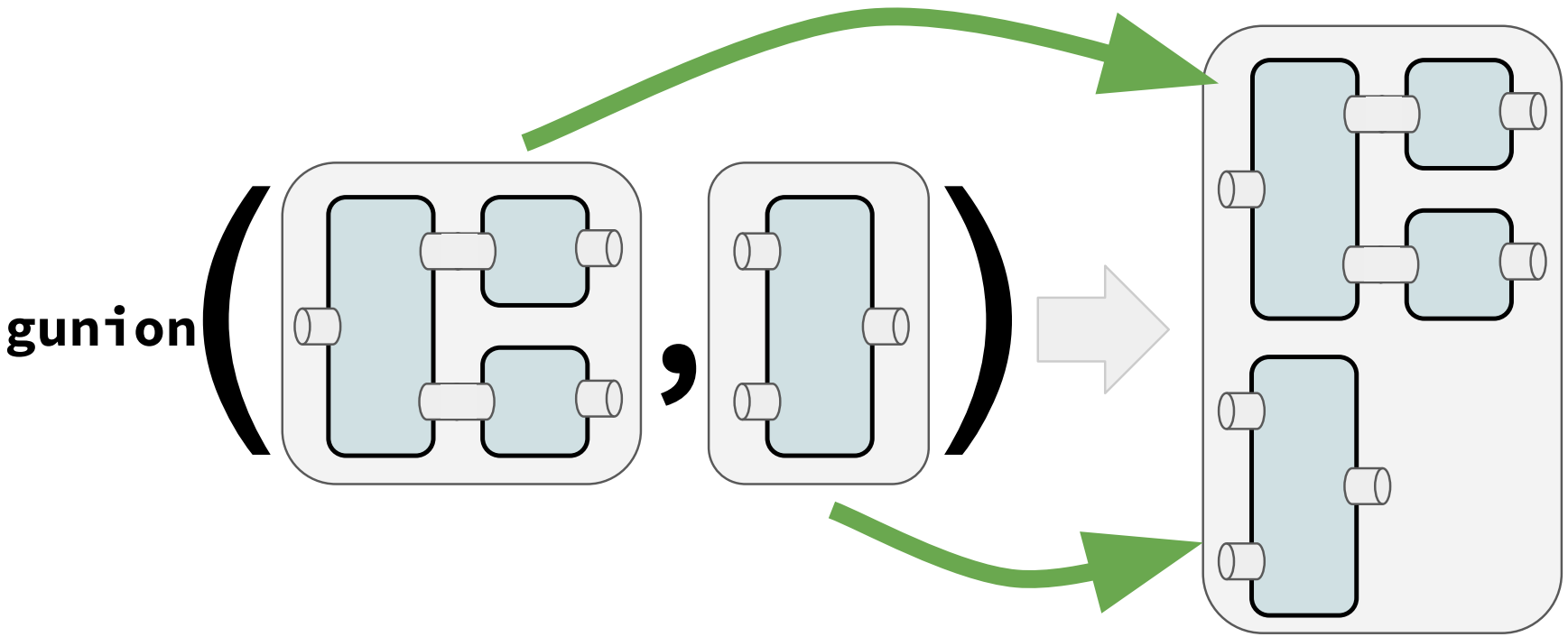
- The %>>%-operator concatenates `Graphs` and `PipeOps`



THE STRUCTURE

Graph Operations

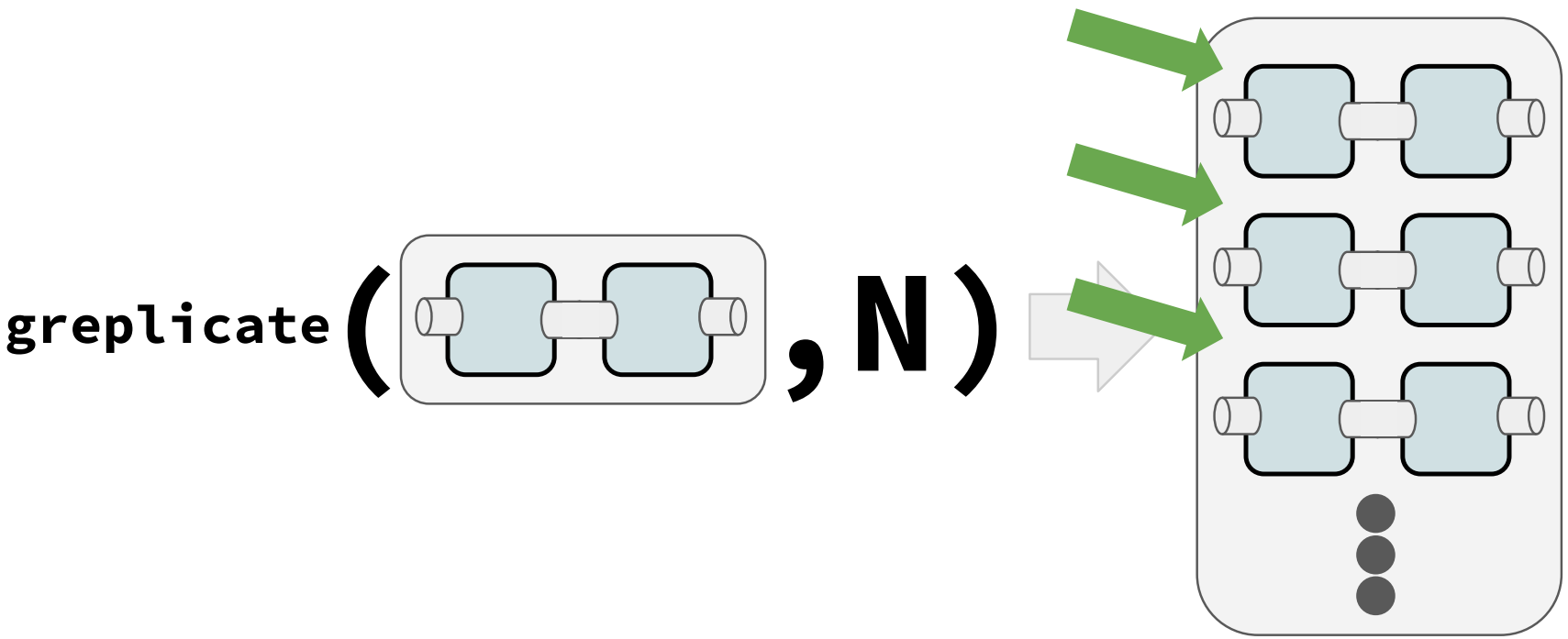
- The %>>%-operator concatenates `Graphs` and `PipeOps`
- The `gunion()`-function unites `Graphs` and `PipeOps`



THE STRUCTURE

Graph Operations

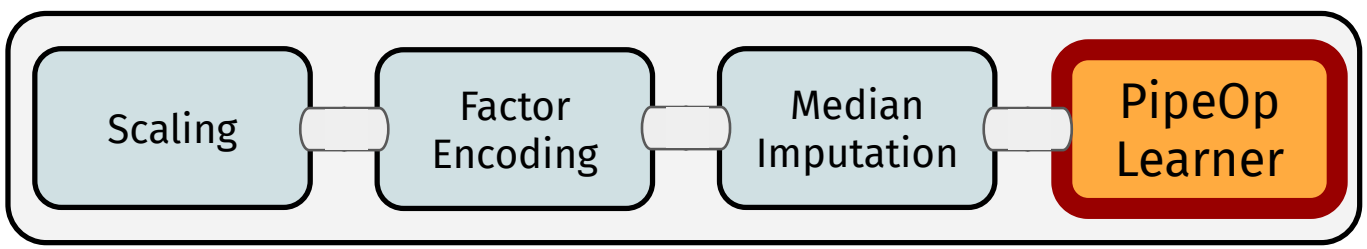
- The %>>%-operator concatenates `Graphs` and `PipeOps`
- The `gunion()`-function unites `Graphs` and `PipeOps`
- The `greplicate()`-function unites copies of `Graphs` and `PipeOps`



