

Package ‘mlr3tuning’

July 28, 2020

Title Tuning for 'mlr3'

Version 0.2.0

Description Implements methods for hyperparameter tuning with 'mlr3', e.g. Grid Search, Random Search, or Simulated Annealing. Various termination criteria can be set and combined. The class 'AutoTuner' provides a convenient way to perform nested resampling in combination with 'mlr3'.

License LGPL-3

URL <https://mlr3tuning.mlr-org.com>,
<https://github.com/mlr-org/mlr3tuning>

BugReports <https://github.com/mlr-org/mlr3tuning/issues>

Depends R (>= 3.1.0)

Imports bbottk (>= 0.2.0), checkmate (>= 2.0.0), data.table, lgr, mlr3, mlr3misc, paradox (>= 0.3.0), R6

Suggests bibtex, GenSA, mlr3pipelines, nloptr, rpart, testthat

RdMacros mlr3misc

Encoding UTF-8

NeedsCompilation no

RoxygenNote 7.1.1

Collate 'AutoTuner.R' 'ObjectiveTuning.R' 'mlr_tuners.R' 'Tuner.R'
 'TunerDesignPoints.R' 'TunerFromOptimizer.R' 'TunerGenSA.R'
 'TunerGridSearch.R' 'TunerNLopt.R' 'TunerRandomSearch.R'
 'TuningInstanceMulticrit.R' 'TuningInstanceSingleCrit.R'
 'assertions.R' 'helper.R' 'reexport.R' 'sugar.R' 'zzz.R'

Author Marc Becker [cre, aut] (<<https://orcid.org/0000-0002-8115-0400>>),
 Michel Lang [aut] (<<https://orcid.org/0000-0001-9754-0393>>),
 Jakob Richter [aut] (<<https://orcid.org/0000-0003-4481-5554>>),
 Bernd Bischl [aut] (<<https://orcid.org/0000-0001-6002-6980>>),
 Daniel Schalk [aut] (<<https://orcid.org/0000-0003-0950-1947>>)

Maintainer Marc Becker <marcbecker@posteo.de>

Repository CRAN

Date/Publication 2020-07-28 13:30:04 UTC

R topics documented:

mlr3tuning-package	2
AutoTuner	3
mlr_terminators	5
mlr_tuners	5
mlr_tuners_design_points	6
mlr_tuners_gensa	8
mlr_tuners_grid_search	10
mlr_tuners_nloptr	12
mlr_tuners_random_search	14
ObjectiveTuning	16
tnr	17
trm	18
trms	18
Tuner	19
TuningInstanceMultiCrit	21
TuningInstanceSingleCrit	23

Index	27
--------------	-----------

mlr3tuning-package *mlr3tuning: Tuning for 'mlr3'*

Description

Implements methods for hyperparameter tuning with 'mlr3', e.g. Grid Search, Random Search, or Simulated Annealing. Various termination criteria can be set and combined. The class 'AutoTuner' provides a convenient way to perform nested resampling in combination with 'mlr3'.

Author(s)

Maintainer: Michel Lang <michellang@gmail.com> ([ORCID](#))

Authors:

- Jakob Richter <jakob1richter@gmail.com> ([ORCID](#))
- Bernd Bischl <bernd_bischl@gmx.net> ([ORCID](#))
- Daniel Schalk <daniel.schalk@stat.uni-muenchen.de> ([ORCID](#))
- Marc Becker <marcbecker@posteo.de> ([ORCID](#))

See Also

Useful links:

- <https://mlr3tuning.mlr-org.com>
- <https://github.com/mlr-org/mlr3tuning>
- Report bugs at <https://github.com/mlr-org/mlr3tuning/issues>

AutoTuner

AutoTuner

Description

The AutoTuner is a [mlr3::Learner](#) which wraps another [mlr3::Learner](#) and performs the following steps during `$train()`:

1. The hyperparameters of the wrapped (inner) learner are trained on the training data via resampling. The tuning can be specified by providing a [Tuner](#), a [bbotk::Terminator](#), a search space as [paradox::ParamSet](#), a [mlr3::Resampling](#) and a [mlr3::Measure](#).
2. The best found hyperparameter configuration is set as hyperparameters for the wrapped (inner) learner.
3. A final model is fit on the complete training data using the now parametrized wrapped learner.

During `$predict()` the AutoTuner just calls the predict method of the wrapped (inner) learner.

Note that this approach allows to perform nested resampling by passing an [AutoTuner](#) object to `mlr3::resample()` or `mlr3::benchmark()`. To access the inner resampling results, set `store_tuning_instance = TRUE` and execute `mlr3::resample()` or `mlr3::benchmark()` with `store_models = TRUE` (see examples).

Super class

[mlr3::Learner](#) -> AutoTuner

Public fields

`instance_args (list())`

All arguments from construction to create the [TuningInstanceSingleCrit](#).

`tuner (Tuner)`.

