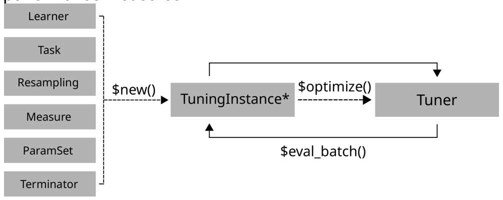
Hyperparameter Tuning with mlr3tuning::CHEAT SHEET

Class Overview

The package provides a set of R6 classes which allow to (a) define general hyperparameter (HP) tuning instances and (b) run algorithms which optimize on these. (a) is called a TuningInstanceSingleCrit or TuningInstaneMultiCrit, which define a blackbox optimization function that maps HP candidate configurations to resampled performance values for arbitrary performance measures.



Learner

Task

Resampling

Measure

ParamSet

Terminator

$new()

TuningInstance*

$optimize()

Tuner

$eval_batch()

ParamSet - Parameters and Ranges

Scalar doubles, integers, factors or logicals are combined to define a multivariate tuning space.

```
tune_ps = ParamSet$new(list(
  ParamInt$new(id, lower, upper),
  ParamDbl$new(id, lower, upper),
  ParamFct$new(id, levels),
  ParamLgl$new(id)))
```

id is the Param identifier. lower/upper define numerical ranges, levels is for categories.

Transformations for Rescaling

```
tune_ps$trafo = function(x, param_set) {
x$id =  2^{x$id}; return(x)}
```

Apply a custom transformation before passing the param to the `Learner.

Parameter Dependencies

Dependencies prevent invalid learner configurations.

```
tune_ps$add_dep(id, on, cond)
```

Adds a dependency for param id so that param id depends on param on, optional to condition cond.

Terminators - When to stop

Construction: trm(.key, ...)

- evals (n_evals)
  After a given amount of iterations.
- clock_time (secs, stop_time)
  After a given absolute time.
- model_time (secs)
  After a given training time.
- perf_reached (level)
  After a specific performance was reached.
- stagnation (iters, threshold)
  After the performance stagnated for given iterations.

```
as.data.table(mlr_terminators)
```

Lists all available terminators.

TuningInstance* - Search Scenario

Evaluator and container for resampled performances of HP configurations during tuning. The main (internal) function eval_batch(xdt) calls benchmark() to evaluate a table of HP configurations.
Also stores archive of all evaluated experiments and the final result.

```
instance = TuningInstanceSingleCrit$new(
  task, learner, resampling, measure,
  tune_ps, terminator)
```

Set store_benchmark_result = TRUE to store resamplings of evaluations and store_models = TRUE to store associated models.

Example

```
# optimize hyperpar of RBF SVM on logscale
learner = lrn("classif.svm", kernel = "radial",
  type = "C-classification")

tune_ps = ParamSet$new(list(
  ParamDbl$new("cost", lower = -8, upper = 8),
  ParamDbl$new("gamma", lower = -8, upper = 8)))
tune_ps$trafo = function(x, param_set) {
  x$cost = 2^x$cost; x$gamma = 2^x$gamma; x}
evals20 = trm("evals", n_evals = 20)

instance = TuningInstanceSingleCrit$new(
  task, learner, resampling, measure, tune_ps,
  evals20)
tuner = tnr("random_search")
tuner$optimize(instance)
instance$result
```

Use TuningInstanceMultiCrit for multi-criteria tuning.

Tuner - Search Strategy

Tuning strategy. Generates candidate configurations and passes these to TuningInstance for evaluation until termination. Creation: tnr(.key, ...)

- grid_search (resolution, batch_size)
  Grid search.
- random_search (batch_size)
  Random search.
- gensa (smooth, temperature)
  Generalized Simulated Annealing.
- nloptr (algorithm)
  Non-linear optimization.
- design_points (batch_size, design)
  User supplied settings.

```
as.data.table(mlr_tuners)
```

Lists all available tuners.

Executing the Tuning

```
tuner$optimize(instance)
```

Starts the tuning. Tuner generates candidate configurations and passes these to the $eval_batch() method of the TuningInstance* until the budget of the Terminator is exhausted.

```
instance$archive$data()
```

Returns all evaluated configurations and their resampling results. Use unnest to display HP with (x_domain) trafo applied.

Example

```
instance$archive$data()
## >     cost gamma classif.ce   x_domain batch_nr
## > 1:  3.13  5.55       0.56  <list[2]>        1
## > 2: -1.94  1.32       0.10  <list[2]>        2
```

uhash refers to instance$archive$benchmark_result.

```
instance$result
```

Returns list with optimal configurations and estimated performance.

```
learner$param_set$values =
  instance$result_learner_param_vals
```

Set optimized HP in Learner.

AutoTuner - Tune before Train

Wraps learner and performs integrated tuning.

```
at = AutoTuner$new(
  learner, resampling, measure, tune_ps,
  terminator, tuner)
```

Inherits from class Learner. Training starts tuning on the training set. After completion the learner is trained with the "optimal" configuration on the given task.

```
at$train(task)
at$predict(task, row_ids)
```

Nested Resampling

Resampling the AutoTuner results in nested resampling with an inner and outer loop.

Example

```
resampling_inner = rsmp("holdout")

at = AutoTuner$new(learner, resampling_inner,
  measure, tune_ps, evals20, tuner,
  store_tuning_instance = TRUE)

resampling_outer = rsmp("cv", folds = 2)
rr = resample(task, at, resampling_outer,
  store_models = TRUE)

as.data.table(rr)
## >             learner         resampling iteration
## > 1:  <AutoTuner[37]> <ResamplingCV[19]>         1
## > 2:  <AutoTuner[37]> <ResamplingCV[19]>         2
```

```
rr$aggregate()
```

Aggregates performances of outer folds.

```
as.data.table(rr)$learner[[1]]$tuning_result
```

Retrieves inner tuning results.

Logging and Parallelization

```
lgr::get_logger("bbotk")$set_threshold("<level>")
```

Change log-level only for mlr3tuning.

```
future::plan(strategy)
```

Sets the parallelization backend. Speeds up tuning by running iterations in parallel.

mlr-org.com, cheatsheets.mlr-org.com