LEARNERS AND GRAPHS

PipeOpLearner

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



LEARNERS AND GRAPHS

PipeOpLearner

- `Learner` as a `PipeOp`
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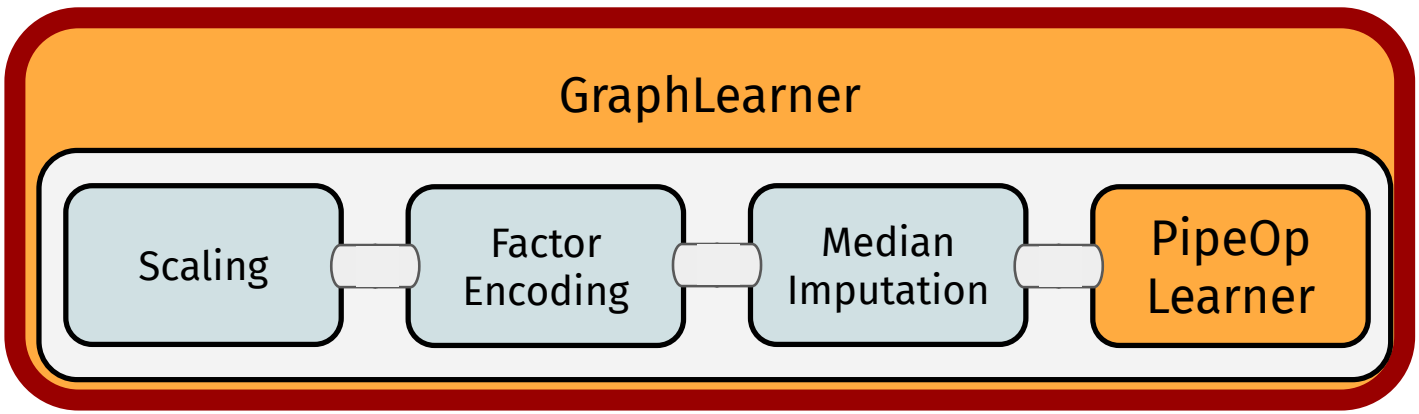
GraphLearner

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

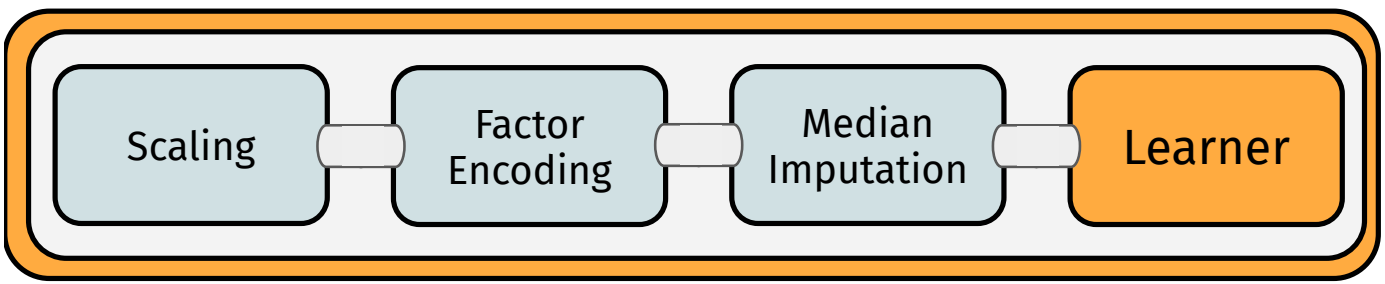


Linear Pipelines

MLR3PIPELINES IN ACTION

Linear Preprocessing Pipeline

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



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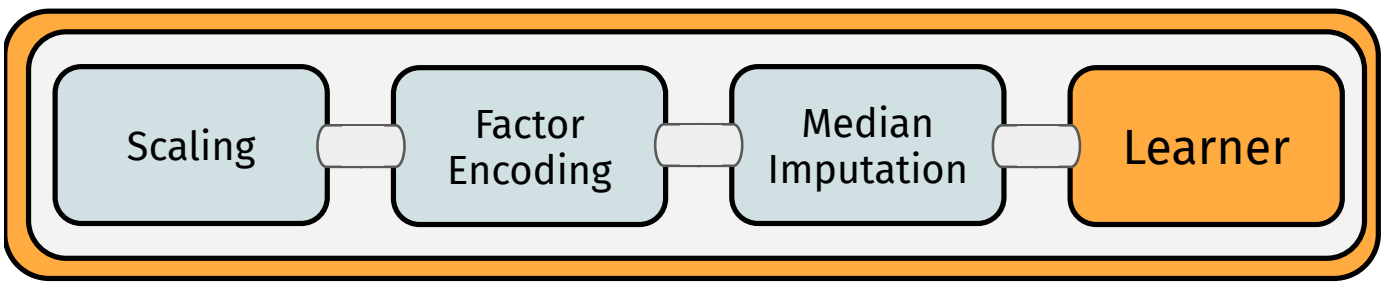
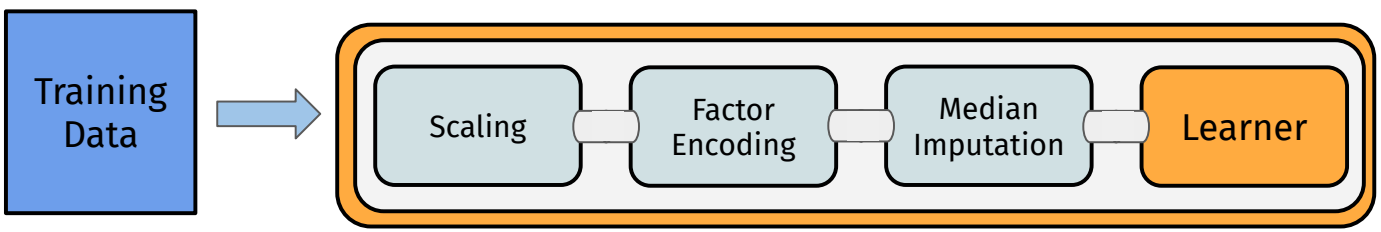