`store_tuning_instance (logical(1))`

If TRUE (default), stores the internally created [TuningInstanceSingleCrit](#) with all intermediate results in slot `$tuning_instance`.

Active bindings

`archive bbotk::Archive`

Archive of the [TuningInstanceSingleCrit](#).

`learner (mlr3::Learner)`

Trained learner

`tuning_instance (TuningInstanceSingleCrit)`

Internally created tuning instance with all intermediate results.

`tuning_result (named list())`

Short-cut to result from [TuningInstanceSingleCrit](#).

`param_set paradox::ParamSet`.

Methods

Public methods:

- `AutoTuner$new()`
- `AutoTuner$clone()`

Method new(): Creates a new instance of this `R6` class.

Usage:

```
AutoTuner$new(learner, resampling, measure, search_space, terminator, tuner)
```

Arguments:

`learner` (`mlr3::Learner`)

Learner to tune, see `TuningInstanceSingleCrit`.

`resampling` (`mlr3::Resampling`)

Resampling strategy during tuning, see `TuningInstanceSingleCrit`. This `mlr3::Resampling` is meant to be the **inner** resampling, operating on the training set of an arbitrary outer resampling. For this reason it is not feasible to pass an instantiated `mlr3::Resampling` here.

`measure` (list of `mlr3::Measure`)

Performance measure to optimize.

`search_space` (`paradox::ParamSet`)

Hyperparameter search space, see `TuningInstanceSingleCrit`.

`terminator` (`bbotk::Terminator`)

When to stop tuning, see `TuningInstanceSingleCrit`.

`tuner` (`Tuner`)

Tuning algorithm to run.

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
AutoTuner$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

Examples

```
library(mlr3)
library(paradox)
task = tsk("iris")
learner = lrn("classif.rpart")
resampling = rsmp("holdout")
measure = msr("classif.ce")
search_space = ParamSet$new(
  params = list(ParamDbl$new("cp", lower = 0.001, upper = 0.1)))

terminator = trm("evals", n_evals = 5)
tuner = tnr("grid_search")
at = AutoTuner$new(
  learner, resampling, measure, search_space, terminator,
  tuner)
```

```
at$store_tuning_instance = TRUE

at$train(task)
at$model
at$learner

# Nested resampling
at = AutoTuner$new(learner, resampling, measure, search_space, terminator,
  tuner)
at$store_tuning_instance = TRUE

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

# Aggregate performance of outer results
rr$aggregate()

# Retrieve inner tuning results.
rr$data$learner[[1]]$tuning_result
```

mlr_terminators

Re-export of mlr_terminators See [bbotk::mlr_terminators](#).

Description

Re-export of `mlr_terminators`

See [bbotk::mlr_terminators](#).

mlr_tuners

Dictionary of Tuners

Description

A simple [mlr3misc::Dictionary](#) storing objects of class [Tuner](#). Each tuner has an associated help page, see `mlr_tuners_[id]`.

This dictionary can get populated with additional tuners by add-on packages.

For a more convenient way to retrieve and construct tuner, see [tnr\(\)](#)/[tnrs\(\)](#).

Usage

`mlr_tuners`

Format

[R6::R6Class](#) object inheriting from [mlr3misc::Dictionary](#).

Methods

See [mlr3misc::Dictionary](#).

See Also

Sugar functions: [tnr\(\)](#), [tnrs\(\)](#)

Examples

```
mlr_tuners$get("grid_search")
tnr("random_search")
```

mlr_tuners_design_points
TunerDesignPoints

Description

Subclass for tuning w.r.t. fixed design points.

We simply search over a set of points fully specified by the user. The points in the design are evaluated in order as given.

Dictionary

This [Tuner](#) can be instantiated via the [dictionary mlr_tuners](#) or with the associated sugar function [tnr\(\)](#):

```
mlr_tuners$get("design_points")
tnr("design_points")
```

Parallelization

In order to support general termination criteria and parallelization, we evaluate points in a batch-fashion of size `batch_size`. Larger batches mean we can parallelize more, smaller batches imply a more fine-grained checking of termination criteria. A batch contains of `batch_size` times `resampling$iters` jobs. E.g., if you set a batch size of 10 points and do a 5-fold cross validation, you can utilize up to 50 cores.

Parallelization is supported via package [future](#) (see [mlr3::benchmark\(\)](#)'s section on parallelization for more details).

Logging

All [Tuners](#) use a logger (as implemented in [lgr](#)) from package [bbotk](#). Use `lgr::get_logger("bbotk")` to access and control the logger.

Parameters

`batch_size integer(1)`
 Maximum number of configurations to try in a batch.

`design data.table::data.table`
 Design points to try in search, one per row.

Super classes

`mlr3tuning::Tuner -> mlr3tuning::TunerFromOptimizer -> TunerDesignPoints`

Methods

Public methods:

- `TunerDesignPoints$new()`
- `TunerDesignPoints$clone()`

Method new(): Creates a new instance of this **R6** class.

