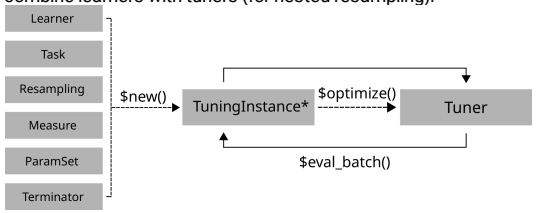
Hyperparameter Tuning with mlr3tuning::CHEAT SHEET

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 (HPCs) to resampled performance values; (b) run black-box optimzers; (c) combine learners with tuners (for nested resampling).



[NB: In many table prints we suppres cols for readability.]

ParamSet - Parameters and Ranges

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

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

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

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

Or, use `to_tune()` to set SS for each param in `Learner`. SS is auto-generated when learner is tuned. Params can be arbitrarily transformed by setting a global trafo in SS, or `p_*` shortforms, `logscale = TRUE` is short for most common choice.

Terminators - When to stop

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

- `evals` (`n_evals`)
  After iterations.
- `run_time` (`secs`)
  After training time.
- `clock_time` (`stop_time`)
  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) # list all
```

TuningInstance* - Search Scenario

Evaluator and container for resampled performances of HPCs. The (internal) `eval_batch(xdt)` calls `benchmark()` to eval a table of HPCs. Stores archive of all evaluated experiments and final result.

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

`store_benchmark_result = TRUE` to store resampled evals and `store_models = TRUE` for fitted models.

Example

```
# optimize HPs of RBF SVM on logscale
learner = lrn("classif.svm", kernel = "radial", type = "C-classification")
ss = ps(cost = p_dbl(1e-4, 1e4, logscale = TRUE),
  gamma = p_dbl(1e-4, 1e4, logscale = TRUE))
evals = trm("evals", n_evals = 20)
instance = TuningInstanceSingleCrit$new(task, learner, resampling, measure, evals,
        ss)
tuner = tnr("random_search")
tuner$optimize(instance)
instance$result
# >        cost     gamma learner_param_vals  x_domain classif.ce
# > 1: 5.852743 -7.281365          <list[4]> <list[2]>       0.04
```

Use `TuningInstanceMultiCrit` for multi-criteria tuning.

Tuner - Search Strategy

Generates HPCs and passes to tuning instance for evaluation until termination. Creation: `tnr(.key, ...)`

- `grid_search` (`resolution`, `batch_size`)
  Grid search.
- `random_search` (`batch_size`)
  Random search.
- `design_points` (`design`)
  Search at predefined points.
- `random_search` (`batch_size`)
  Random search.
- `nloptr` (`algorithm`)
  Non-linear optimization.
- `gensa` (`smooth`, `temperature`)
  Generalized Simulated Annealing.
- `irace`
  Iterated racing.

```
as.data.table(mlr_tuners) # list all
```

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.

Execute Tuning and Access Results

```
tuner$optimize(instance)
as.data.table(instance$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 # datatable row with optimal HPC and estimated perf
```

Get evaluated HPCs and performances; and result. `x_domain_*` cols contain HP values after trafo (if any).

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

Set optimal HPC in `Learner`.

Example

```
learner = lrn("classif.svm", type = "C-classification", kernel = "radial",
  cost = to_tune(1e-4, 1e4, logscale = TRUE),
  gamma = 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
# >       cost     gamma learner_param_vals  x_domain classif.ce
# > 1: 5.270814 -4.414869          <list[4]> <list[2]>       0.08
```

Access tuning result.

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

Use shortcut to create `AutoTuner`.

Nested Resampling

Just resample `AutoTuner`; now has inner and outer loop.

Example

```
inner = rsmp("holdout")
at = auto_tuner(method = "gensa", learner, inner, measure, term_evals = 20)
outer = rsmp("cv", folds = 2)
rr = resample(task, at, outer, 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)
# >    iteration      cost      gamma classif.ce learner_param_vals  x_domain
# > 1:         1 1.222198 -0.4974749       0.08          <list[4]> <list[2]>
# > 2:         2 2.616557 -3.1440039       0.08          <list[4]> <list[2]>
```

Check inner tuning results for stable HPs.

```
rr$score()
# >              learner  iteration             prediction classif.ce
# > 1:  <AutoTuner[40]>          1 <PredictionClassif[19]> 0.05333333
# > 2:  <AutoTuner[40]>          2 <PredictionClassif[19]> 0.02666667
```

Predictive performances estimated on the outer resampling.

```
extract_inner_tuning_archives(rr)
# >    iteration      cost   gamma classif.ce  runtime      resample_result
# > 1:         1  -7.4572  4.1506       0.68    0.013 <ResampleResult[20]>
# > 21:        2   1.0056  0.4003       0.12    0.014 <ResampleResult[20]>
```

All evaluated HP configurations.

```
rr$aggregate()
#> classif.ce
#>       0.04
```

Aggregates performances of outer resampling iterations.

```
rr = tune_nested(method = "grid_search", task,
  learner, inner, outer, measure, term_evals = 20)
```

Use shortcut to execute nested resampling.