MLR3PIPELINES IN ACTION

Linear Preprocessing Pipeline

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

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



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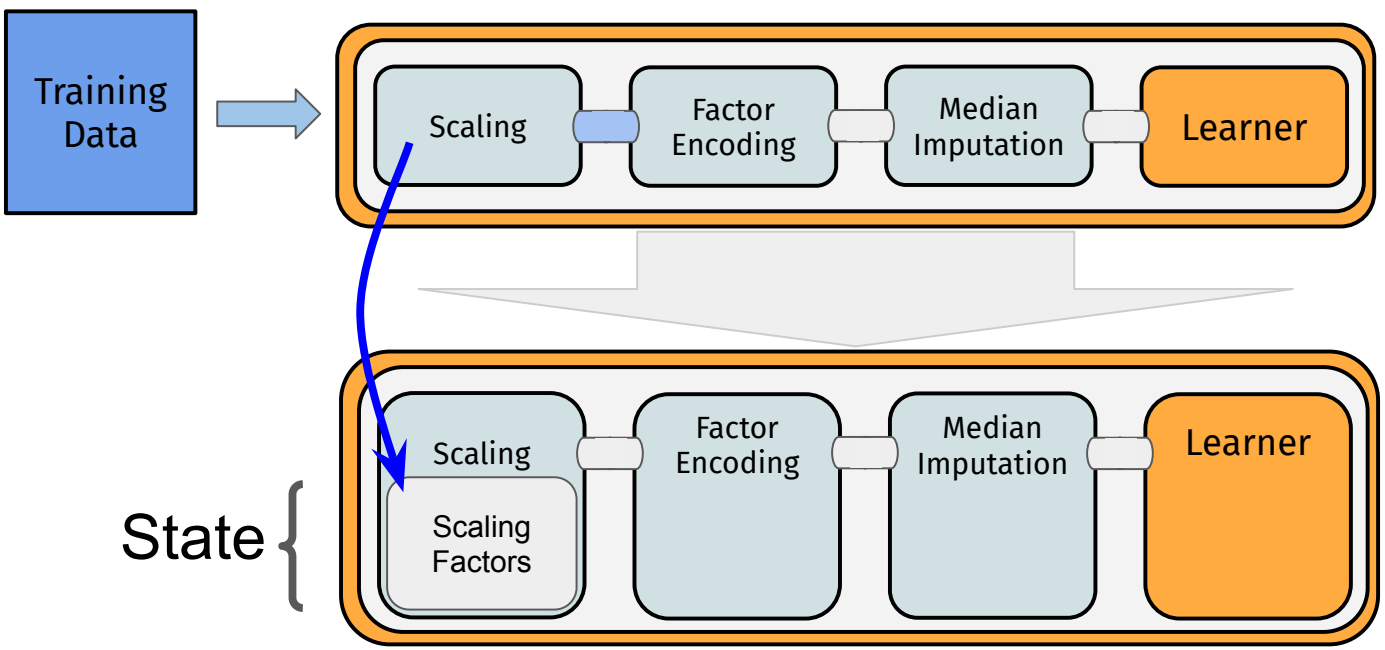

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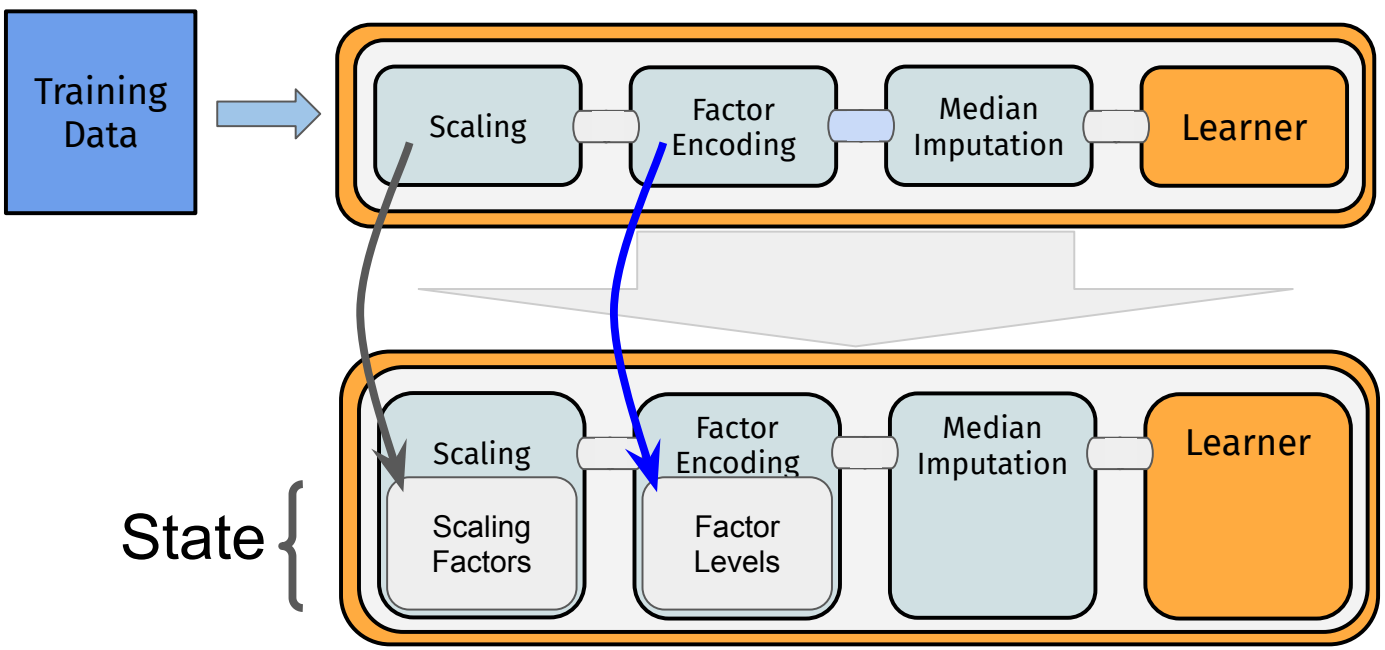

MLR3PIPELINES IN ACTION

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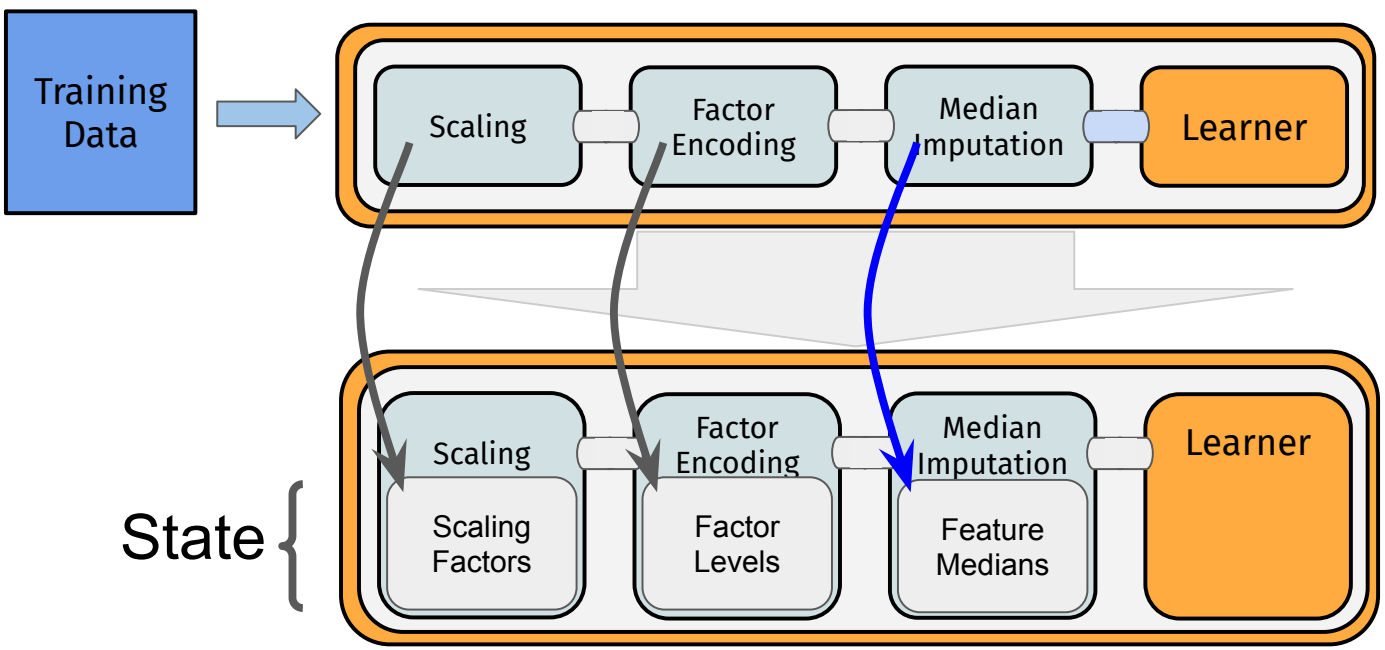