Usage:

`TunerDesignPoints$new()`

Method clone(): The objects of this class are cloneable with this method.

Usage:

`TunerDesignPoints$clone(deep = FALSE)`

Arguments:

`deep` Whether to make a deep clone.

Examples

```
library(mlr3)
library(paradox)
library(data.table)
search_space = ParamSet$new(list(
  ParamDbl$new("cp", lower = 0.001, upper = 0.1)
))
terminator = trm("evals", n_evals = 3)
instance = TuningInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  search_space = search_space,
  terminator = terminator
)
design = data.table(cp = c(0.1, 0.01))
tt = tnr("design_points", design = design)
# modifies the instance by reference
tt$optimize(instance)
# returns best configuration and best performance
```

```
instance$result
# allows access of data.table of full path of all evaluations
instance$archive
```

mlr_tuners_gensa *TunerGenSA*

Description

Subclass for generalized simulated annealing tuning calling [GenSA:::GenSA\(\)](#) from package [GenSA](#).

Dictionary

This [Tuner](#) can be instantiated via the [dictionary mlr_tuners](#) or with the associated sugar function [tnr\(\)](#):

```
mlr_tuners$get("gensa")
tnr("gensa")
```

Logging

All [Tuners](#) use a logger (as implemented in [lgr](#)) from package [bbotk](#). Use [lgr::get_logger\("bbotk"\)](#) to access and control the logger.

Parameters

```
smooth logical(1)
temperature numeric(1)
acceptance.param numeric(1)
verbose logical(1)
trace.mat logical(1)
```

For the meaning of the control parameters, see [GenSA:::GenSA\(\)](#). Note that we have removed all control parameters which refer to the termination of the algorithm and where our terminators allow to obtain the same behavior.

Super classes

```
mlr3tuning::Tuner -> mlr3tuning::TunerFromOptimizer -> TunerGenSA
```

Methods

Public methods:

- [TunerGenSA\\$new\(\)](#)
- [TunerGenSA\\$clone\(\)](#)

Method new(): Creates a new instance of this [R6](#) class.

Usage:

```
TunerGenSA$new()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
TunerGenSA$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Source

Tsallis C, Starilo DA (1996). “Generalized simulated annealing.” *Physica A: Statistical Mechanics and its Applications*, 233(1-2), 395–406. doi: [10.1016/s03784371\(96\)002713](https://doi.org/10.1016/s03784371(96)002713).

Xiang Y, Gubian S, Suomela B, Hoeng J (2013). “Generalized Simulated Annealing for Global Optimization: The GenSA Package.” *The R Journal*, 5(1), 13. doi: [10.32614/rj2013002](https://doi.org/10.32614/rj2013002).

Examples

```
library(mlr3)
library(paradox)
search_space = ParamSet$new(list(
  ParamDbl$new("cp", lower = 0.001, upper = 0.1)
))
terminator = trm("evals", n_evals = 3)
instance = TuningInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  search_space = search_space,
  terminator = terminator
)
tt = tnr("gensa")

# modifies the instance by reference
tt$optimize(instance)

# returns best configuration and best performance
instance$result

# allows access of data.table of full path of all evaluations
instance$archive
```

mlr_tuners_grid_search
TunerGridSearch

Description

Subclass for grid search tuning.

The grid is constructed as a Cartesian product over discretized values per parameter, see [paradox::generate_design_grid\(\)](#). The points of the grid are evaluated in a random order.

Dictionary

This [Tuner](#) can be instantiated via the [dictionary mlr_tuners](#) or with the associated sugar function [tnr\(\)](#):

```
mlr_tuners$get("grid_search")
tnr("grid_search")
```

Parallelization

In order to support general termination criteria and parallelization, we evaluate points in a batch-fasion of size `batch_size`. Larger batches mean we can parallelize more, smaller batches imply a more fine-grained checking of termination criteria. A batch contains of `batch_size` times `resampling$iters` jobs. E.g., if you set a batch size of 10 points and do a 5-fold cross validation, you can utilize up to 50 cores.

Parallelization is supported via package [future](#) (see [mlr3::benchmark\(\)](#)'s section on parallelization for more details).

Logging

All [Tuners](#) use a logger (as implemented in [lgr](#)) from package [bbotk](#). Use `lgr::get_logger("bbotk")` to access and control the logger.

Parameters

```
resolution integer(1)
  Resolution of the grid, see paradox::generate\_design\_grid\(\).
param_resolutions named integer()
  Resolution per parameter, named by parameter ID, see paradox::generate\_design\_grid\(\).
batch_size integer(1)
  Maximum number of points to try in a batch.
```

Super classes

[mlr3tuning::Tuner](#) -> [mlr3tuning::TunerFromOptimizer](#) -> [TunerGridSearch](#)

Methods

Public methods:

- `TunerGridSearch$new()`
- `TunerGridSearch$clone()`

Method new(): Creates a new instance of this `R6` class.

Usage:

```
TunerGridSearch$new()
```

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
TunerGridSearch$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

Examples

```
library(mlr3)
library(paradox)
search_space = ParamSet$new(list(
  ParamDbl$new("cp", lower = 0.001, upper = 0.1)
))
terminator = trm("evals", n_evals = 3)
instance = TuningInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  search_space = search_space,
  terminator = terminator
)
tt = tnr("grid_search")

# modifies the instance by reference
tt$optimize(instance)

# returns best configuration and best performance
instance$result

# allows access of data.table of full path of all evaluations
instance$archive
```

<code>mlr_tuners_nloptr</code>	<i>TuneNLoptr</i>
--------------------------------	-------------------

Description

TunerNLoptr class that implements non-linear optimization. Calls `nloptr::nloptr` from package `nloptr`.

Details

The termination conditions `stopval`, `maxtime` and `maxeval` of `nloptr::nloptr()` are deactivated and replaced by the `bbotk::Terminator` subclasses. The x and function value tolerance termination conditions (`xtol_rel = 10^-4`, `xtol_abs = rep(0.0, length(x0))`, `ftol_rel = 0.0` and `ftol_abs = 0.0`) are still available and implemented with their package defaults. To deactivate these conditions, set them to -1.

Dictionary

This Tuner can be instantiated via the dictionary `mlr_tuners` or with the associated sugar function `tnr()`:

```
mlr_tuners$get("nloptr")
tnr("nloptr")
```

Logging

All Tuners use a logger (as implemented in `lgr`) from package `bbotk`. Use `lgr::get_logger("bbotk")` to access and control the logger.

Parameters

```
algorithm character(1)
x0 numeric()
eval_g_ineq function()
xtol_rel numeric(1)
xtol_abs numeric(1)
ftol_rel numeric(1)
ftol_abs numeric(1)
```

For the meaning of the control parameters, see `nloptr::nloptr()` and `nloptr::nloptr.print.options()`.

The termination conditions `stopval`, `maxtime` and `maxeval` of `nloptr::nloptr()` are deactivated and replaced by the `Terminator` subclasses. The x and function value tolerance termination conditions (`xtol_rel = 10^-4`, `xtol_abs = rep(0.0, length(x0))`, `ftol_rel = 0.0` and `ftol_abs = 0.0`) are still available and implemented with their package defaults. To deactivate these conditions, set them to -1.

Super classes

`mlr3tuning::Tuner` -> `mlr3tuning::TunerFromOptimizer` -> `TunerNloptr`

Methods

Public methods:

- `TunerNloptr$new()`
- `TunerNloptr$clone()`

Method `new()`: Creates a new instance of this `R6` class.

Usage:

`TunerNloptr$new()`

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

`TunerNloptr$clone(deep = FALSE)`

Arguments:

`deep` Whether to make a deep clone.

Source

Johnson SG (2020). “The NLOpt nonlinear-optimization package.” <http://github.com/stevengj/nlopt>.

Examples

```
## Not run:
library(mlr3)
library(paradox)
library(data.table)
search_space = ParamSet$new(list(
  ParamDbl$new("cp", lower = 0.001, upper = 0.1)
))
# We use the internal termination criterion xtol_rel
terminator = trm("none")
instance = TuningInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  search_space = search_space,
  terminator = terminator
)
tt = tnr("nloptr", x0 = 0.1, algorithm = "NLOPT_LN_BOBYQA")
# modifies the instance by reference
tt$optimize(instance)
# returns best configuration and best performance
instance$result
# allows access of data.table of full path of all evaluations
```

```
instance$archive
## End(Not run)
```

mlr_tuners_random_search
TunerRandomSearch

Description

Subclass for random search tuning.

The random points are sampled by [paradox::generate_design_random\(\)](#).

Dictionary

This [Tuner](#) can be instantiated via the [dictionary mlr_tuners](#) or with the associated sugar function [tnr\(\)](#):

```
mlr_tuners$get("random_search")
tnr("random_search")
```

Parallelization

In order to support general termination criteria and parallelization, we evaluate points in a batch-fashion of size `batch_size`. Larger batches mean we can parallelize more, smaller batches imply a more fine-grained checking of termination criteria. A batch contains of `batch_size` times `resampling$iters` jobs. E.g., if you set a batch size of 10 points and do a 5-fold cross validation, you can utilize up to 50 cores.

Parallelization is supported via package [future](#) (see [mlr3::benchmark\(\)](#)'s section on parallelization for more details).

Logging

All [Tuners](#) use a logger (as implemented in [lgr](#)) from package [bbotk](#). Use `lgr::get_logger("bbotk")` to access and control the logger.

Parameters

```
algorithm character(1)
x0 numeric()
eval_g_ineq function()
xtol_rel numeric(1)
xtol_abs numeric(1)
ftol_rel numeric(1)
```

