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



- \$train(input): Named list
- \$predict(input): Named list
- Sstate: 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 |
| PipeOpCoIApply | "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 |
| Fulllist:as.data.table(mlr_pipeops) | | |

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:

```
qr = 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

Linear Graphs

Concatenate POs with %>>%:

Example

task = **tsk**("penguins") qr = po("scale") %>% po("encode") %>% po("imputemean") %>>% lrn("classif.rpart") grl = GraphLearner\$new(gr) grl%graph%pipeops%scale grlStrain(task) orlSpredict(task) rr = resample(task, grl, rsmp("cv", folds = 3))

Debugging and Intermediate Results

grl\$graph\$keep_results = TRUE

Store intermediate results of PipeOps.

grl\$graph\$pipeops\$encode\$.result

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

grl\$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")

grl = GraphLearnerSnew(gr) tune ps = ParamSetSnew(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"), tt, tune_ps)
```

```
tuper = 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"))
```

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

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.



features: gr1 = GraphLearner\$new(gr). See slots \$encapsulate for debugging and \$model for results after training.