MLR3PIPELINES IN ACTION

Linear Preprocessing Pipeline

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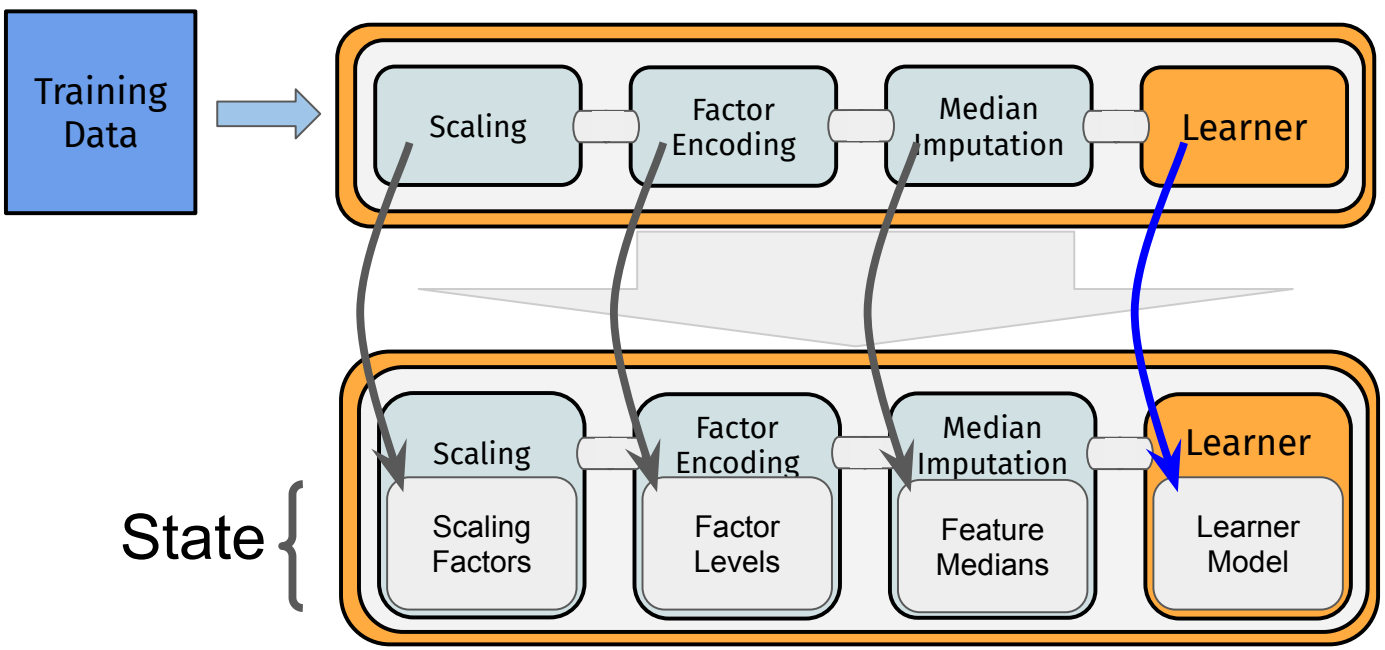
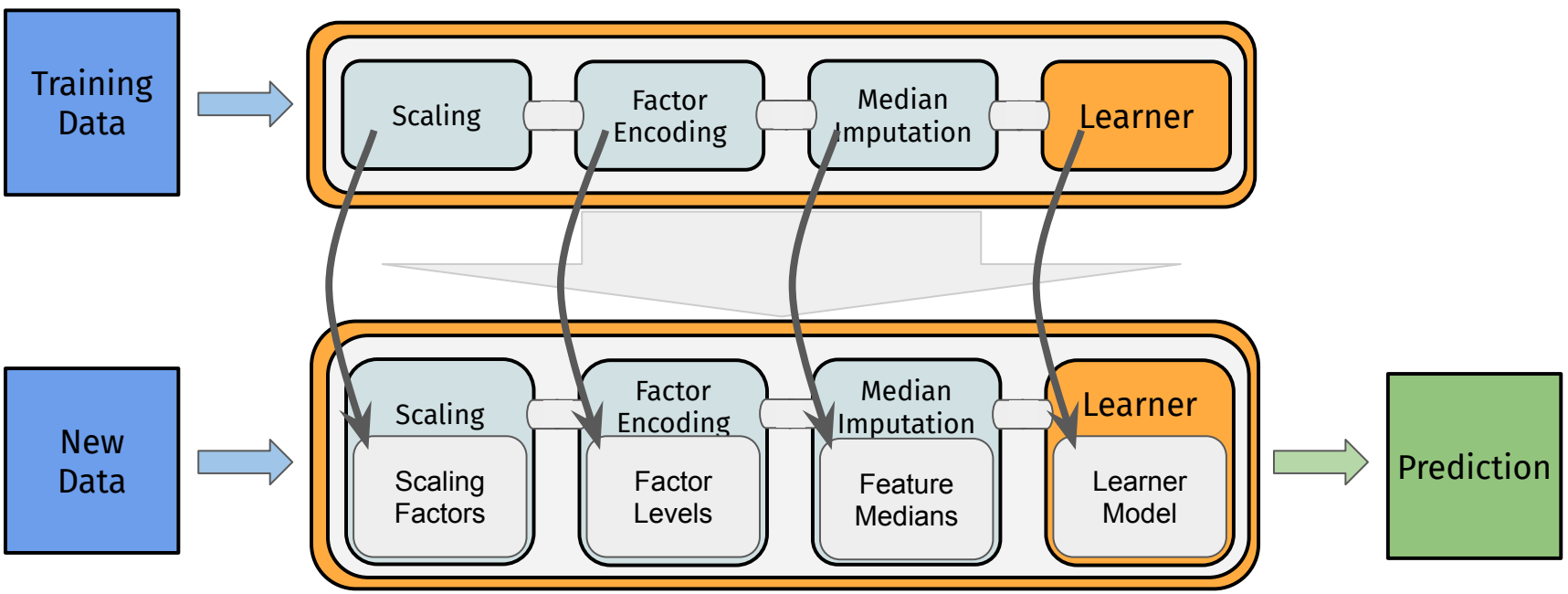


MLR3PIPELINES IN ACTION

Linear Preprocessing Pipeline

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

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

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

```
#> Petal.Length  Petal.Width Sepal.Length  Sepal.Width
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MLR3PIPELINES IN ACTION

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#>     4.163367     1.424451     5.921098     3.098387
```