```
ftol_abs numeric(1)
```

For the meaning of the control parameters, see `nloptr::nloptr()` and `nloptr::nloptr.print.options()`.

The termination conditions `stopval`, `maxtime` and `maxeval` of `nloptr::nloptr()` are deactivated and replaced by the `Terminator` subclasses. The `x` and function value tolerance termination conditions (`xtol_rel = 10^-4`, `xtol_abs = rep(0.0, length(x0))`, `ftol_rel = 0.0` and `ftol_abs = 0.0`) are still available and implemented with their package defaults. To deactivate these conditions, set them to `-1`.

Super classes

```
mlr3tuning::Tuner -> mlr3tuning::TunerFromOptimizer -> TunerRandomSearch
```

Methods

Public methods:

- `TunerRandomSearch$new()`
- `TunerRandomSearch$clone()`

Method `new()`: Creates a new instance of this `R6` class.

Usage:

```
TunerRandomSearch$new()
```

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
TunerRandomSearch$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

Source

Bergstra J, Bengio Y (2012). “Random Search for Hyper-Parameter Optimization.” *Journal of Machine Learning Research*, **13**(10), 281–305. <http://jmlr.org/papers/v13/bergstra12a.html>.

Examples

```
library(mlr3)
library(paradox)
search_space = ParamSet$new(list(
  ParamDbl$new("cp", lower = 0.001, upper = 0.1)
))
terminator = trm("evals", n_evals = 3)
instance = TuningInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  search_space = search_space,
```

```

    terminator = terminator
)
tt = tnr("random_search")

# modifies the instance by reference
tt$optimize(instance)

# returns best configuration and best performance
instance$result

# allows access of data.table of full path of all evaluations
instance$archive

```

ObjectiveTuning

ObjectiveTuning

Description

Stores the objective function that estimates the performance of hyperparameter configurations. This class is usually constructed internally by the [TuningInstanceSingleCrit](#) / [TuningInstanceMultiCrit](#).

Super class

[bbotk::Objective](#) -> ObjectiveTuning

Public fields

- task ([mlr3::Task](#)).
- learner ([mlr3::Learner](#)).
- resampling ([mlr3::Resampling](#)).
- measures (list of [mlr3::Measure](#)).
- store_models (logical(1)).
- store_resample_results (logical(1)).

Methods

Public methods:

- [ObjectiveTuning\\$new\(\)](#)
- [ObjectiveTuning\\$clone\(\)](#)

Method new(): Creates a new instance of this [R6](#) class.

Usage:

```
ObjectiveTuning$new(
  task,
  learner,
  resampling,
  measures,
  store_models = FALSE,
  check_values = TRUE,
  store_resample_results = TRUE
)
```

Arguments:

- task** ([mlr3::Task](#))
 - Task to operate on.
- learner** ([mlr3::Learner](#)).
- resampling** ([mlr3::Resampling](#))
 - Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits.
- measures** (list of [mlr3::Measure](#))
 - Measures to optimize. If NULL, **mlr3**'s default measure is used.
- store_models** (logical(1)).
- check_values** (logical(1))
 - Should parameters before the evaluation and the results be checked for validity?
- store_resample_results** (logical(1))
 - Store resample results in archive?

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
ObjectiveTuning$clone(deep = FALSE)
```

Arguments:

- deep** Whether to make a deep clone.

Description

This function complements [mlr_tuners](#) with functions in the spirit of [mlr3::mlr_sugar](#).

Usage

```
tnr(.key, ...)
tnrs(.keys, ...)
```

Arguments

.key	(character(1))
	Key passed to the respective dictionary to retrieve the object.
...	(named list()) Named arguments passed to the constructor, to be set as parameters in the paramdox::ParamSet , or to be set as public field. See mlr3misc::dictionary_sugar_get() for more details.

.keys	(character())
	Keys passed to the respective dictionary to retrieve multiple objects.

Value

- [Tuner](#) for `tnr()`
- list of [Tuner](#) for `tnrs()`

Examples

```
tnr("random_search")
```

`trm`

Re-export of trm See [bbotk::trm](#).

Description

Re-export of `trm`

See [bbotk::trm](#).

`trms`

Re-export of trms See [bbotk::trms](#).

Description

Re-export of `trms`

See [bbotk::trms](#).

Tuner

Tuner

Description

Abstract Tuner class that implements the base functionality each tuner must provide. A tuner is an object that describes the tuning strategy, i.e. how to optimize the black-box function and its feasible set defined by the [TuningInstanceSingleCrit](#) / [TuningInstanceMultiCrit](#) object.

A tuner must write its result into the [TuningInstanceSingleCrit](#) / [TuningInstanceMultiCrit](#) using the `assign_result` method of the [bbottk::OptimInstance](#) at the end of its tuning in order to store the best selected hyperparameter configuration and its estimated performance vector.

Private Methods

- `.optimize(instance) -> NULL`
Abstract base method. Implement to specify tuning of your subclass. See technical details sections.
- `.assign_result(instance) -> NULL`
Abstract base method. Implement to specify how the final configuration is selected. See technical details sections.

