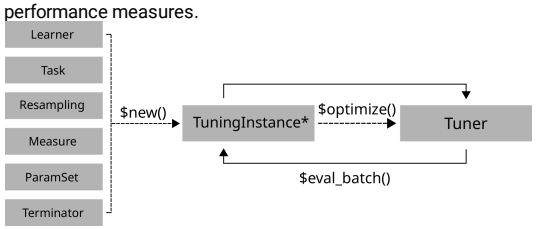
Hyperparameter Tuning with mlr3tuning::CHEAT SHEET

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.



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,
  terminator, tune_ps)
```

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$new(
  task, learner, resampling, measure, evals20,
  tune_ps)
tuner = tnr("random_search")
tuner$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.

```
as.data.table(instance$archive)
```

Returns all evaluated configurations and their resampling results. The `x_domain_*` columns contain HP values after the transformation.

Example

```
as.data.table(instance$archive)
## >     cost gamma classif.ce     uhash x_domain_cost x_domain_gamma
## > 1:  3.13  5.55       0.56  b8744...          3.13           5.55
## > 2: -1.94  1.32       0.10  f5623...         -1.94           1.32
```

`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, terminator,
  tuner, tune_ps)
```

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, evals20, tuner, tune_ps,
  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.