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

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

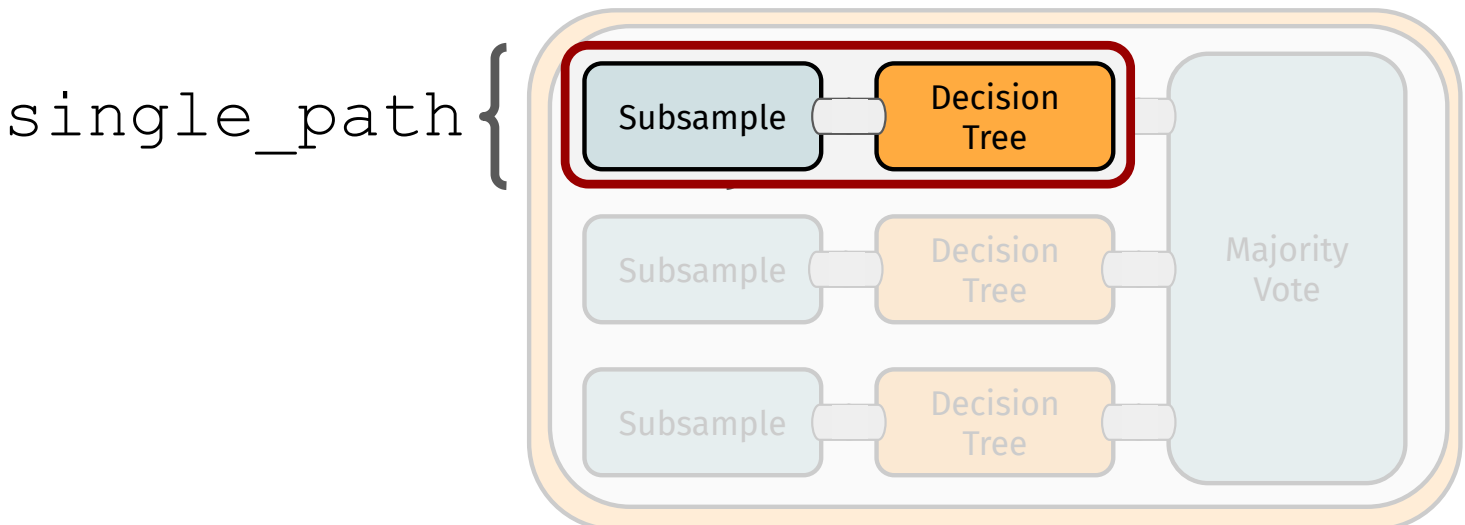
```
#>    Species Petal.Length Petal.Width Sepal.Length Sepal.Width
#> 1:  setosa    0.3362663    0.140405    0.8613268   1.1296201
#> 2:  setosa    0.3362663    0.140405    0.8275493   0.9682458
#> 3:  setosa    0.3122473    0.140405    0.7937718   1.0327956
```

Nonlinear Pipelines

MLR3PIPELINES IN ACTION

Ensemble Method: Bagging

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

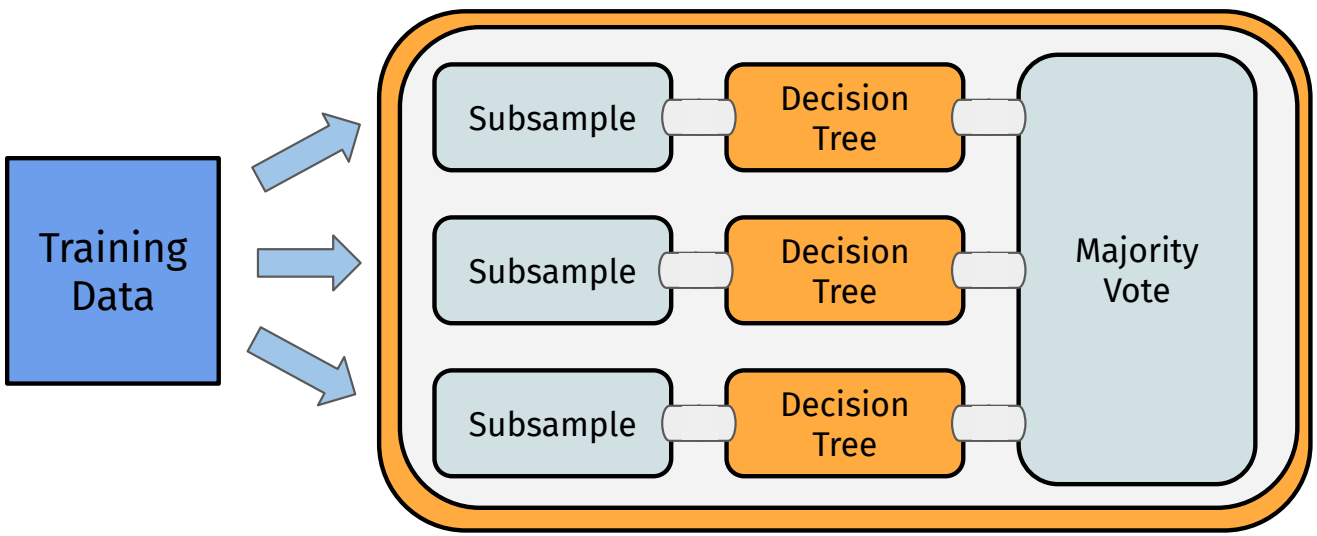


MLR3PIPELINES IN ACTION

Ensemble Method: Bagging

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

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



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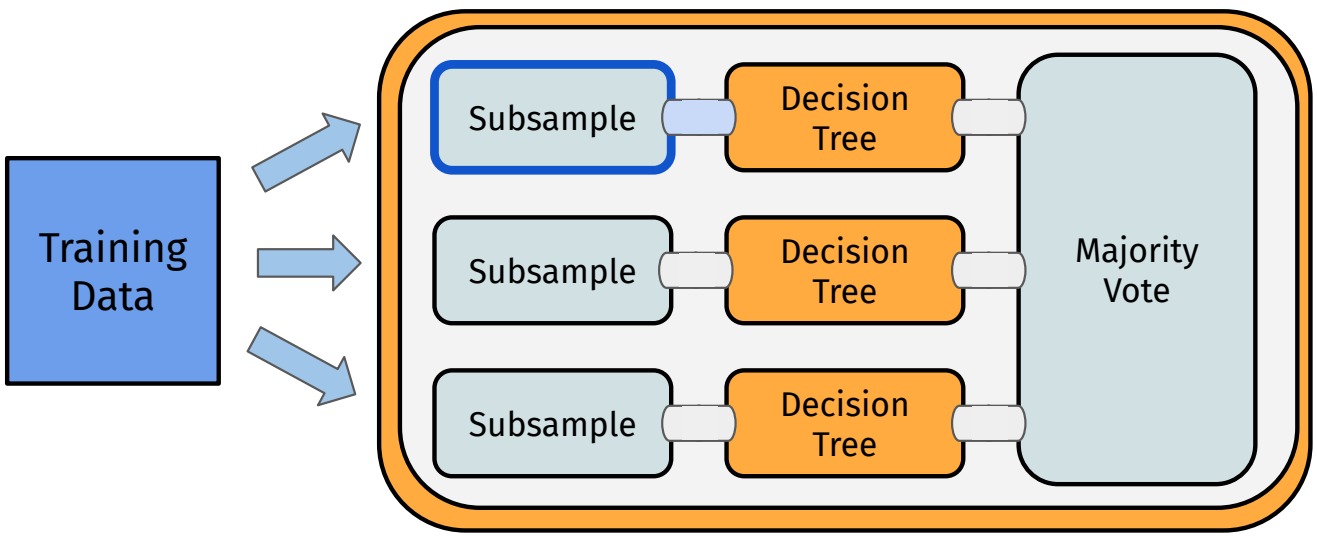