Technical Details and Subclasses

A subclass is implemented in the following way:

- Inherit from Tuner.
- Specify the private abstract method `$.tune()` and use it to call into your optimizer.
- You need to call `instance$eval_batch()` to evaluate design points.
- The batch evaluation is requested at the [TuningInstanceSingleCrit](#) / [TuningInstanceMultiCrit](#) object instance, so each batch is possibly executed in parallel via [mlr3::benchmark\(\)](#), and all evaluations are stored inside of `instance$archive`.
- Before the batch evaluation, the [bbottk::Terminator](#) is checked, and if it is positive, an exception of class "terminated_error" is generated. In the later case the current batch of evaluations is still stored in `instance`, but the numeric scores are not sent back to the handling optimizer as it has lost execution control.
- After such an exception was caught we select the best configuration from `instance$archive` and return it.
- Note that therefore more points than specified by the [bbottk::Terminator](#) may be evaluated, as the Terminator is only checked before a batch evaluation, and not in-between evaluation in a batch. How many more depends on the setting of the batch size.
- Overwrite the private super-method `.assign_result()` if you want to decide yourself how to estimate the final configuration in the instance and its estimated performance. The default behavior is: We pick the best resample-experiment, regarding the given measure, then assign its configuration and aggregated performance to the instance.

Public fields

```
param_set (paradox::ParamSet).
param_classes (character()).
properties (character()).
packages (character()).
```

Methods

Public methods:

- `Tuner$new()`
- `Tuner$format()`
- `Tuner$print()`
- `Tuner$optimize()`
- `Tuner$clone()`

Method new(): Creates a new instance of this [R6](#) class.

Usage:

```
Tuner$new(param_set, param_classes, properties, packages = character())
```

Arguments:

<code>param_set (paradox::ParamSet)</code>	Set of control parameters for tuner.
<code>param_classes (character())</code>	Supported parameter classes for learner hyperparameters that the tuner can optimize, subclasses of <code>paradox::Param</code> .
<code>properties (character())</code>	Set of properties of the tuner. Must be a subset of <code>mlr_reflections\$tuner_properties</code> .
<code>packages (character())</code>	Set of required packages. Note that these packages will be loaded via <code>requireNamespace()</code> , and are not attached.

Method format(): Helper for print outputs.

Usage:

```
Tuner$format()
```

Method print(): Print method.

Usage:

```
Tuner$print()
```

Returns: (character()).

Method optimize(): Performs the tuning on a `TuningInstanceSingleCrit` or `TuningInstanceMultiCrit` until termination. The single evaluations and the final results will be written into the `bbotk::Archive` that resides in the `TuningInstanceSingleCrit/TuningInstanceMultiCrit`. The final result is returned.

Usage:

```
Tuner$optimize(inst)
```

Arguments:

inst ([TuningInstanceSingleCrit](#) | [TuningInstanceMultiCrit](#)).

Returns: `data.table::data.table`.

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
Tuner$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

Examples

```
library(mlr3)
library(paradox)
search_space = ParamSet$new(list(
  ParamDbl$new("cp", lower = 0.001, upper = 0.1)
))
terminator = trm("evals", n_evals = 3)
instance = TuningInstanceSingleCrit$new(
  task = tsk("iris"),
  learner = lrn("classif.rpart"),
  resampling = rsmp("holdout"),
  measure = msr("classif.ce"),
  search_space = search_space,
  terminator = terminator
)
# swap this line to use a different Tuner
tt = tnr("random_search")
# modifies the instance by reference
tt$optimize(instance)
# returns best configuration and best performance
instance$result
# allows access of data.table / benchmark result of full path of all
# evaluations
instance$archive
```

TuningInstanceMultiCrit

Multi Criteria Tuning Instance

Description

Specifies a general multi-criteria tuning scenario, including objective function and archive for Tuners to act upon. This class stores an `ObjectiveTuning` object that encodes the black box objective function which a `Tuner` has to optimize. It allows the basic operations of querying the objective

at design points (`$eval_batch()`), storing the evaluations in the internal Archive and accessing the final result (`$result`).

Evaluations of hyperparameter configurations are performed in batches by calling `mlr3::benchmark()` internally. Before a batch is evaluated, the `bbotk::Terminator` is queried for the remaining budget. If the available budget is exhausted, an exception is raised, and no further evaluations can be performed from this point on.

The tuner is also supposed to store its final result, consisting of a selected hyperparameter configuration and associated estimated performance values, by calling the method `instance$assign_result`.

Super classes

```
bbotk::OptimInstance -> bbotk::OptimInstanceMultiCrit -> TuningInstanceMultiCrit
```

Active bindings

```
result_learner_param_vals (list())
List of param values for the optimal learner call.
```

Methods

Public methods:

- `TuningInstanceMultiCrit$new()`
- `TuningInstanceMultiCrit$assign_result()`
- `TuningInstanceMultiCrit$clone()`

Method `new()`: Creates a new instance of this `R6` class.

