

Dataflow programming with mlr3pipelines::CHEAT SHEET

Introduction

Combine ML operations to flexible pipelines and processing graphs, which can be configured trained, resampled, tuned as any regular learner. The main purpose of a Graph is to build combined preprocessing and model fitting pipelines that can be used as a Learner.



Each operation in the above example is a PipeOp which transforms the data in each step. PipeOps are chained with the %>% operator.

PipeOp

Flow operation with \$train() and \$predict() step.



Construction example: `pca = po("pca")`

- \$train(input): Named list
- \$predict(input): Named list
- \$state: Learned parameters
- \$param_set: See hyperparameters

Popular PipeOps

Class	Key	Operation
PipeOpRemoveConstants	"removeconstants"	Repair Tasks
PipeOpScale	"scale"	Scale Features
PipeOpImputeMean	"impute"	Impute NAs
PipeOpFilter	"filter"	Feature Filter
PipeOpEncode	"encode"	Factor Encoding
PipeOpPCA	"pca"	PCA
PipeOpSelect	"select"	Restrict Columns
PipeOpColApply	"colapply"	Transform Columns
PipeOpClassBalancing	"classbalancing"	Imbalanced Data
PipeOpLearner	"learner"	Use Learner
PipeOpLearnerCV	"learner_cv"	Crossval Learner
PipeOpMutate	"mutate"	Feature Engineering
PipeOpChunk	"chunk"	Split Data
PipeOpSubsample	"subsample"	Subsample Rows
PipeOpFeatureUnion	"featureunion"	Combine Features
PipeOpFixFactors	"fixfactors"	Handle Unknown Levels
PipeOpNOP	"nop"	Do Nothing

Full list: `as.data.table(mlr_pipelines)`

cheatdown on [GitHub](#)

Graph

Connects PipeOps with edges to control data flow during training and prediction. Input is sent to sources (no in-edges), output is read from sinks (no out-edges).

Important methods and slots:

- Display: `print(gr)`, `gr$plot(html = TRUE)`
- Accessing PipeOps: `gr$pipeops`
Named list of all contained POs.

Graph Construction

The %>% operator takes either a PipeOp or a Graph on each of its sides and connects all left-hand outputs to the right-hand inputs. For full control, connect PipeOps explicitly:

```
gr = Graph$new()
gr$add_pipeop(po("pca"))
gr$add_pipeop(lrn("classif.rpart"))
gr$add_edge("pca", "classif.rpart")
```

GraphLearner

GraphLearner behave like Learner and enable all mlr3 features: `gr1 = GraphLearner$new(gr)`. See slots \$encapsulate for debugging and \$model for results after training.

Linear Graphs

Concatenate POs with %>%:

Example

```
task = tsk("penguins")
gr = po("scale") %>% po("encode") %>%
  po("imputemean") %>% lrn("classif.rpart")
gr1 = GraphLearner$new(gr)
# access the scale pipeop:
gr1$graph$pipeops$scale
gr1$train(task)
gr1$predict(task)
rr = resample(task, gr1, rsm("cv", folds = 3))
```

Debugging and Intermediate Results

```
gr1$graph$keep_results = TRUE
```

Store intermediate results of PipeOps.

```
gr1$graph$pipeops$encode$.result
```

Returns intermediate result of \$train() and \$predict(), e.g. modified task returned by encode pipeop.

```
gr1$state
```

Internal state of graph learner. Contains fitted models in \$model.

Hyperparameters

For POs: Exactly as in a Learner.

```
enc = po("encode")
enc$param_set
enc$param_set$values = list(method="one-hot")
po("encode", param_vals = list(method="one-hot"))
```

For Graph / GraphLearner: All HPs are collected in a global ParamSet stored in \$param_set. IDs are prefixed with the respective PipeOp's id.

Tuning

Can jointly tune any Pipeline.

Example

```
gr = po("encode") %>% lrn("classif.rpart")
gr1 = GraphLearner$new(gr)
tune_ps = ParamSet$new(list(
  ParamFct$new("encode.method",
    levels = c("one-hot", "poly")),
  ParamDbl$new("classif.rpart.cp",
    lower = 0, upper = 0.05)
))
tt = trm("evals", n_evals = 20)
rs = rsm("holdout")
inst = TuningInstanceSingleCrit$new(task, gr1, rs,
  mtr("classif.ce"), tt, tune_ps)
tuner = trn("random_search")
tuner$optimize(inst)
```

Usage of AutoTuner is identical.

Feature Engineering

PipeOpMutate adds new features. This works by providing expressions in a list.

Example

```
task = tsk("iris")
mutations = list(
  Sepal.Sum = ~ Sepal.Length + Sepal.Width)
mutate = po("mutate", param_vals =
  list(mutation = mutations))
GraphLearner$new(mutate %>% lrn("classif.rpart"))
```

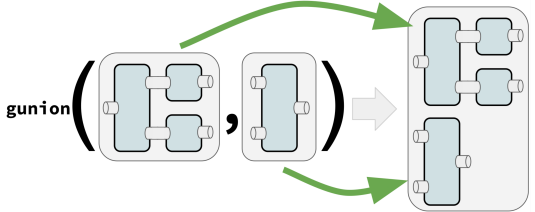
Logging

```
lg = lgr::get_logger("mlr3pipelines")
lg$set_threshold("<level>")
```

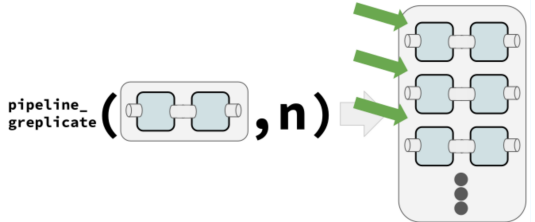
Change log-level only for mlr3pipelines.

Nonlinear Graphs

gunion() arranges PipeOps or Graphs next to each other in a disjoint graph union.



pipeline_greplicate() creates a new Graph containing n copies of the input (PipeOp or Graph).



PipeOpFeatureUnion aggregates features from all input tasks into a single Task.

Example

```
# train on orig and pca features
gunion(list(po("nop"), po("pca"))) %>%
  po("featureunion") %>% lrn("classif.rpart")
```

Example

```
pr = po("subsample") %>% lrn("classif.rpart")
bagging = ppl("greplicate", pr, n = 10) %>%
  po("classifavg", innum = 10)
```

Branching

Controls the path execution. Only one branch can be active. Which one is controlled by a hyperparameter. Unbranching ends the forking.

Example

```
gr = ppl("branch", list(
  pca = po("pca"), scale = po("scale"))
)
# set the "pca" path as the active one:
gr$param_set$values$branch.selection = "pca"
```

Tuning the branching selection enables powerful model selection.