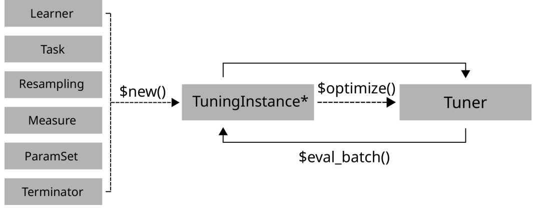
Hyperparameter Tuning with mlr3tuning::CHEAT SHEET

Class Overview

The package provides a set of R6 classes which allow to (a) define general hyperparameter (HP) tuning instances, i.e., the black-box objective that maps HP configurations to resampled performance values; (b) run black-box optimzers; (c) combine learners with tuners (for nested resampling).



ParamSet - Parameters and Ranges

Scalar doubles, integers, factors or logicals are combined to define a multivariate search space (SS).

```
tune_ps = ps(
  <id> = p_int(lower, upper),
  <id> = p_dbl(lower, upper),
  <id> = p_dct(levels),
  <id> = p_lgl())
```

`id` is Param identifier. `lower`/`upper` for ranges, `levels` for categories.

```
learner = lrn("classif.rpart",
  cp = to_tune(0.001, 0.1, logscale = TRUE),
  minsplit = to_tune(1, 10))
learner$param_set$search_space() # only for inspection
```

Or, use `to_tune()` to set SS for each param in `Learner`. SS is auto-generated when learner is tuned. `logscale = TRUE` for log scale.

Terminators - When to stop

Construction: `trm(.key, ...)`

- `evals` (`n_evals`)
  After iterations.
- `run_time` (`secs`)
  After training time.
- `clock_time` (`secs`)
  At given timepoint.
- `perf_reached` (`level`)
  After performance was reached.
- `stagnation` (`iters`, `threshold`)
  After performance stagnated.
- `combo(list_of_terms, any=TRUE`
  Combine terminators with AND or OR.

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

tune_ps = ps(
  cost = p_dbl(1e-4, 1e4, logscale = TRUE),
  gamma = p_dbl(1e-4, 1e4, logscale = TRUE))

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.
- `irace`
  Iterated racing.

```
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.

Access Results

```
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
```

```
instance$result
```

Returns list with optimal configurations and estimated performance.

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

Set optimized HP in `Learner`.

Example

```
learner = lrn("classif.svm", type = "C-classification", kernel = "radial",
  cost = to_tune(1e-4, 1e4, logscale = TRUE))
instance = tune(method = "grid_search", task = tsk("iris"), learner = learner,
  resampling = rsmp ("holdout"), measure = msr("classif.ce"), resolution = 5)
```

Use `tune()`-shortcut.

AutoTuner - Tune before Train

Wraps learner and performs integrated tuning.

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

```
at$learner
```

Returns tuned learner trained on full data set.

```
at$tuning_result
```

Access tuning result.

```
at = auto_tuner(method = "grid_search", learner,
  resampling, measure, term_evals = 20)
```

Use shortcut to create `AutoTuner`.

Nested Resampling

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

Example

```
inner_resampling = rsmp("holdout")

at = auto_tuner(method = "random_search", learner, inner_resampling,
  measure, term_evals = 20)

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

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

```
extract_inner_tuning_results(rr)
```

Check inner tuning results for stable HPs.

```
rr$score()
```

Predictive performances estimated on the outer resampling.

```
extract_inner_tuning_archives(rr)
```

All evaluated HP configurations.

```
rr$aggregate()
```

Aggregates performances of outer resampling iterations.

```
rr = tune_nested(method = "grid_search", task,
  learner = learner, inner_resampling,
  outer_resampling, measure, term_evals = 20)
```

Use shortcut to execute nested resampling.

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