This defines the resampled performance of a learner on a task, a feasibility region for the parameters the tuner is supposed to optimize, and a termination criterion.

Usage:

```
TuningInstanceMultiCrit$new(
  task,
  learner,
  resampling,
  measures,
  search_space,
  terminator,
  store_models = FALSE,
  check_values = FALSE,
  store_resample_results = TRUE
)
```

Arguments:

`task` (`mlr3::Task`)

Task to operate on.

`learner` (`mlr3::Learner`).

`resampling` (`mlr3::Resampling`)

Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits.

`measures` (list of [mlr3::Measure](#))
 Measures to optimize. If NULL, **mlr3**'s default measure is used.

`search_space` ([paradox::ParamSet](#)).
`terminator` ([Terminator](#)).
`store_models` (logical(1)).
`check_values` (logical(1))
 Should parameters before the evaluation and the results be checked for validity?

`store_resample_results` (logical(1))
 Store resample results in archive?

Method `assign_result()`: The [Tuner](#) object writes the best found points and estimated performance values here. For internal use.

Usage:

```
TuningInstanceMultiCrit$assign_result(xdt, ydt, learner_param_vals = NULL)
```

Arguments:

`xdt` (data.table::data.table())
 x values as data.table. Each row is one point. Contains the value in the *search space* of the [TuningInstanceMultiCrit](#) object. Can contain additional columns for extra information.
`ydt` (data.table::data.table())
 Optimal outcomes, e.g. the Pareto front.
`learner_param_vals` (list())
 Fixed parameter values of the learner that are neither part of the

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
TuningInstanceMultiCrit$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

TuningInstanceSingleCrit

Single Criterion Tuning Instance

Description

Specifies a general single-criteria tuning scenario, including objective function and archive for Tuners to act upon. This class stores an [ObjectiveTuning](#) object that encodes the black box objective function which a [Tuner](#) has to optimize. It allows the basic operations of querying the objective at design points (`$eval_batch()`), storing the evaluations in the internal Archive and accessing the final result (`$result`).

Evaluations of hyperparameter configurations are performed in batches by calling `mlr3::benchmark()` internally. Before a batch is evaluated, the [bbotk::Terminator](#) is queried for the remaining budget. If the available budget is exhausted, an exception is raised, and no further evaluations can be performed from this point on.

The tuner is also supposed to store its final result, consisting of a selected hyperparameter configuration and associated estimated performance values, by calling the method `instance$assign_result`.

Super classes

`bbotk::OptimInstance -> bbotk::OptimInstanceSingleCrit -> TuningInstanceSingleCrit`

Active bindings

`result_learner_param_vals (list())`
Param values for the optimal learner call.

Methods

Public methods:

- `TuningInstanceSingleCrit$new()`
- `TuningInstanceSingleCrit$assign_result()`
- `TuningInstanceSingleCrit$clone()`

Method new(): Creates a new instance of this `R6` class.

This defines the resampled performance of a learner on a task, a feasibility region for the parameters the tuner is supposed to optimize, and a termination criterion.

Usage:

```
TuningInstanceSingleCrit$new(
  task,
  learner,
  resampling,
  measure,
  search_space,
  terminator,
  store_models = FALSE,
  check_values = FALSE,
  store_resample_results = TRUE
)
```

Arguments:

`task` (`mlr3::Task`)

Task to operate on.

`learner` (`mlr3::Learner`).

`resampling` (`mlr3::Resampling`)

Uninstantiated resamplings are instantiated during construction so that all configurations are evaluated on the same data splits.

`measure` (`mlr3::Measure`)

Measure to optimize.

`search_space` (`paradox::ParamSet`).

`terminator` (`Terminator`).

`store_models` (`logical(1)`).

`check_values` (`logical(1)`)

Should parameters before the evaluation and the results be checked for validity?

`store_resample_results` (`logical(1)`)

Store resample results in archive?

Method assign_result(): The `Tuner` object writes the best found point and estimated performance value here. For internal use.

Usage:

```
TuningInstanceSingleCrit$assign_result(xdt, y, learner_param_vals = NULL)
```

Arguments:

`xdt` (`data.table::data.table()`)

`x` values as `data.table`. Each row is one point. Contains the value in the *search space* of the `TuningInstanceMultiCrit` object. Can contain additional columns for extra information.

`y` (`numeric(1)`)

 Optimal outcome.

`learner_param_vals` (`list()`)

 Fixed parameter values of the learner that are neither part of the

Method clone(): The objects of this class are cloneable with this method.