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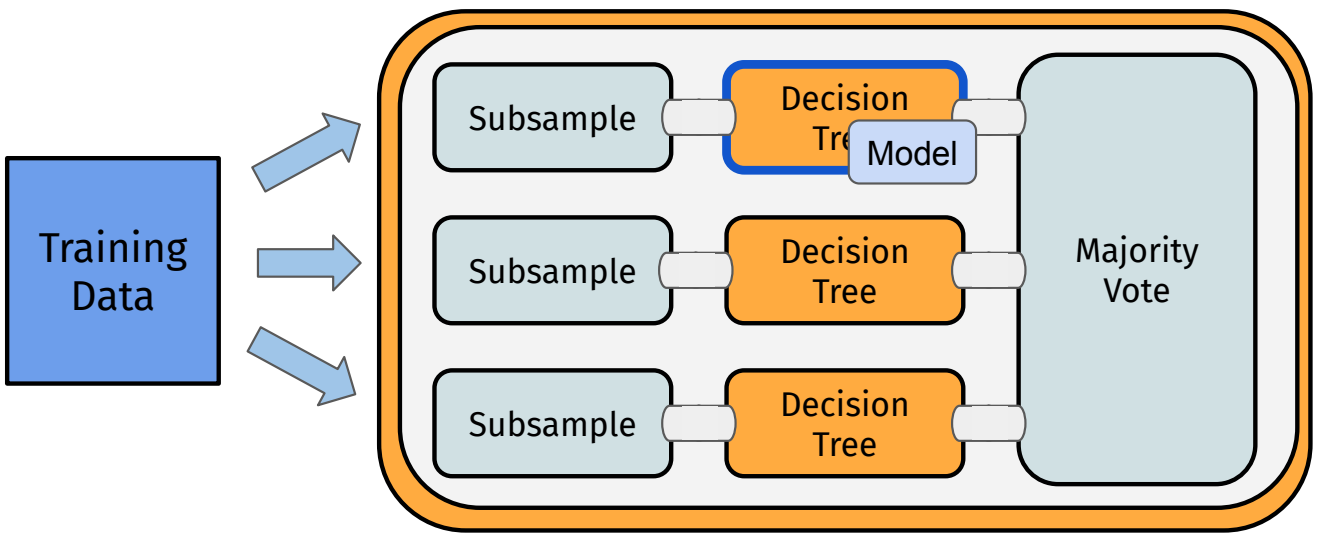

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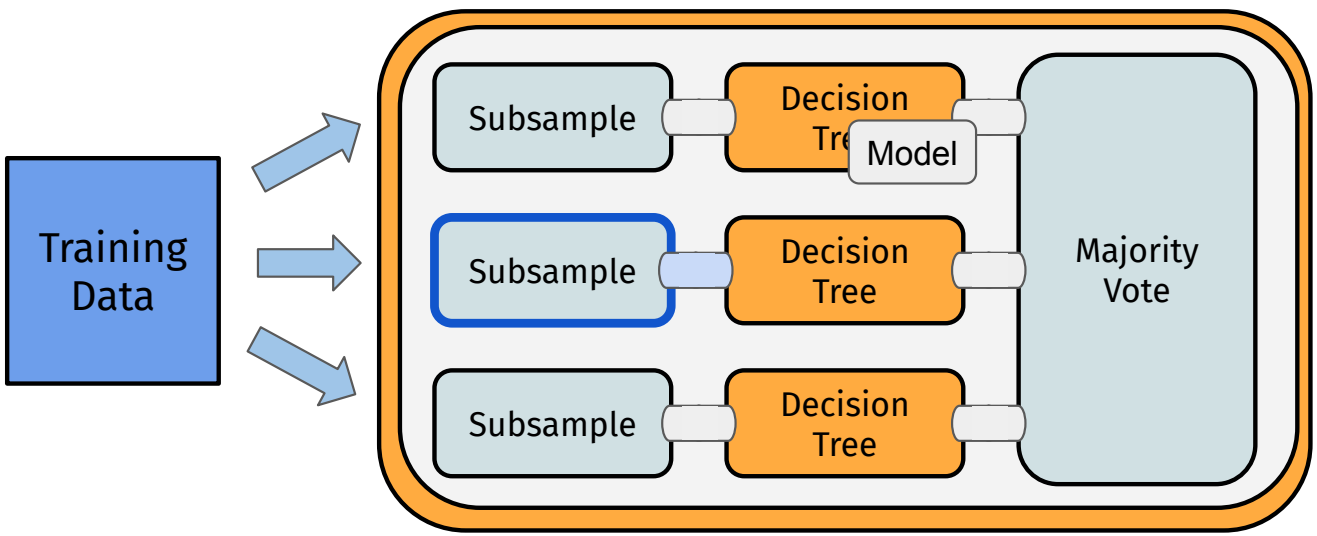

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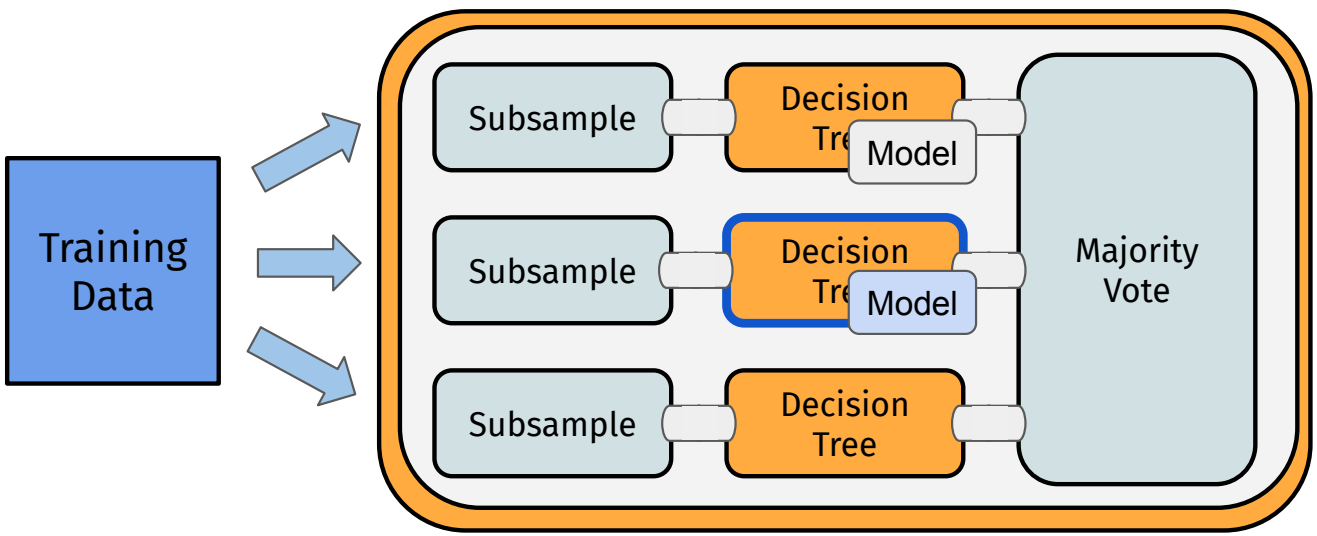

