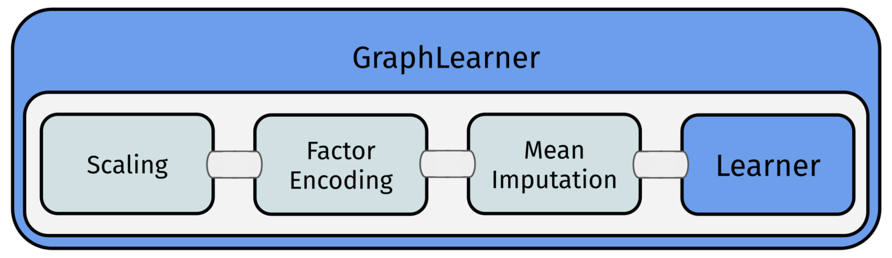
Dataflow programming with mlr3pipelines : : CHEAT SHEET

Introduction

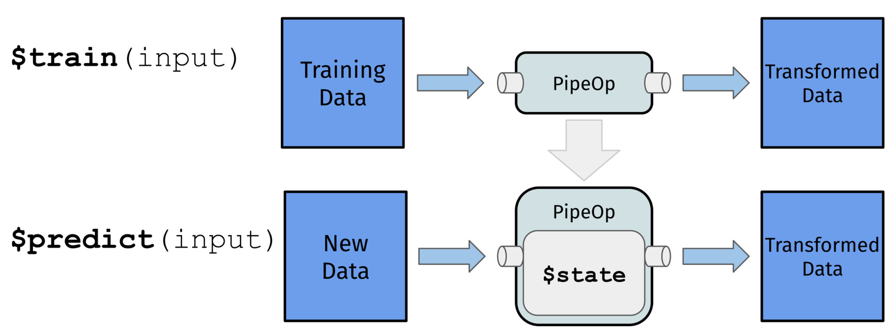
Combine ML operations to flexible pipelines and processing graphs, which can be configured trained, resampled, tuned as any regular learner. The main purpose of a `Graph` is to build combined preprocessing and model fitting pipelines that can be used as a `Learner`.



Each operation in the above example is a `PipeOp` which transforms the data in each step. `PipeOp` s 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"	Fearure 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_pipeops)`

Graph

Connects `PipeOp` s 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$plot(html = TRUE)`
- ▶ Accessing `PipeOp` s: `gr$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 `PipeOp` s 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. : `grl = GraphLearner$new(gr)`

See slots `$encapsulate` for debugging and `$model` for results after training.

Linear Graphs

Concatenate POs with `%>>%` :

Example

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

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")
grl = 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 = rsmp("holdout")
inst = TuningInstanceSingleCrit$new(task, grl, rs,
  msr("classif.ce"), tune_ps, tt)
tuner = tnr("random_search")
tuner$optimize(inst)
```

Usage of `AutoTuner` is identical.

Feature Engineering

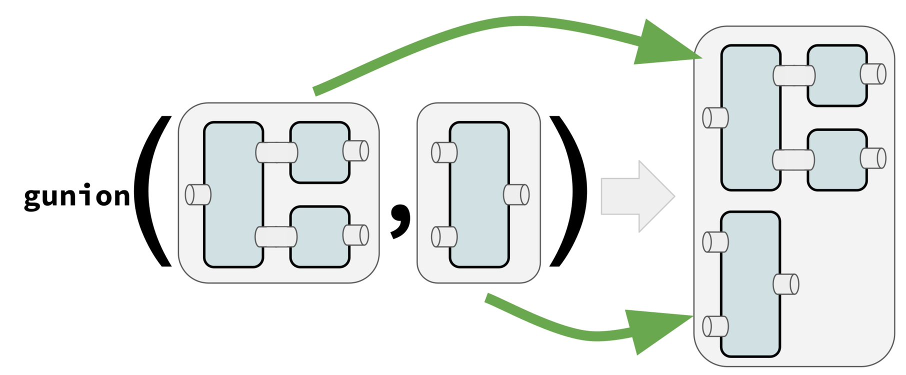
`PipeOpMutate` adds new features. This works by providing expressions in a `list` .

Example

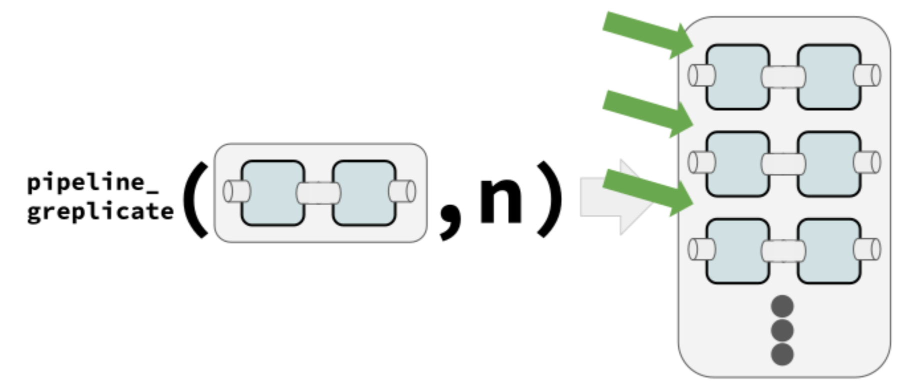
```
task = tsk("iris")
mutations = list(
  Sepal.Sum = ~ Sepal.Length + Sepal.Width)
mutate = po("mutate", param_vals =
  list(mutation = mutations))
GraphLearner$new(mutate %>>% lrn("classif.rpart"))
```

Nonlinear Graphs

`gunion()` arranges `PipeOp` s or `Graph` s 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 - Feature Union

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

Example - Bagging Ensemble

```
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 - Preprocessing

```
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