Usage:

```
TuningInstanceSingleCrit$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

Examples

```
library(data.table)
library(paradox)
library(mlr3)

# Objects required to define the performance evaluator:
task = tsk("iris")
learner = lrn("classif.rpart")
resampling = rsmp("holdout")
measure = msr("classif.ce")
param_set = ParamSet$new(list(
  ParamDbl$new("cp", lower = 0.001, upper = 0.1),
  ParamInt$new("minsplit", lower = 1, upper = 10))
)

terminator = trm("evals", n_evals = 5)
inst = TuningInstanceSingleCrit$new(
  task = task,
  learner = learner,
  resampling = resampling,
  measure = measure,
  search_space = param_set,
  terminator = terminator
)

# first 4 points as cross product
design = CJ(cp = c(0.05, 0.01), minsplit = c(5, 3))
inst$eval_batch(design)
inst$archive
```

```

# try more points, catch the raised terminated message
tryCatch(
  inst$eval_batch(data.table(cp = 0.01, minsplit = 7)),
  terminated_error = function(e) message(as.character(e))
)

# try another point although the budget is now exhausted
# -> no extra evaluations
tryCatch(
  inst$eval_batch(data.table(cp = 0.01, minsplit = 9)),
  terminated_error = function(e) message(as.character(e))
)

inst$archive

### Error handling
# get a learner which breaks with 50% probability
# set encapsulation + fallback
learner = lrn("classif.debug", error_train = 0.5)
learner$encapsulate = c(train = "evaluate", predict = "evaluate")
learner$fallback = lrn("classif.featureless")

param_set = ParamSet$new(list(
  ParamDbl$new("x", lower = 0, upper = 1)
))

inst = TuningInstanceSingleCrit$new(
  task = tsk("wine"),
  learner = learner,
  resampling = rsmp("cv", folds = 3),
  measure = msr("classif.ce"),
  search_space = param_set,
  terminator = trm("evals", n_evals = 5)
)

tryCatch(
  inst$eval_batch(data.table(x = 1:5 / 5)),
  terminated_error = function(e) message(as.character(e))
)

archive = inst$archive$data()

# column errors: multiple errors recorded
print(archive)

```

Index

* datasets
 mlr_tuners, 5

AutoTuner, 3, 3

 bbotk::Archive, 3, 20
 bbotk::mlr_terminators, 5
 bbotk::Objective, 16
 bbotk::OptimInstance, 19, 22, 24
 bbotk::OptimInstanceMultiCrit, 22
 bbotk::OptimInstanceSingleCrit, 24
 bbotk::Terminator, 3, 4, 12, 19, 22, 23
 bbotk::trm, 18
 bbotk::trms, 18

 data.table::data.table, 7, 21
 dictionary, 6, 8, 10, 12, 14, 18

 GenSA::GenSA(), 8

 mlr3::benchmark(), 3, 6, 10, 14, 19, 22, 23
 mlr3::Learner, 3, 4, 16, 17, 22, 24
 mlr3::Measure, 3, 4, 16, 17, 23, 24
 mlr3::mlr_sugar, 17
 mlr3::resample(), 3
 mlr3::Resampling, 3, 4, 16, 17, 22, 24
 mlr3::Task, 16, 17, 22, 24
 mlr3misc::Dictionary, 5, 6
 mlr3misc::dictionary_sugar_get(), 18
 mlr3tuning (mlr3tuning-package), 2
 mlr3tuning-package, 2
 mlr3tuning::Tuner, 7, 8, 10, 13, 15
 mlr3tuning::TunerFromOptimizer, 7, 8, 10,
 13, 15
 mlr_reflections\$tuner_properties, 20
 mlr_terminators, 5
 mlr_tuners, 5, 6, 8, 10, 12, 14, 17
 mlr_tuners_design_points, 6
 mlr_tuners_gensa, 8
 mlr_tuners_grid_search, 10
 mlr_tuners_nloptr, 12

 mlr_tuners_random_search, 14

 nloptr::nloptr, 12
 nloptr::nloptr(), 12, 15
 nloptr::nloptr.print.options(), 12, 15

 ObjectiveTuning, 16

 paradox::generate_design_grid(), 10
 paradox::generate_design_random(), 14
 paradox::Param, 20
 paradox::ParamSet, 3, 4, 18, 20, 23, 24

 R6, 4, 7, 8, 11, 13, 15, 16, 20, 22, 24

 R6::R6Class, 5
 requireNamespace(), 20

 Terminator, 12, 15, 23, 24
 tnr, 17
 tnr(), 5, 6, 8, 10, 12, 14
 tnrs (tnr), 17
 tnrs(), 5, 6
 trm, 18
 trms, 18
 Tuner, 3–6, 8, 10, 12, 14, 18, 19, 21, 23, 25
 TunerDesignPoints
 (mlr_tuners_design_points), 6
 TunerGenSA (mlr_tuners_gensa), 8
 TunerGridSearch
 (mlr_tuners_grid_search), 10
 TunerNLopt (mlr_tuners_nloptr), 12
 TunerRandomSearch
 (mlr_tuners_random_search), 14
 TuningInstanceMultiCrit, 16, 19–21, 21,
 23, 25
 TuningInstanceSingleCrit, 3, 4, 16, 19–21,
 23