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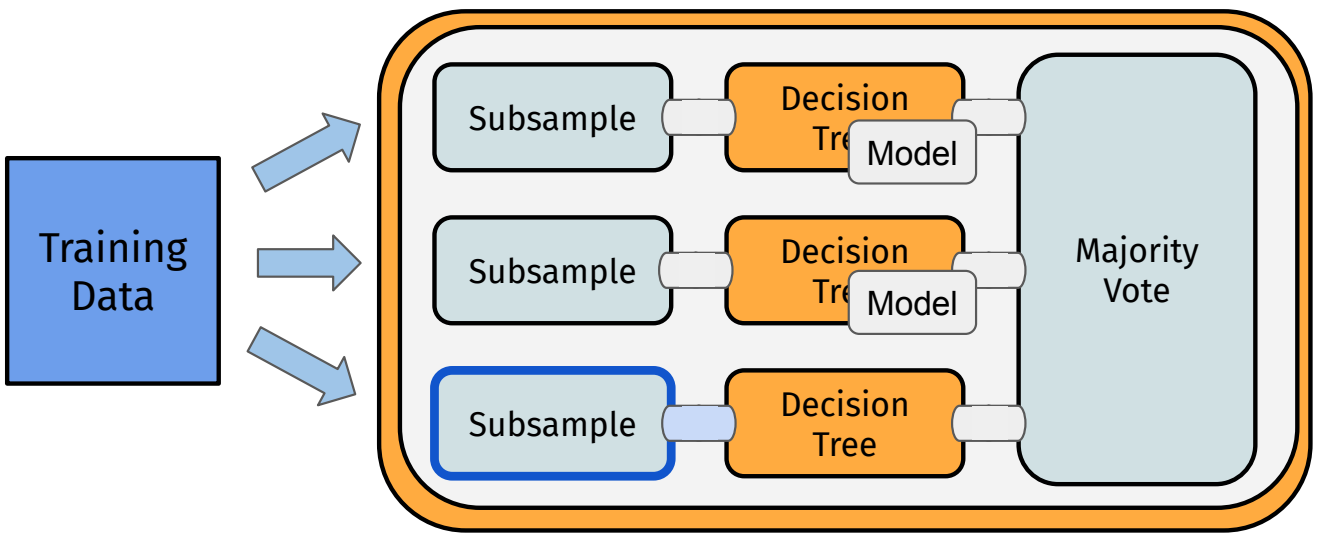

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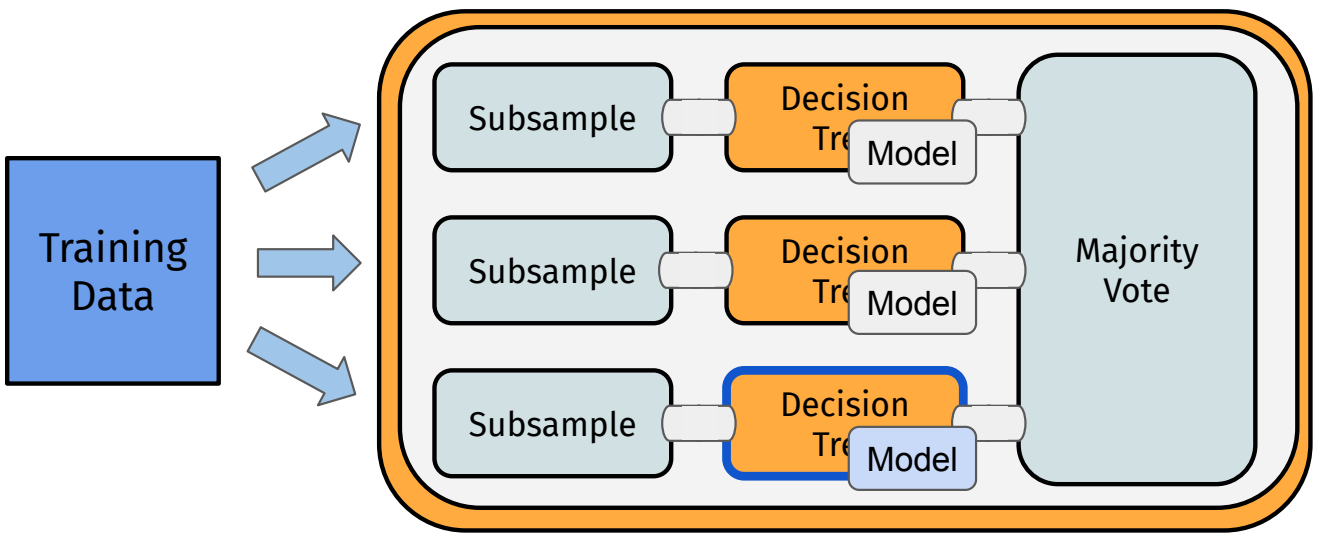

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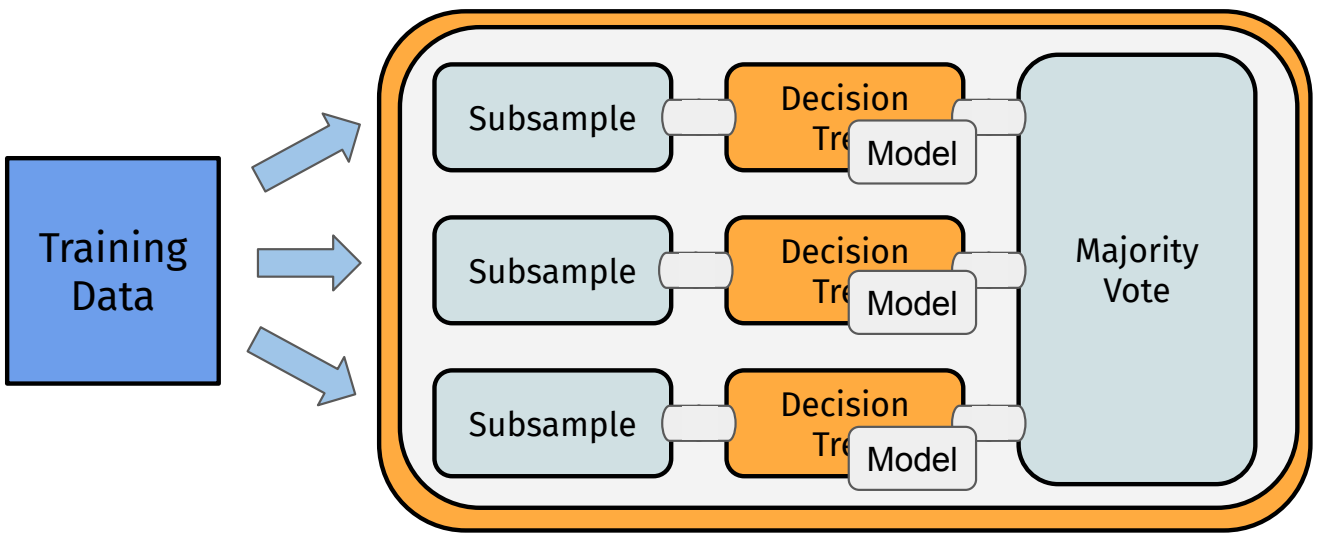
single_path = po("subsample") %>>% lrn("classif.rpart")

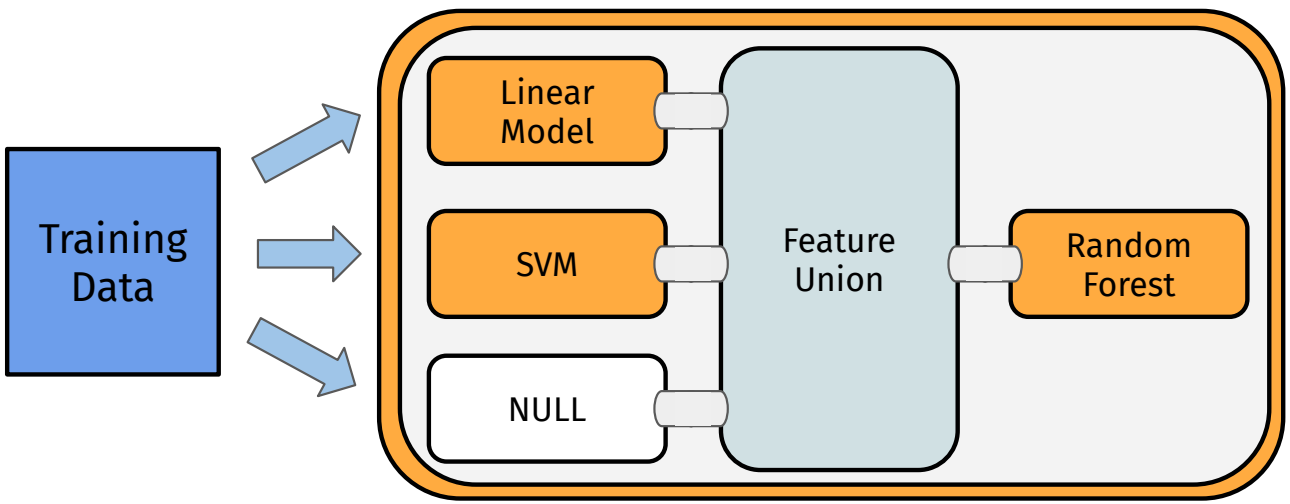
graph_bag = greplicate(single_path, n = 3) %>>%
  po("classifavg")
```



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")
```

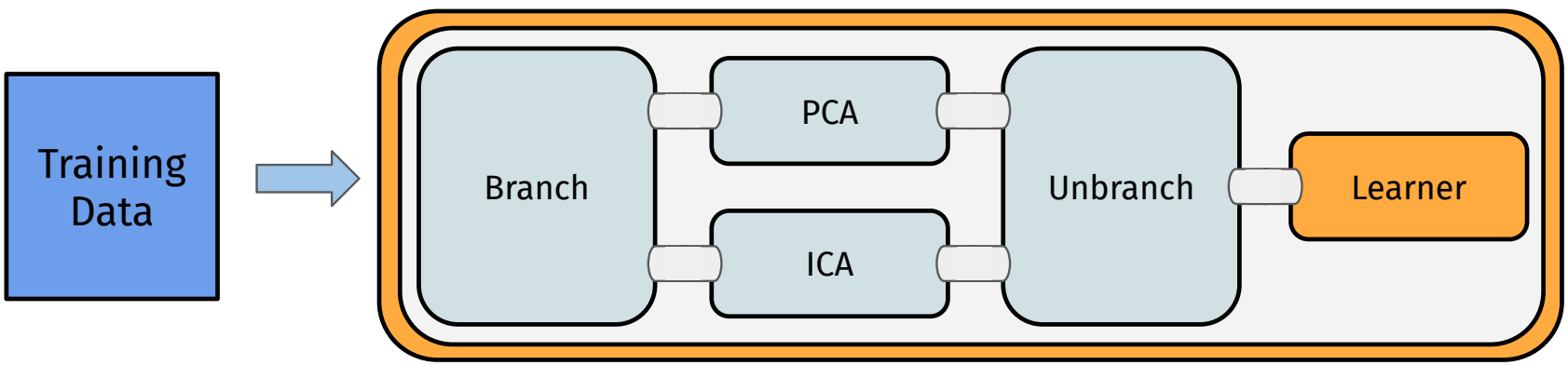


MLR3PIPELINES IN ACTION

Branching

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

Execute only one of several alternative paths

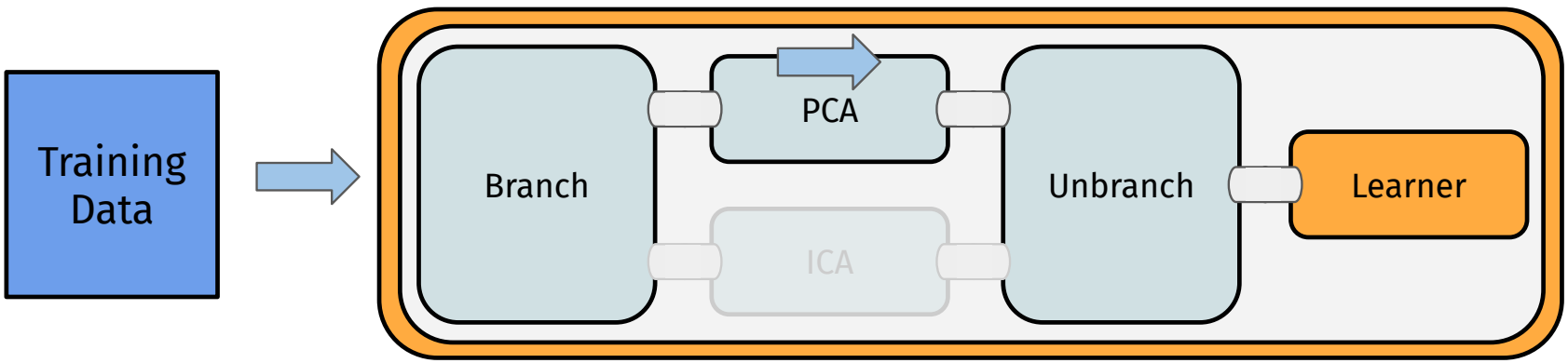


MLR3PIPELINES IN ACTION

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 = "pca"
```

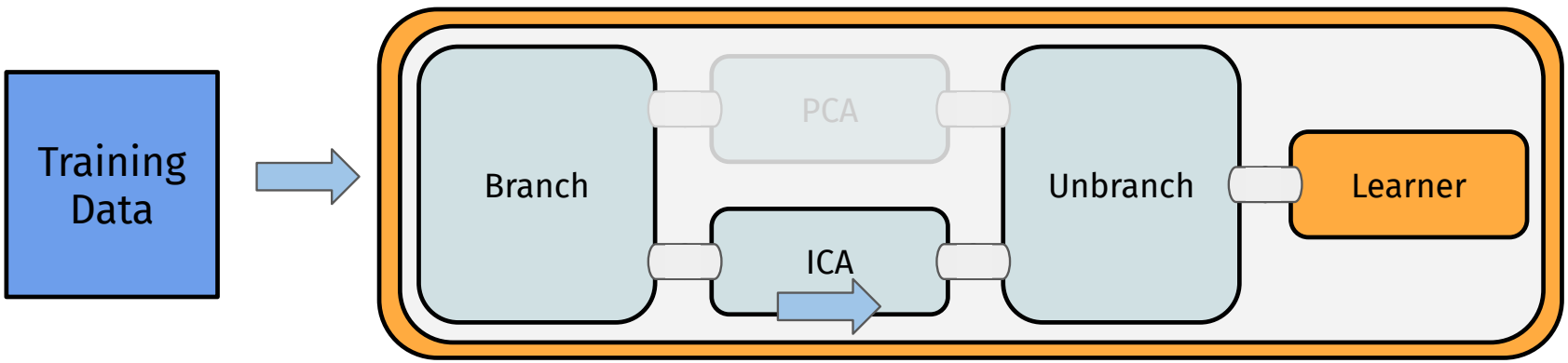


MLR3PIPELINES IN ACTION

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*
- $\Rightarrow$ 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
  - `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